Publishable Report

SABATLE

Safety Assessment of Flow Battery Electrolytes

(01/2021-03/2023)

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1. Executive Summary

The SABATLE project was one of the first of its kind to adapt and employ the use of the Safe-and-Sustainable-by-Design approach to energy storage systems. As energy storage system we chose organic flow batteries, which aim at replacing the electrolyte, namely commercially available vanadium against biobased redox active molecules. The SSbD considerations included the value chain from cradle to grave, included social LCA impacts as well as toxicity testing of some compounds. Application of the SSbD approach showed that by analysis of all process steps, the safety of the overall process can be significantly increased. The main outcome of the project was a case study which was presented at the EuroNanoforum in Lund 2023 and submitted for publication in December 2023. It highlighted that the implementation of SSbD during technology development is capable to design better processes from both economic, ecologic and safety point of view. Another important outcome of the project was the analysis of current LCA methods to assess flow battery technoeconomic and environmental performance where we identified several methodological shortcomings which were summarized in a ChemSusChem Paper published in early 2023. In addition, the project was presented to a variety of stakeholders and was disseminated in many conferences on national and international level (e.g. American Chemical Society meeting). SABATLE also served as the seed for two more funding initiatives which both started in September 2023 (Safera SUESS, SSbD, LCA of post-lithium ion batteries and EIC VanillaFlow, toxicity of redox active molecules).

The project partners covered a large company (Mondi AG), an SME (Biobide), an internationally recognized research network (BioNanoNet) and two universities (University of Graz and Graz University of Technology).

2. Approach and concept

The approach in the project was the conceptualization of the SSbD approach (Fig.1) including the assessment of materials which will be used during the whole project lifetime. The concept also includes interactions with relevant stakeholders and government/institutional bodies

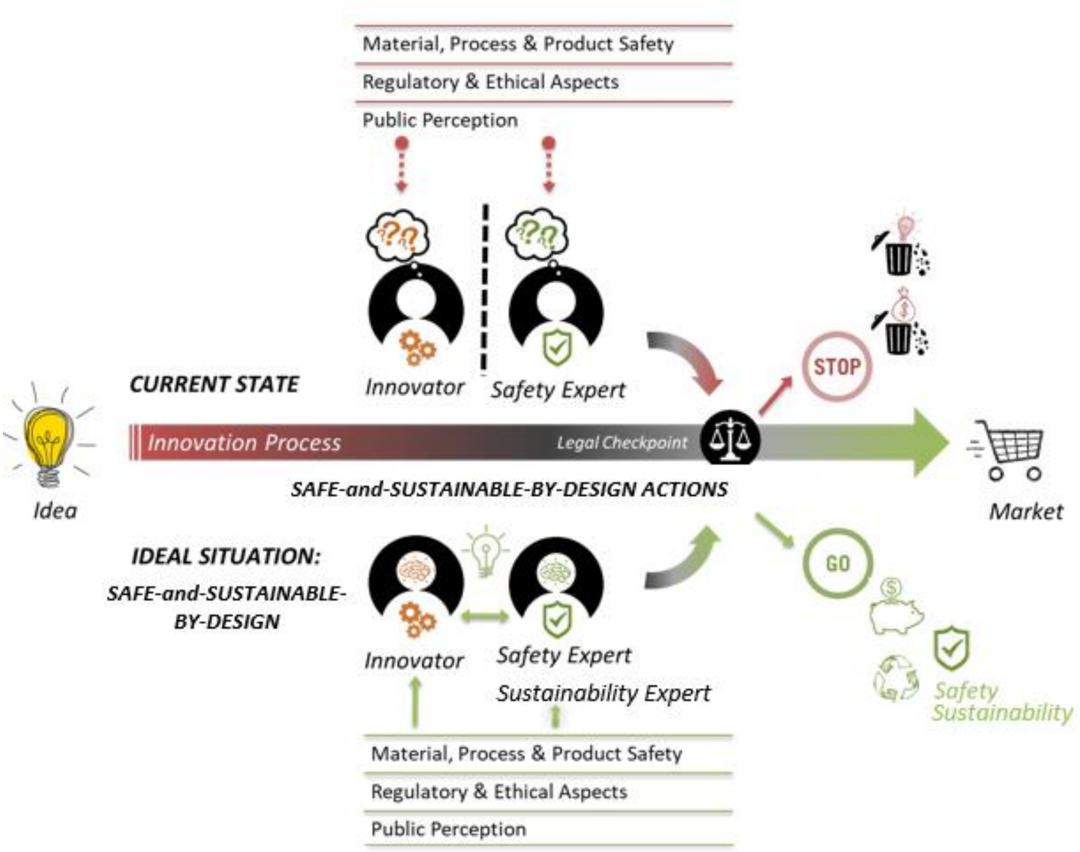

Figure 1: Illustration of the SSbD concept compared to a traditional innovation process.

The fundamental SSbD approach in SABATLE was complemented by sustainability criteria (full life cycle, toxicity) and paves the way to safe and more sustainable innovations. SSbD can be seen as a pre-market approach, as it is identifying potentially harmful chemicals for humans and the environment. Consequently, risks are quantified and mitigation measures are developed and implemented. In general, sustainability is achieved by minimizing the ecologic footprint of all used chemicals in respect to climate change and ecosystems, resource efficiency and biodiversity over the whole life cycle.[1] This holistic innovation process allows for looking at the innovation processes from different viewpoints. However, the improvement of the EHS performance (environment, health, safety) must be balanced with the reduction of climate impacts and must consider also the technological performance and its economic boundaries (Figure 2). We developed a concept which is based on iterative processes, considering the individual steps during the product life cycle and which can be used also beyond the project lifetime of SABATLE.

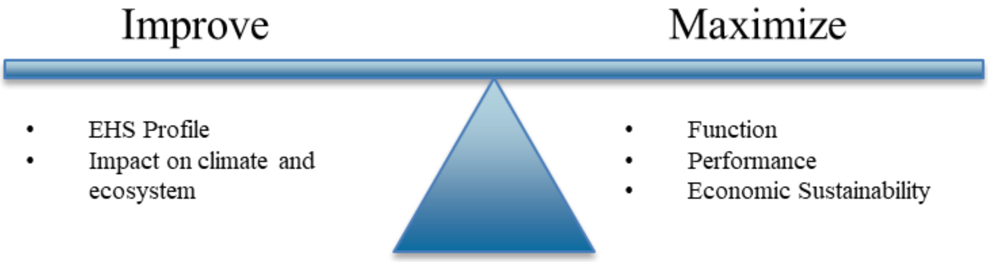

Figure 2: Profile balancing approach

We performed an extensive literature search to design the concept on the basis of the state of the art. The key documents were identified and a project specific concept was finalized , which is depicted in Figure 3. As there were not any specific guidelines for flow batteries, (and still do not exist), general considerations of the regulatory framework were implemented into the flow battery topic. Available data concerning the used raw materials and the value chains were considered as well as the CO2 footprint, climate/eco impact (via LCA), end of life scenarios, circularity as well as safety concerns. We were anticipating at project start already potential regulatory adaptions at project start.

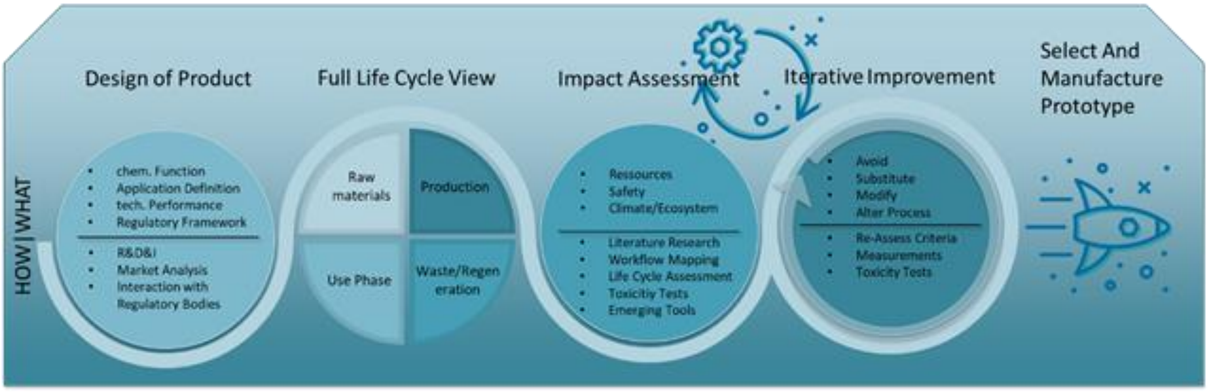

Figure 3: SaSbD Concept for SABATLE

The starting point for the concept was the study of Schlemmer et.al., which described the basic principle of the planned product.[2] A workflow mapping was established by the partners (see Figure 4).

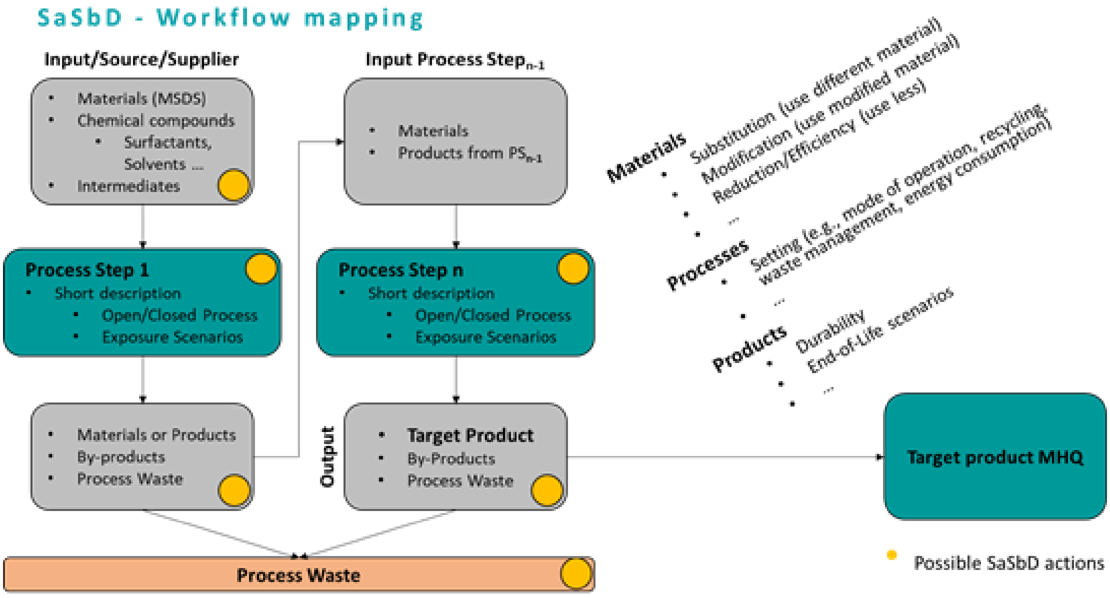

Figure 4:. Workflow mapping of the SaSbD approach

Description of the processes and the implementation of iterative process improvements

<u>The following points were identified for improvements in the process which were then later implemented:</u>

- Use of a continuous process instead of a batch process.
- Inert atmosphere improves performance of process.
- Reaction is exothermic, and the generated heat can be used in other sections of the synthesis leading to a lower overall energy consumption.
- Use of green and more sustainable solvents for the production as well as quantitative recovery of the solvents/reagents
- Adaption of core structure of the redox active molecules to reduce toxicity for humans and the environment

In the course of the project, there was significant progress on the European level concerning holistic SSbD concepts, which resulted in a EC recommendation, published on 08.12.2022.[1]
The aim of this recommendation is to develop new chemicals and materials, to optimize/redesign production processes and to improve the safety and sustainabiliyt of currently used materials and chemicals. Case studies are the main means to test the suitability of the recommendation. SABATLE is actually a pre-case study in teh context of this recommendation. In the last months of the project, the

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[1] https://research-and-innovation.ec.europa.eu/system/files/2022-12/Commission%20recommendation%20-%20establishing%20a%20European%20assessment%20framework%20for%20safe%20and%20sustainable%20by%20design.PDF

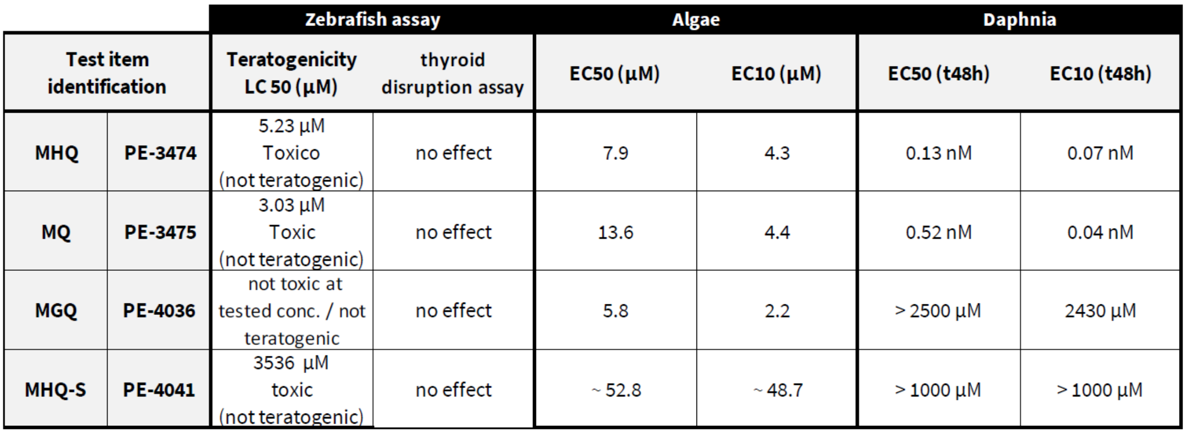
partners intensively worked to reflect the concept developed in SABATLE onto the published framework by the EC to establish guidelines and recommendations particularly for SMEs. The results were presented at the EuroNanoForum in Lund (June 2023) and are part of a publication (submitted december 2023), whose results are excerpted below.

3. Toxicity Testing

The main goal concerning toxicity and ecotoxicity screening is to assess the hazard potential of the first generation materials and of those which have been proposed and further developed on the basis of the SSbD concept (2^nd^ generation). Investigations regarding human toxicity were conducted using zebrafish (e.g. developmental toxicity, endocrine disruption potential) at different concentrations. Ecotoxicity was investigated with algae, daphnia and zebrafish based biological assays according to the ecotoxicity screening assays based on OECD guidelines –OECD 201: Freshwater Alga and Cyanobacteria, Growth Inhibition Test, OECD 202: *Daphnia sp*. Acute Immobilisation Test, OECD 236: Fish Embryo Acute Toxicity (FET) Test).

The first generation materials were not teratogenic (definition teratogenity index smaller than 2) but show toxicity to humans. Neither of the compounds are furthermore endocrine disruptors (Figure 6). There are hardly any changes visible even at very high doses. However, regarding ecotoxicity the performance of the1st generation materials was not very good, and particularly daphnia is extremely sensitive towards these materials. The SSbD concept was then applied and led to two more core structures whose toxicity was further investigated. The 2nd generation materials were equipped on one hand with negatively charged functionalities (MHQS) and on the other hand with nitrogen containing groups (MGQ). While MHQS is still slightly toxic to humans (3500 µM) but not featuring ecotoxicity, MGQ does not feature any toxicity to humans nor to the environment. Only algal growth is compromised by all components whereas MHQS performs best in this category. A summary is provided in Table 2.

Table 1: overview on toxicological data of the investigated materials, with MQ and MHQ being first generation materials and MGQ and MHQS being second generation materials.



		Zebrafish assay		Algae		Daphnia	
Test item identification		**Teratogenicity LC 50 (µM)**	**thyroid disruption assay**	**EC50 (µM)**	**EC10 (µM)**	**EC50 (t48h)**	**EC10 (t48h)**
MHQ	**PE-3474**	5.23 µM Toxico (not teratogenic)	no effect	7.9	4.3	0.13 nM	0.07 nM
MQ	**PE-3475**	3.03 µM Toxic (not teratogenic)	no effect	13.6	4.4	0.52 nM	0.04 nM
MGQ	**PE-4036**	not toxic at tested conc. / not teratogenic	no effect	5.8	2.2	> 2500 µM	2430 µM
MHQ-S	**PE-4041**	3536 µM toxic (not teratogenic)	no effect	~ 52.8	~ 48.7	> 1000 µM	> 1000 µM

4. Life Cycle assessment

In the course of the project we performed an extensive literature survey on LCA in the flow battery area. The results on the methodology and shortcomings have been summarized in recent publication: “How green are redox flow batteries?” published in the journal ChemSusChem[3]. The main findings were that assessment for different flow battery technologies depends on many factors which have not been standardized in LCA Analysis of flow batteries. This comprises the energy mix used for charging, the system boundaries, the operating conditions, and the technoeconomic performance. Standardization of these items is highly necessary to make a quantitative assessment of flow battery systems.

4.1 Streamlined LCA

The environmental impacts of products or services can be assessed by means of LCA (ISO 14040 and 14044, 2006) [4, 5]. The method itself is widely acknowledged and defines four phases to perform an assessment [6]:

- the goal and scope definition
- the life cycle inventory (LCI)
- the life cycle impact assessment (LCIA)
- and the interpretation phase.

For product systems in an early development stage, preliminary screenings based on material and energy balances can be performed using modeling tools which require less accurate datasets, like generic datasets and standard modules for transportation and energy production [7-10].

A contribution analysis provides insights into the materials and energy inputs contributing most to the total impact of the product system. In the present work a contribution analysis of MHQ is performed to identify improvement potentials to avoid unintended impacts and reduce environmental impacts. Hereby the functional unit is defined as 1 kg MHQ electrolyte to be used in RFBs produced in Austria with the system boundaries cradle-to-gate (Fig. 5). Importantly, the currently employed LCA method cannot distinguish between the subtypes of quinones (e.g., MHQ, MQ, MGQ, MHQS). However, a streamlined LCA was performed for different routes of MHQ-generation. Due to data unavailability for the MTHF in generic LCA databases, THF was considered for both routes.

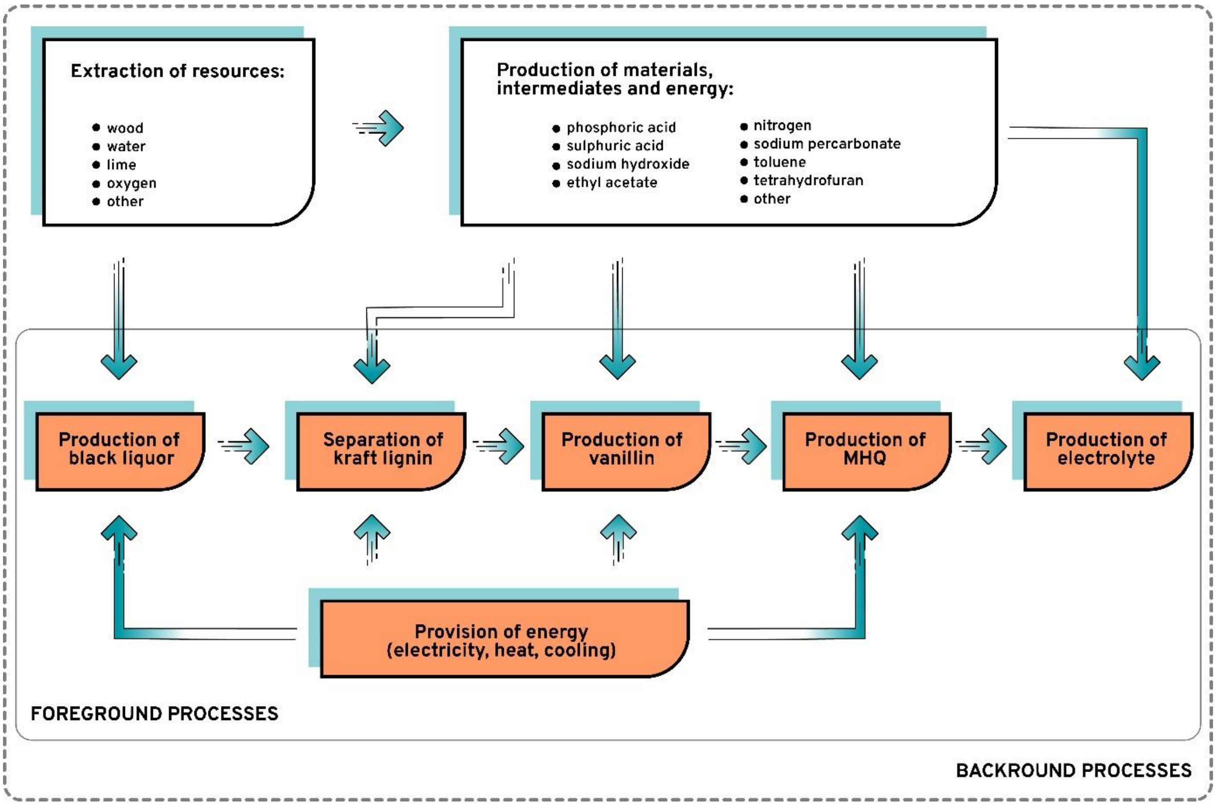


Figure 5: Simplified illustration of the system boundaries from cradle-2-gate including foreground and background processes.

In the LCI phase, the inputs and outputs of all the processes from cradle-2-gate are collected. Different sources are used to collect the data for the foreground processes depicted in Figure 5. The inventories for the extraction of kraft lignin from black liquor are taken from Culbertson and colleagues [11, 12]. For the inventories of the vanillin extraction from kraft lignin a techno-economic study by Khwanjaisakun et al. was used [13]. The inventories of the MHQ production and electrolyte composition are provided by the experts from the SABATLE project consortium. The LCIA was performed using the software SimaPro 9.2.0.1 and Ecoinvent v3.7.1 for background processes. In the LCIA phase, the actual impacts on the environment are calculated by first selecting impact categories, category indicators and characterization models [4, 5]. For the present study, the potential contribution to climate change with the impact category Global Warming Potential (GWP) using the characterization model IPCC 2013 GWP 100a V1.03 was calculated. Since the hotspots can differ depending on which impact category is investigated [3], the impacts are also calculated using the EF 3.0 V1.01 LCIA method including the impact categories climate change, ozone depletion, ionizing radiation, photochemical ozone formation, particulate matter, human toxicity (cancer and non-cancer), acidification, eutrophication (freshwater, marine and terrestrial), ecotoxicity, freshwater, land use, water use and resource use (fossils and minerals and metals).

4.2 Generic SLCA

The potential social risks in the MHQ value chain were investigated by means of generic SLCA. In SLCA the focus of investigation is the stakeholders potentially affected through the activities or behaviors "of organizations linked to the life cycle of the product or service and from the use of the product itself" [14]. For products in the early development stages, the actual companies that will produce the products are rarely known. In such cases the social risks on a country level can be investigated with a 2nd-level SLCA as proposed by Groiß-Fürtner et al. [15]. That means that the countries involved in the production of the foreground processes are identified and potential risks are analyzed by collecting data for relevant indicators on a country level [16, 17]. The first step is therefore to identify the countries which are potentially involved in the value chain of MHQ. The first step of the value chain under investigation is to extract the kraft lignin from black liquor (LignoBoost®, Valmet, Finland), a side stream in the pulp and paper production [18]. The main producers of kraft lignin are Finland, USA, Brazil, and Canada [18, 19]. Vanillin is one of the most important flavoring chemicals with a total vanillin output of 20 million kg from three major routes (85% petroleum-based, 15% from lignin and <1% from vanillin bean). Currently, all commercially available lignin-based vanillin is produced from lignosulfonate by Borregaard [18]. In this study, it is therefore assumed that the vanillin is either produced in the facilities where the kraft lignin is coming from or as a future scenario where we assume that kraft lignin, the synthesis of vanillin, as well as the MHQ production, will be done in Austria. After the identification of the affected regions relevant indicators need to be identified [20, 21]. Here we follow the suggestions in the framework for SSbD where the potential social impacts of the stakeholder groups workers, local communities and consumers are the ones most often considered with a total of eleven social aspects [22, 23]. In this context the focus lies on developing safe and sustainable chemicals or materials. Therefore, the objective of the generic SLCA is to identifying social risks of a potential future value chain of MHQ, to provide insights and recommendations on tackling critical social aspects already before a value chain is set up. The social aspects and indicators chosen for this study are summarized in Table 2. Due to the early stage of development of the MHQ and the limited availability of primary data, some social aspects, i.e., fair pay, working hours, community involvement, responsible communication and consumer health and safety, are not analyzed further. Though the stakeholder group society was included since the focus is on the social risks of a potential lignin source and corruption is one aspect covered in this category.

The data collection was performed following the recommendations given in the methodological sheets of the United Nations Environment Programme guidelines [24]. Generic data was collected from publicly available data sources, e.g., the international labour organization (ILO), to quantify the selected indicators (see Table 3). The data gathered was then normalized to standardize the results on a scale of 0 to 1, where 0 is considered the best and 1 the worst value within the countries identified [25, 26].

Table 2: Selected social indicators according to the SSbD Framework (Joint Research Council of the European Commission). Adapted from Caldeira et al. (2022) [22].

Stakeholder group	Social aspect	Indicator	Source
Workers	Child labour	Realization of Children's rights Index	https://www.humanium.org/en/rcri/ [27]
	Forced labour	Estimated Proportion Living in Modern Slavery	https://www.globalslaveryindex.org/2018/data/maps/ [28]
	Health and safety	Fatal occupational injuries	https://www.ilo.org/ [29]
		Non-fatal occupational injuries	https://www.ilo.org/ [29]
		Coverage of essential health services	https://vizhub.healthdata.org/sdg/ [30]
	Freedom of association and collective bargaining	Collective bargaining coverage	https://www.ilo.org/ [29]
		Global right index	https://www.globalrightsindex.org/de/2023 [31]
	Equal opportunities / discrimination	Gender inequality index	https://hdr.undp.org/ [32]
Local community	Local employment	Unemployment rate	https://www.ilo.org/ [29]
Society	Corruption	Corruption Perception Index	https://www.transparency.org/en/cpi/2018 [33]

4.3 Environmental hotspots analysis of streamlined LCA reveals energy input as major contributor to MHQ´s overall GWP

In Figure 6, the material and energy contributions of the MHQ electrolyte to GWP, and its major contributors in the upstream processes, i.e., the MHQ production and the vanillin synthesis from kraft lignin, are illustrated. The main contributor to the total GWP attributed to the MHQ-based electrolyte is the MHQ production process itself, which is responsible for almost 100% of the released CO_2. This is in significant part due to the kraft lignin-based vanillin, which is responsible for almost 60% of the GWP attributed to the MHQ. The GWP is determined largely by the required energy inputs (e.g., cooling, electricity and heat) needed for vanillin production (in total responsible for about 60% of the GWP attributed to vanillin; energy inputs required for its upstream products are not considered here). When all energy inputs required for the production process (from kraft lignin to the MHQ-based electrolyte) are considered, their contribution to the electrolyte's total GWP amounts to about 80% - hence, the demanded energy represents the main hotspot in terms of GWP.

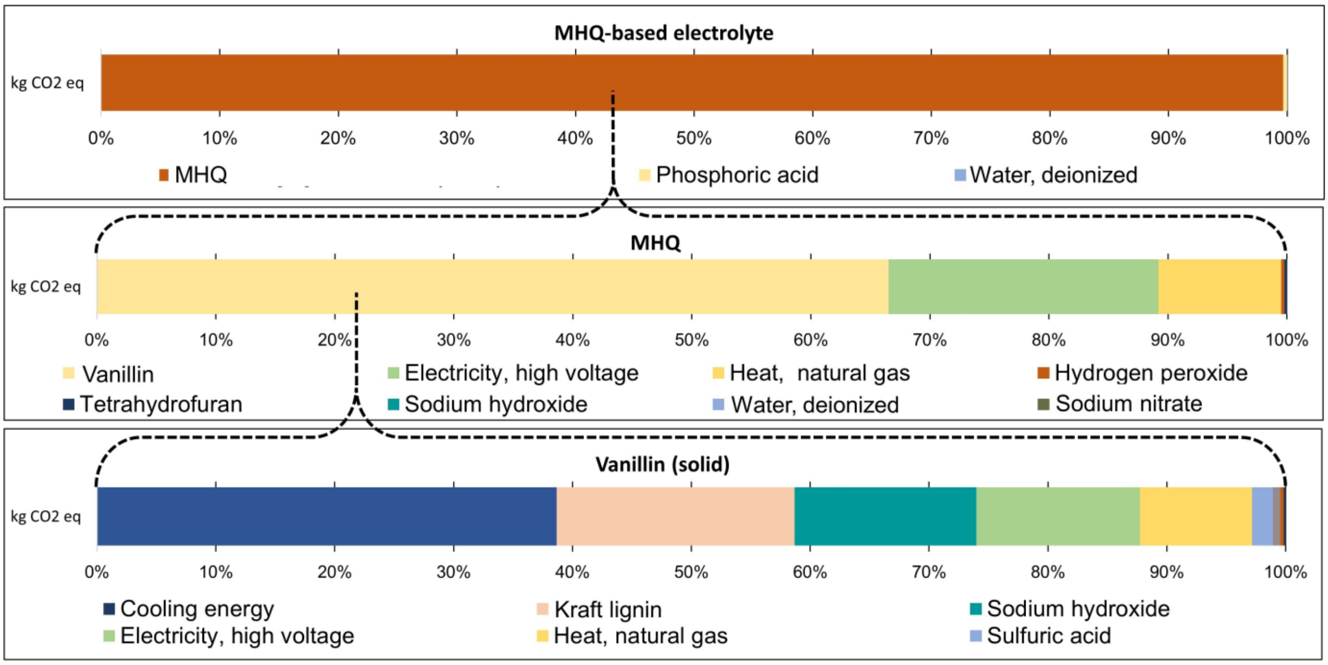


Figure 6: Environmental hotspots in terms of global warming potential (GWP) of the MHQ-electrolyte.

Apart from the impacts related to the energy demand, the progress in quinone development also impacted the total GWP. When compared to Route A of MHQ synthesis, due to a slightly lower synthesis yield, a higher amount of vanillin-input was assumed in Route B, which in consequence increased the overall impact on GWP (Figure 7). However, this is still connected to high uncertainties regarding the vanillin-related input data, including that the (slightly) different quantities used might also be attributable to design and data characteristics typical in early phases of technology development (see [7]). On the contrary, the assumed input change in chemicals from toluene and sodium percarbonate to sodium nitrate and hydrogen peroxide would result in a decrease of associated GWP impacts.

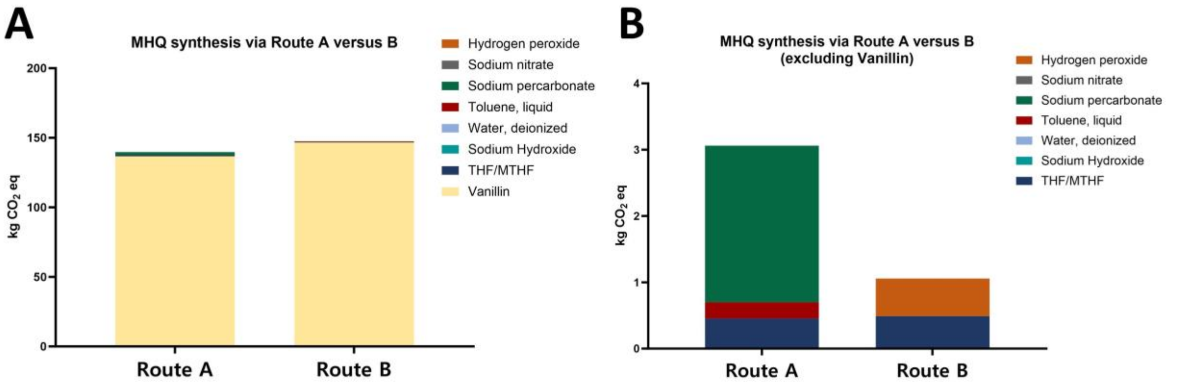


Figure 7: MHQ synthesis comparison of Route A and B based on kg CO_2 eq (A) and zoom in, disregarding vanillin (B). Abbreviations: eq – equivalents

5. Social hotspots analysis revealed major country-specific differences about safety and welfare of workers

The potential social risks of countries involved in the kraft lignin production for selected social aspects are summarized in Figure 8. The results show that Brazil forms a hotspot in most indicators (8/10). Also, Canada and the United States relate to higher social risks regarding collective bargaining coverage, global rights index, and fatal occupational injuries. The collective bargaining coverage depicts the extent to which employees are covered by one or more collective agreements on pay and/or conditions of employment [29]. The global rights index documents violations of internationally recognized collective labor rights by governments and employers [31]. According to the data from ILO, workers in Finland are at higher risk when it comes to health and safety, according to a high number of non-fatal accidents reported (Figure 9A). Austria appeared as the country with the lowest risks for almost all investigated indicators (Figure 9A-C).

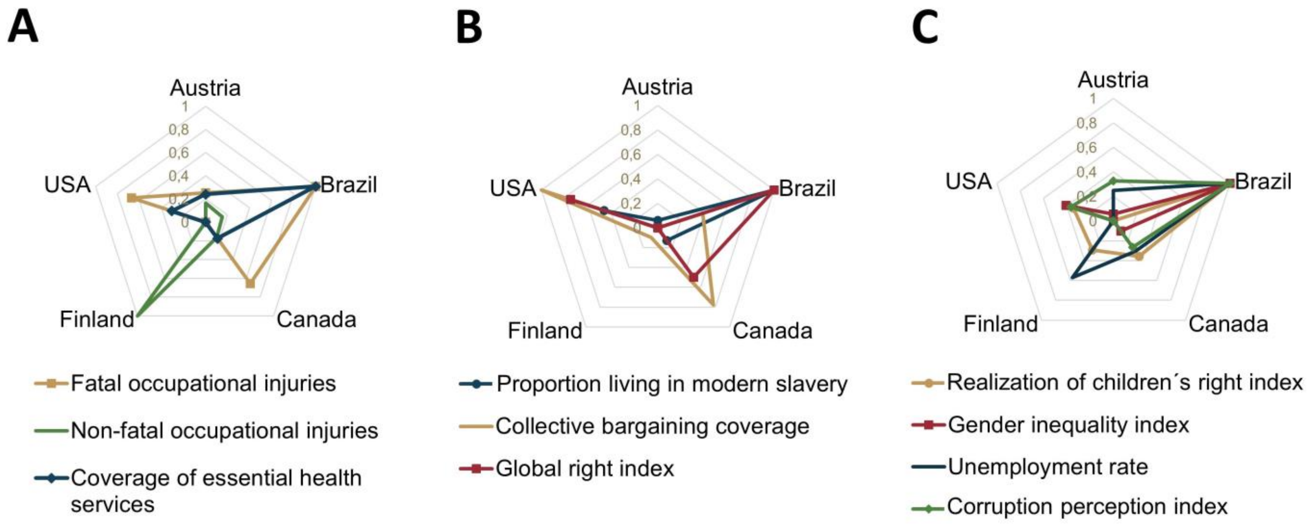


Figure 8: Social risks or opportunities in different indicators, highlighting hotspot countries (A-C). Normalized values from 0: lower to 1: higher social risks. Data extracted from [27-33].

6. Discussion

The here introduced SSbD concept was applied to a specific set of quinones derived from bio-based vanillin, which can be used in flow battery systems. The goal of this procedure was to consider materials performance and connect it to sustainability data, including toxicity testing and putting it into relation of social and environmental performance.

6.1 Safety and sustainability of quinone synthesis was improved by greener solvent choice and omission of toluene and less toxic quinone variant generation

The omission of hazardous chemicals, such as toluene in this case, which was omitted in route B of MHQ synthesis, improves the safety of the production process. Additionally, to the here provided listing of hazard potential, tools such as VEGA QSAR [34] could improve the assessment and classification further. The starting point for this study was MHQ, which is obtained by Dakin oxidation from vanillin in alkaline media. Although the reaction is rapid, the use of THF is a major drawback due to environmental concerns. Consequently, THF was exchanged to the more sustainable ether MTHF. The use of MTHF as a solvent achieves near identical yields as THF (75%). MTHF has been described as a greener alternative, as it can be manufactured from renewable sources, hence presenting with improved life cycle footprint. Quantitative measurements **revealed 97% reduced emissions for MTHF**, compared to conventional THF [35]. Additionally, **MTHF is classified as less toxic** than THF by the European Medicines Agency [36]. Also, as a side product, it is economically competitive for THF. Moreover, another advantage of MTHF use in the context of MHQ synthesis is the better drying properties of MTHF over THF, **facilitating the quantitative recovery** of the solvent after phase separation. This presents as another positive economic factor, due to facilitating circularity of the used solvent. The higher boiling point (80°C) compared to THF (64°C) provides a larger reaction window and **improves the safety** of the process. Albeit it must be noted, that the here used LCA cannot depict differences due to the change of used solvent at the current stage. To properly assess MTHF in the LCA, extensive literature and data research would be warranted, which is beyond the scope of this project.

The newly synthesized quinones (MGQ and MHQS) presented with **superior ecotoxicity outcome** and are hence recommended for further use. Further, the compounds had a **lower toxicity** than other redox active materials used in RFBs such **as vanadium oxides** [37].

6.2 Improving energy efficiency to improve GWP of kraft lignin to vanillin synthesis

As **the main outcome** of the streamlined LCA was **poor energy efficiency**, this should be a prime focus for amelioration. However, it should be noted that the mass and energy balances **had to be derived from limited available data sources** [13, 38], with the respective approaches not yet primarily aimed at targets, such as increasing energy efficiency or circularity. Thus, the **current results do not reveal the extent of potential savings** or how, the yet to be combined and upscaled, MHQ electrolyte production process from kraft lignin would perform when compared to the already established vanadium electrolyte production. However, they do give an indication, based on current knowledge, on where the key levers in process development lie and how to reduce its GWP. Accordingly, the focus should be on **increasing resource efficiency in MHQ electrolyte production** and upstream processes.

The presented two synthesis variants give indication that these adaptations to the processing are serving as cases for the implementation of the SSbD concept, more specifically applying the re-design aspects. However, these changes currently seem of secondary relevance when compared to the kraft lignin-based vanillin input. Looking at the results regarding the impact categories of the environmental footprint (EF) method, the picture is similar in respect to vanillin being a hotspot in all other impact categories as well. In other words, the focus should be on increasing energy efficiency and establishing closed-loop operations in general.

6.3 Monitoring and improving conditions in country of lignin origin to enhance social impact

It should be noted that the results in Figure 8 only depict a comparison between the countries considered for supplying the kraft lignin to identify social aspects where special attention must be paid. If the kraft lignin is provided by a company from a country with higher risks in a respective indicator, then measures should be implemented to ensure that the social impact is kept as low as possible. Such measures may include investigating if the supplying company ensures a save working environment and good working conditions. Also, standards and management practices should be in place to avoid corruption, forced labor or discrimination at respective supplying companies. Regarding the extremely positive and negative risk scores (e.g., Figure 9A) on reporting of non-fatal occupational injuries, the data should be considered with caution as Finland [39] has a much more rigorously enforced policy than other countries. The USA for example is aware of underreporting of workplace injuries and illnesses, which Pransky and colleagues have pinpointed to fear repercussions (cf. other social aspects in the USA in Figure 9, such as poor collective bargaining coverage) [40].

6.4 Preparing to adhere to the potential legal regulations for sustainable batteries

Batteries take a key role in the transition towards a zero-emission mobility landscape and the effective storage of intermittent renewable energy sources. Their importance is further highlighted in the European Parliament´s report "New EU regulatory framework for batteries", which emerged from the Thinktank in July 2021. The new proposal on sustainable batteries aims to ensure that batteries entering the EU market are to be sustainable and safe throughout their entire life cycle [41]. In summary, the EU's focus on batteries as the keystone of its climate-neutral journey is underpinned by three interlinked objectives: Harmonizing regulations, promoting circularity, and prioritizing sustainability.

However, guidelines for RFBs are not included in the scope of the proposed regulatory directive. Nonetheless, the **general considerations have been translated** to the present technology and thus considered in the **SSbD concept and application**. This includes **information about raw materials** and **the supply chain in general**, carbon footprint, climate, and ecosystem impact by means of life-cycle-assessment, **considerations of end-of-life scenarios** and waste management, circularity, and information about safety risks. By anticipating these steps in the current study, we are striving to be prepared for the potential implementation of regulations in the future.

6.5. Relation to the recently published SSbD framework

The Joint Research Centre (JRC) of the European Commission (EC) recently published a review and framework for SSbD [22, 42], which shall support the transition towards safer and more sustainable chemicals and materials. **The present study was conducted before the publication of these documents**, hence the exact stepwise approach described within them was not applied, however, **specific steps of its implementation already anticipated in the concept**. In future studies, we will consider the framework as a guiding measure to assess and improve SSbD. Case studies applying the JRC SSbD framework to RFBs will improve the domain of battery design in the terms of safety and sustainability tremendously.

7. Conclusion

In conclusion, the study accompanied and improved the design process for bio-based compounds used in the electrolyte of novel RFBs. The key highlights, actions and pitfalls were identified and are presented in Figure 9. Social impacts were identified early in the process chain in the form of country specific concerns regarding the sourcing of lignin. Streamlined LCA revealed that the conversion of lignin to vanillin is the biggest energy demanding factor. However, **in literature only one dataset** was available, which did not consider reuse of thermal energy. Further, **fossil-based fuels** were used as **primary energy sources**; the use of **renewable energy** in the processes **was not considered**. We are currently working to **generate our own dataset** together with our industrial partners. Concerning direct improvements of sustainability, it can be highlighted that a **greener choice of solvents for the quinone** synthesis was achieved, while the most promising candidates regarding ecotoxicity were identified. Taken together, the **implemented changes improved the RFBs in terms of sustainability** and the newly acquired knowledge for impact points in the process chain will further enable better control and development advances. It should be emphasized that the main objective of the study was to highlight a **concept for SSbD implementation into battery development**. The technology has continued to improve, and more sustainable processes are now available, which are being analyzed and will be published in the near future.

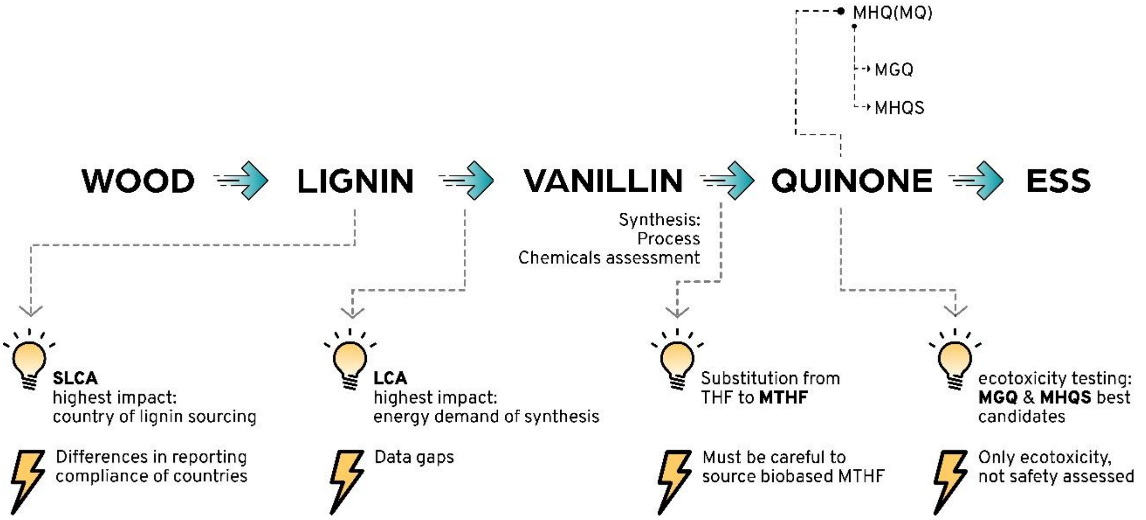


Figure 9: Schematic scheme of the process chain, highlighting the major findings and pitfalls.

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