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# Safe-and-sustainable-by-design redox active molecules for energy storage applications

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## Abstract

**Background** Sustainability aspects have become a main criterion for design next to performance of material and product. Particularly the emerging field of energy storage and conversion is striving towards more sustainable solutions. However, implementing sustainability considerations during the design and development phase of energy materials and products is challenging due to the complexity and broadness of the different dimensions of sustainability.

**Results** Here, we demonstrate that by using the principles of Safe-and-Sustainable-by-Design (SSbD), a concept can be formulated. This concept served as the basis for selecting and evaluating criteria and performance parameters aimed at enhancing the safety and sustainability aspects of redox active molecules in an organic redox flow battery. Following an iterative approach, the collected data provided valuable insights enabling us to fine-tune and enhance the materials and processes in alignment with the identified parameters. (Social) life cycle assessment focused on the workflow from sourcing, processing and generation of intermediate products to the quinone used in the redox flow batteries and revealed important insights, highlighting critical steps in the process chain. Additionally, we identified two specific points of intervention regarding solvent and quinone choice, based on sustainability parameters. The proposed solvent change resulted in a greener alternative [changed from tetrahydrofuran (THF) to 2-methyltetrahydrofuran (MTHF)], and the ecotoxicity testing revealed MGQ and MHQS to be improved options. However, we also faced severe challenges regarding access to reliable LCA data on the raw material sourcing.

**Conclusion** Taken together, the modified designs led to safer and more sustainable redox active materials for both humans and the environment at lab scale. Implementing the results mentioned above to further expedite the technology will ultimately pave the way to more sustainable energy storage applications. This study proved the value of implementing of an SSbD concept in battery development is the main result of this study.

**Keywords** Safe-and-sustainable-by-design, Safe-by-design, Redox flow battery, Energy storage system, Quinone, Electrolyte, Ecotoxicity, Social life cycle assessment, Life cycle assessment

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## Background

The past several years have been dominated by rapid changes in European energy policies, triggered by climate change and, recently, geopolitics [1, 2]. The increasing share of renewables in electricity generation is a major challenge for grid operators, as supply often does not match demand and consumers are not always located close to power generation sites. Seasonal changes further exacerbate this mismatch. The main challenge we are currently facing, is to manage this efficiently via backup solutions. While there is a plethora of ideas and concepts available (e.g., energy quarters, island solutions) to counteract this, the lack of energy storage systems (ESS), and in particular batteries remains a hinderance [3]. Most battery technologies rely on critical raw materials (CRMs), which are not available in sufficient quantities in the European Union (EU) [4–8]. This involves metals used in lithium-ion battery (LIB) technology (e.g., lithium, cobalt), as well as vanadium used in redox flow battery (RFB) technology.

These batteries can be used to ameliorate fluctuations in the grid. Both LIB and RFB technologies have recently been reviewed regarding their assets from a technological perspective [9, 10]. Safety issues of LIBs are extensively described and include ignition due to thermal runaways, often caused by dendrite formation. This leads to separator damage, failure and subsequently a short circuit [11]. In addition, recycling of LIBs poses several concerns, causing major problems in the recycling value chains [12]. Vanadium, used in RFBs, in turn is rather safe with respect to fire hazards, but comes with high inherent toxicity at even small doses [13]. As these CRMs cannot be mined in Europe, mining and transport of these materials compromise the ecological benefits of these technologies [14].

To assess environmental and social impacts regarding the entire life cycle of a particular product or process, (social) life cycle assessment (LCA) is performed. However, LCA of ESS faces several challenges which are yet to be improved and mastered [15]. These challenges include, but are not limited to, availability and quality of technical performance data and LCA data, selection of system boundaries, choice of impact categories, classification of recycled material (including its quality) and the number of available studies. Recently, a review has outlined the challenges that must be addressed for the RFB ecosystem [16]. Due to the novelty level of the technology, only a limited number of LCA studies are available. The data gap further expands due to the lack of toxicological data for both humans and the environment, which may impede life cycle considerations.

It is therefore essential to focus on assessing and improving safety and sustainability aspects of new technologies used in ESSs, employing the concept of Safe-by-Design (SbD) and Safe-and-Sustainable-by-Design (SSbD). The results discussed here are an outcome of the SABATLE project [17], whose conception already incorporated the importance of SbD and SSbD into the proposal. Based on delivered concepts within EU-funded projects (such as R2R Biofluidics [18], Hi-Response [19], INSPIRED [20], Smart-4-Fabry [21]), the approach to address requirements for safety and sustainability was further developed in-depth by considering strategic documents [22, 23] and tailoring to the ESS material sector, more specifically to the biobased electrochemical species for RFBs.

The concept of SbD has been recently extended by sustainability criteria to cover a full life cycle view (Fig. 1) to pave the way for SSbD innovations [24–27]. By focusing on the delivered purpose of a product, rather than its exact form, innovation can occur more broadly and a wide range of possible candidates for application can be considered [22]. In addition, a thorough understanding of the regulatory requirements with which the product must comply will help to create the ideal starting conditions. This prevents late failures in the innovation

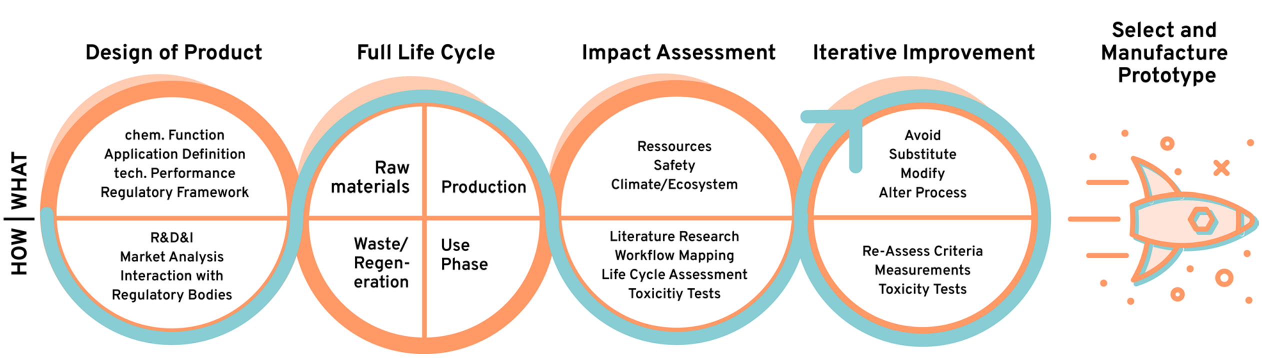


**Fig. 1** Safety and sustainability as an iterative design framework. Simplified workflow for where and how Safe-and-Sustainable-by-Design during the design and innovation phase of a novel product (whether material, chemical or multicomponent product) can be applied

process. Combined with an early business perspective, this increases the focus on the conditions and needs of the current market, as well as the barriers and challenges that need to be overcome to enter the market.

In this study, safety and sustainability criteria and performance parameters were selected and assessed in parallel to the development process of the electrolyte used here for RFBs. A potential solution to address the above-mentioned technical issues is the use of redox active biobased materials, which can either be employed as redox active electrodes or as redox active species in electrolyte formulations. Quinones are among the best investigated biobased materials in this context as they possess a highly reversible redox potential [28]. Some of these redox active biobased materials and/or their precursors can be obtained in large scale from industrial side streams [29]. Lignin in particular has attracted considerable interest recently, which led to several approaches being currently followed up to valorize lignin and its depolymerization products in energy storage systems [30, 31]. However, some of these redox active biobased materials, such as viologens or benzoquinone, feature significant toxicity for both humans and the environment. In addition to these inherent toxicity properties, the solvents used in synthesis processes often present sustainability and safety concerns as well [32].

Hence, this research showcases that the implementation of the SSbD and the generation of project-specific concepts, such as for SABATLE, can lead to the creation of more eco-friendly materials in RFBs, offering guidance for the development of environmentally sustainable solutions.

## Materials and methods

Additional information for Materials and methods can be found in the Supplemental Material.

### General approach

By gathering information to assess the performance of candidate products against safety and sustainability criteria, the life cycle was mapped under given system boundaries using a workflow mapping template (Fig. 2).

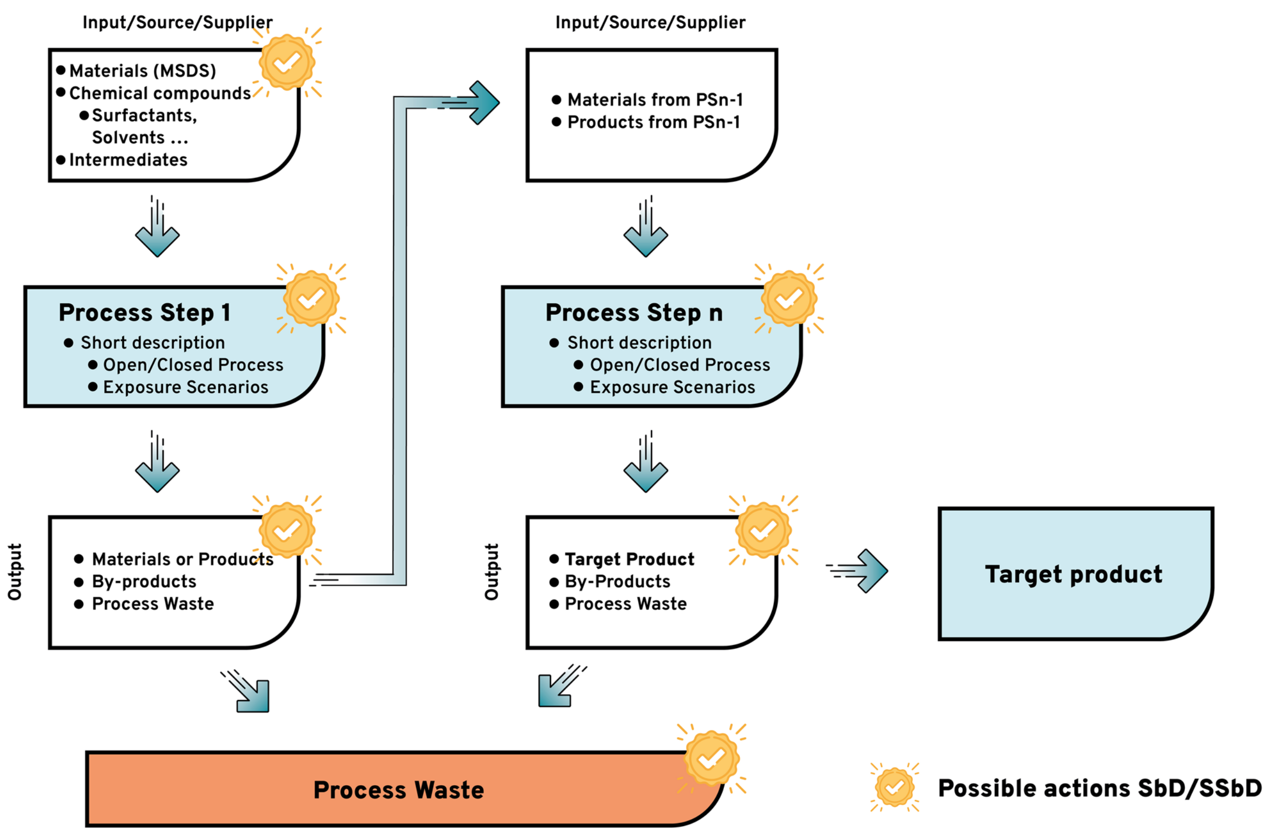


**Fig. 2** Workflow mapping template for materials, processes, and products life cycle. Workflow mapping offers a comprehensive depiction of the processes in question, along with a clear record of the input and output for all materials and (intermediate) products, as well as any generated process waste. In general, the model concept is intended to provide innovators and Safe-and-Sustainable-by-Design (SSbD) experts with a comprehensive overview of the entire process chain and should be updated accordingly during the analysis. Possible action points for SSbD are indicated by a *yellow dot*. *MSDS* material safety data sheet, *PS* process step; *PS1* first process step; *PSn* nth process step

Assessment of the performance impact of each candidate product throughout its life cycle encompassed various dimensions related to SSbD. The analysis involved identifying all utilized chemicals in the production and/or recycling process, as well as in waste streams. Potential emissions and effects of potential exposure to hazardous chemicals on human health and the environment were thoroughly evaluated. This assessment drew upon data from sources such as the European Chemicals Agency (ECHA) database, LCA inventories, and ecotoxicity testing. A comprehensive mapping of the resources used and consumed was performed. Analysis of end-of-life recovery and process waste handling was omitted, as it is beyond the scope of this work. This evaluation was performed by expert interviews and aimed to promote a circular economy approach. The analysis further encompassed a wide range of potential environmental impacts, including energy consumption, damage to ecosystems during resource extraction and emissions of pollutants and greenhouse gas within predefined system boundaries. This assessment employed a streamlined LCA approach to quantify emissions.

In addition to the environmental considerations, an examination of potential social risks associated with the quinone value chain was carried out using a generic social life cycle assessment (sLCA). This analysis delved into various social aspects related to the product's life cycle, aiming to identify and mitigate potential risks.

During the final phase of the approach, an evaluation was conducted, considering the outcomes of prior stages, and deliberating on potential further strategies. This involved a thorough discussion and proposal of mitigation strategies based on the technical parameters and chemical functionality criteria. To pursue improvements, the results of the avoidance strategy criteria were re-evaluated and re-measured to identify the optimal solution under given conditions and predefined system boundaries.

### Materials inventory

As an outcome of the workflow mapping described in Fig. 2 and the derived inventory of the chemicals used in the synthesis of the battery electrolytes (Table 1), safety information was gathered from different sources. As a main source the ECHA database [33] was used. In addition, the Classification, Labeling and Packaging (CLP) inventory [34], which is part of the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) regulation [35], and the PubChem database [36] were consulted.

### Streamlined LCA

The environmental impacts of products or services can be assessed by means of LCA (ISO 14040 and 14044, 2006) [37, 38]. The method itself is widely acknowledged and defines four phases to perform an assessment [39]:

- The goal and scope definition
- The life cycle inventory (LCI)
- The life cycle impact assessment (LCIA)
- 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 [40–43].

**Table 1** Material inventory for chemicals used in the synthesis of battery electrodes

| Input | | Output | |
|---|---|---|---|
| **Chemical (molecular formula)** | **PubChem CID** | **Chemical (molecular formula)** | **PubChem CID** |
| Vanillin, solid | 1183 | MHQ | 69,988 |
| THF | 8028 | THF | 8028 |
| MTHF | 7301 | MTHF | 7301 |
| Sodium hydroxide (NaOH) | 14,798 | Sodium hydroxide (NaOH) | 14,798 |
| Sodium percarbonate ($Na_2CO_3{\cdot}1.5H_2O_2$) | 159,762 | Sodium percarbonate ($Na_2CO_3{\cdot}1.5H_2O_2$) | 159,762 |
| Water, deionized ($H_2O$) | 962 | Water, deionized ($H_2O$) | 962 |
| Toluol | 1140 | Toluol | 1140 |
| | | Sodium Nitrate (NaNO3) | 24,268 |
| Hydrogen peroxide ($H_2O_2$) | 784 | Hydrogen peroxide ($H_2O_2$) | 784 |
| | | Sodium carbonate ($Na_2CO_3$) | 10,340 |
| | | Carbon dioxide ($CO_2$) | 280 |

*CID* compound identification number

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. 3, Supplemental Table 2) [44]. Importantly, the currently employed LCA method cannot distinguish between the subtypes of quinones (e.g., MHQ, MQ, MGQ, MHQS). However, a streamlined

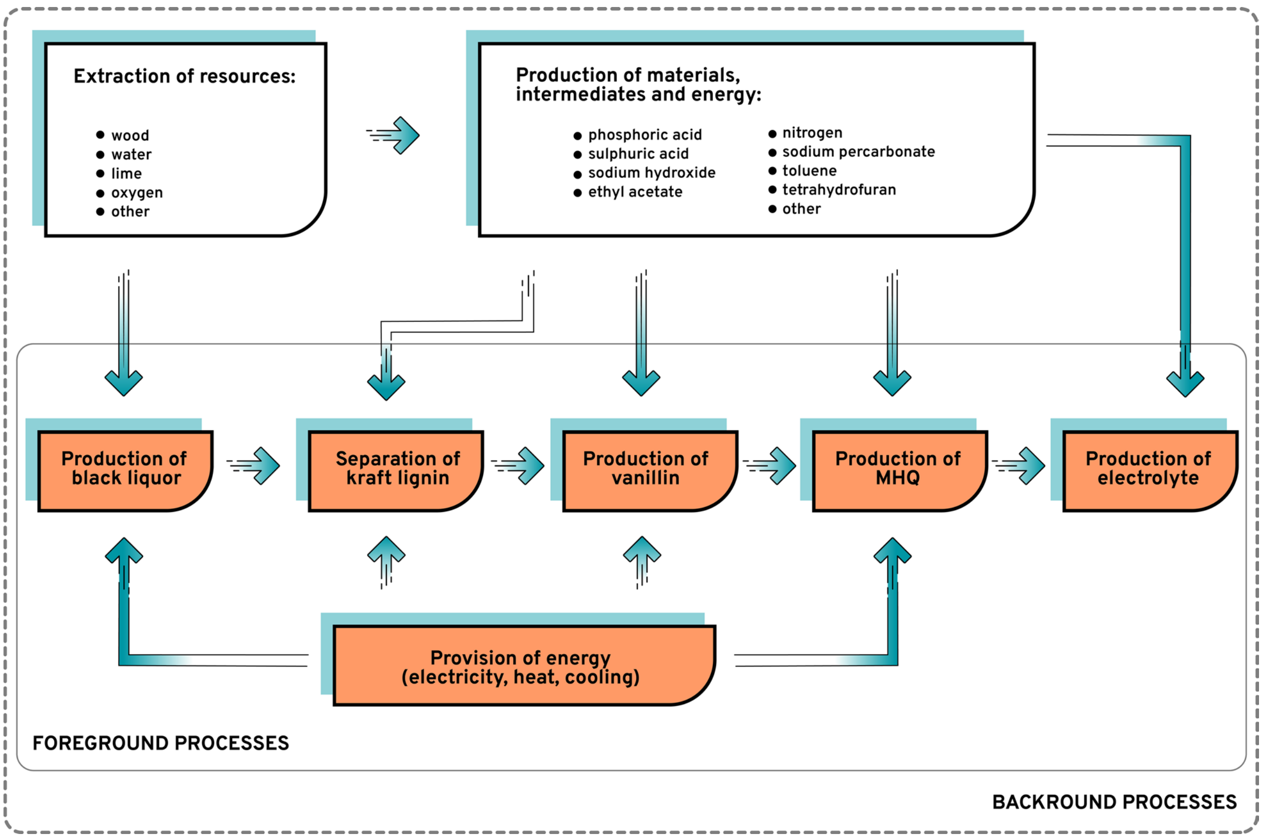


**Fig. 3** Simplified illustration of the system boundaries from cradle-to-gate including foreground and background processes

**Table 2** Selected social indicators according to the SSbD framework (Joint Research Council of the European Commission). Adapted from Caldeira et al. [25]

| Stakeholder group | Social aspect | Indicator | Source |
|---|---|---|---|
| Workers | Child labor | Realization of children's rights index | https://www.humanium.org/en/rcri/ [60] |
| | Forced labor | Estimated proportion Living in modern slavery | https://www.globalslaveryindex.org/2018/data/maps/ [61] |
| | Health and safety | Fatal occupational injuries | https://www.ilo.org/ [62] |
| | | Non-fatal occupational injuries | https://www.ilo.org/ [62] |
| | | Coverage of essential health services | https://vizhub.healthdata.org/sdg/ [63] |
| | Freedom of association and collective bargaining | Collective bargaining coverage | https://www.ilo.org/ [62] |
| | | Global right index | https://www.globalrightsindex.org/de/2023 [64] |
| | Equal opportunities/discrimination | Gender inequality index | https://hdr.undp.org/ [65] |
| Local community | Local employment | Unemployment rate | https://www.ilo.org/ [62] |
| Society | Corruption | Corruption perception index | https://www.transparency.org/en/cpi/2018 [66] |

LCA was performed for different routes of MHQ-generation (Route A versus Route B, compare Supplemental Fig. 2 and Table 3). Due to lack of data availability for the MTHF in generic LCA databases, THF was considered for both routes.

In the LCI phase the inputs and outputs of all the processes from cradle-to-gate were collected. Different sources were used to collect the data for the foreground processes depicted in Fig. 3. The inventories for the extraction of kraft lignin from black liquor were taken from Culbertson and colleagues [45, 46]. For the inventories of the vanillin extraction from kraft lignin a techno-economic study by Khwanjaisakun et al. was used [47]. The inventories of the MHQ production and electrolyte composition were 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 were calculated by first selecting impact categories, category indicators and characterization models [37, 38]. 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 [16], the impacts were 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

**Table 3** Material safety observations from input–output analysis of both synthesis routes A and B

| Route A | Hazard statements | Route B | Hazard statements |
|---|---|---|---|
| Vanillin, solid | Skin Sens. 1<br>Eye Irrit. 2 | Vanillin, solid | Skin Sens. 1<br>Eye Irrit. 2 |
| 2-Methoxyhydroquinone | Acute Tox. 4<br>Skin Irrit. 2<br>Eye Irrit. 2<br>STOT SE 3<br>Aquatic Acute 1 | 2-Methoxyhydroquinone | Acute Tox. 4<br>Skin Irrit. 2<br>Eye Irrit. 2<br>STOT SE 3<br>Aquatic Acute 1 |
| Tetrahydrofuran (THF) | Flam. Liq. 2<br>Acute Tox. 4<br>Eye Irrit. 2<br>STOT SE 3<br>Carc. 2 | 2-Methyltetrahydrofuran (MTHF, for LCA THF) | Flam. Liq. 2<br>Acute Tox. 4<br>Skin Irrit. 2<br>Eye Dam. 1<br>Eye Irrit. 2<br>STOT SE 3 |
| Sodium hydroxide (NaOH) | Skin Corr. 1A | Sodium hydroxide (NaOH) | Skin Corr. 1A |
| Sodium percarbonate ($Na_2CO_3 \cdot 1.5\ H_2O_2$) | Ox. Sol. 2<br>Acute Tox. 4<br>Eye Dam. 1 | | |
| Toluol | Flam. Liq. 2<br>Repr. 2<br>Asp. Tox. 1<br>STOT SE 3<br>STOT RE 2 *<br>Skin Irrit. 2 | | |
| | | Hydrogen peroxide ($H_2O_2$) | Ox. Liq. 1<br>Acute Tox. 4<br>Skin Corr. 1A<br>Eye Dam. 1<br>Acute Tox. 4<br>STOT SE 3<br>Aquatic Chronic 3 |
| | | Sodium nitrate ($NaNO_3$) | Ox. Sol. 2<br>Acute Tox. 4<br>Eye Irrit. 2 |
| Carbon dioxide ($CO_2$) | – | Carbon dioxide ($CO_2$) | – |
| Deionized water ($H_2O$) | – | Deionized water ($H_2O$) | – |

Hazard statements obtained from ECHA (%) [33] or EU REGULATION (EC) No. 1272/2008 (scale) [34]

*Asp.* aspiration, *Carc.* carcinogenicity, *Corr.* corrosion, *Dam.* damage, *Flam.* flammable, *Irrit.* irritation, *Liq.* liquid, *Ox.* oxidizing, *RE* repeated exposure, *Repr.* reproductive toxicity, *SE* single exposure, *Sens.* sensitization, *Sol.* solution, *STOT* specific target organ toxicity, *Tox.* toxicity; according to CLP a lower number indicates a higher hazard [34]. A * indicates that importers/manufacturers are obliged to use the current grading but must classify in a more severe grading if additional information becomes available non-cancer), acidification, eutrophication (freshwater, marine and terrestrial), ecotoxicity, freshwater, land use, water use and resource use (fossils and minerals and metals).

### Generic SLCA

The potential social risks in the MHQ value chain were investigated by means of generic SLCA. In the case of the SLCA, the focus of the investigation is on the interest groups potentially affected by the activities or behaviors "of organizations linked to the life cycle of the product or service and from the use of the product itself" [48]. At the early stage in product development, it is rare to know which companies will ultimately produce the products. 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. [49]. 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 [50, 51]. The first step was 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 [52]. The main producers of kraft lignin are Finland, USA, Brazil, and Canada [52, 53]. 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 [52]. 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 we envision for the future, the kraft lignin, synthesis of vanillin, and MHQ production will be carried out in Austria. After the identification of the affected regions, relevant indicators need to be identified [54, 55]. Here we followed the suggestions provided by the Joint Research Center (JRC) of the European Commission (EC) framework for SSbD, in which the potential social impacts of the stakeholder groups, workers, local communities and consumers are the ones most often considered among stakeholder groups with a total of eleven social aspects [25, 56]. In this context the focus lies on developing safe and sustainable chemicals or materials. Therefore, the objective of the generic SLCA was to identify social risks of a potential future value chain of MHQ, to provide insights and recommendations on tackling critical social aspects even 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. However, the stakeholder group Society was included as the focus is on the social risks of a potential source of lignin, and corruption is an aspect that is dealt with in this category.

The data collection was performed following the recommendations given in the methodological sheets of the United Nations Environment Programme guidelines [57]. Generic data were collected from publicly available data sources, e.g., the International Labour Organization (ILO), to quantify the selected indicators (see Table 2). The data gathered were 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 [58, 59]. This is illustrated in Fig. 8.

## Results

### Analysis of synthesis routes A and B—material safety observations

The hazard potentials shown in Table 3 result from the material safety analysis of the two synthesis routes A and B and their corresponding chemical material inventory. Both synthesis routes A and B have similar inventories, with the main difference being the choice of solvent: THF for route A and MTHF for route B. Additionally, toluene is absent from route B, while hydrogen peroxide and sodium nitrate only occur in Route B.

### Improving sustainability of MHQ synthesis by choosing a greener solvent

THF is often produced from fossil raw materials and thus suggested for replacement according to SSbD principles. To that end, methyl-tetrahydrofuran (MTHF) is a suitable candidate [67]. Compared to THF, MTHF has a slightly lower tendency to form peroxides, however, it still warrants the use of a stabilizer (e.g., butylhydroxytoluol, BHT). Nevertheless, using MTHF in the synthesis of MHQ allows reaching yields as high as those reached by using THF (see Supplemental Fig. 1). Since MTHF can be exclusively produced from biobased feedstock (as it is a side-product of industrial furfuryl alcohol production, which uses lignocellulosic feedstocks (e.g., corncobs, bagasse)), replacing this solvent contributes to increase sustainability of the reaction [68].

### MHQ and MQ present as ecotoxic in *Daphnia* immobilization assay

For toxicity testing, the established *Daphnia* immobilization assay [69], which is used to assess environmental risk assessment of new chemicals, was employed. The results obtained after the treatment of *Daphnia* neonates with

5 concentrations of the tested items to determine the best range for the definitive test are shown in Fig. 4 and Table 4. The DRF experiment in *Daphnia* was considered valid since <10 and >50% immobilization could be detected in the vehicle and positive controls, respectively. Based on the DRF results the test concentrations for the definitive *Daphnia* immobilization assay were selected. MHQ and MQ were highly toxic to the water flea *Daphnia magna*. A 50% immobilization of the investigated daphnids by these two electrolytes was already detected in the upper picomol range.

### Adaptation of quinone synthesis

Due to the severe implication of MHQ and MQ in ecotoxicity assays on daphnids, the synthesis of quinones was modified in an iterative approach. Therefore, the strategy was to modify the MHQ scaffold with other functional groups. One strategy was to employ secondary amines, which can react with the MHQ in an addition–elimination type reaction. In this type of reaction, the methoxy group of the MHQ is cleaved off and a symmetrically substituted diaminoquinone is obtained. Concretely, we reacted the MHQ with NMEA, a secondary amine to receive MGQ (see also Supplemental Fig. 1). This reaction does not require any other solvents than ethanol, and the product precipitates from this solution once the reaction has ended. Neither heating nor cooling is required to run the reaction and after stirring overnight the compound can be collected in the form of red crystals after precipitation.

Additionally, MHQS was synthesized from MHQ. MHQS has previously been described by Preger and colleagues; however, they employed the carcinogenic benzoquinone as a starting product [70]. Here, we developed an electrochemical synthesis route to obtain the MHQS directly from MHQ (Supplemental Fig. 1). The reaction does not rely on the use of toxic solvents. The resulting molecule has a similar performance (though the cyclability was tested in another medium, here phosphoric acid versus sulfuric acid in the work of Preger et al.) as described in literature [70] and features good cyclability as proven by cyclovoltammetry (Supplemental Fig. 4).

### MGQ and MHQS are non-toxic in *Daphnia* immobilization assay

The newly synthesized quinones were subjected to the same ecotoxicity test as their precursor MHQ and MQ. In contrast to these, MGQ and MHQS were evaluated to be non-toxic to daphnids since the percentage of immobilized daphnids did not exceed 20% compared to the control (Fig. 5 and Table 5). The results of the *Daphnia*

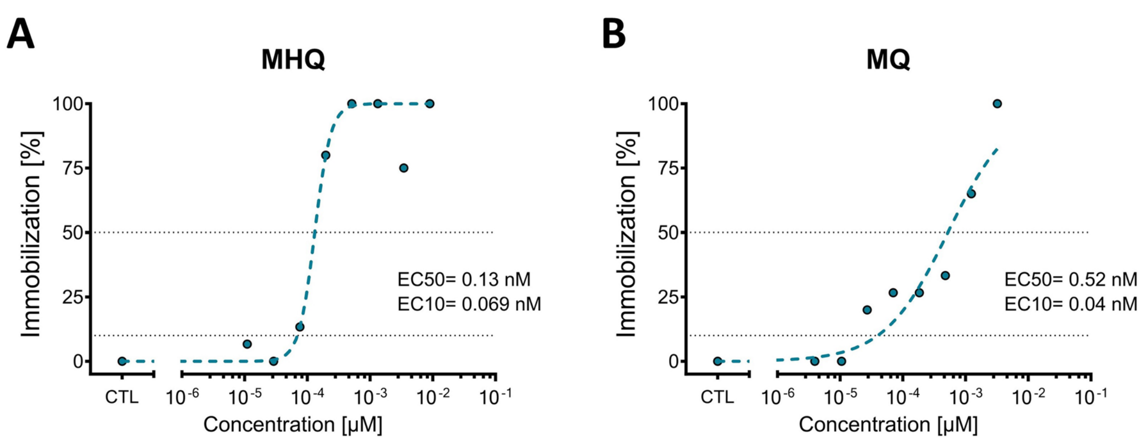


**Fig. 4** Results of the ecotoxicity tests on MHQ (**A**) and MQ (**B**) using Daphnia magna immobilization assay. *CTL* control, *EC* effective concentration

**Table 4** Results of the ecotoxicity tests on MHQ and MQ using Daphnia magna immobilization assay

| Test substance | Concentration in DRF test | Precip (yes μM/no) | Concentrations for *Daphnia* immobilization assay | EC50 48 h | EC10 48 h | Classif. |
|---|---|---|---|---|---|---|
| MHQ | 1, 3, 61, 412, 1070 nM | No | 0.01, 0.03, 0.01, 0.2, 0.5, 1.3, 3.5, 9.0 nM | 0.13 nM | 0.069 nM | Toxic |
| MQ | 1, 8, 22, 146, 986 nM | No | 0.004, 0.01, 0.03, 0.1, 0.2, 0.5, 1.2, 3.2 nM | 0.52 nM | 0.04 nM | Toxic |

*Classif.* classification, *DRF* dose–response finding, *EC* effective concentration, *Precip.* precipitation immobilization are the most divergent outcomes of all four assays since there are striking differences between the toxic MHQ and MQ and the test items MGQ and MHQS, which exhibit very low effect potential towards the mobility impairment of daphnids. Differences in

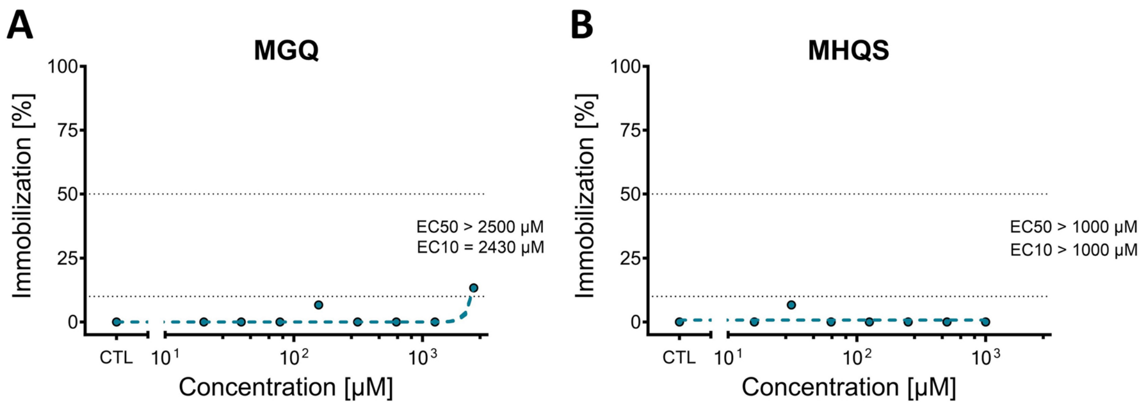


**Fig. 5** Results of the ecotoxicity tests on MGQ (**A**) and MHQS (**B**) using Daphnia magna immobilization assay. *CTL* control, *EC* effective concentration

**Table 5** Results of the ecotoxicity tests on MGQ and MHQS using Daphnia magna immobilization assay

| Test substance | Concentration in DRF test | Precip (yes µM/no) | Concentrations for *Daphnia* immobilization assay | EC50 48 h | EC10 48 h | Classif. |
|---|---|---|---|---|---|---|
| MGQ | 0.1, 1, 10, 100, 1000 µM | 1000 | 20, 39, 78, 156, 313, 625, 1250, 2500 µM | >2500 µM | 2430 µM | Non-toxic |
| MHQS | 0.06, 0.6, 6, 60, 600 µM | 60, 600 | 8, 16, 31, 63, 125, 250, 500, 100 µM | >1000 µM | >1000 µM | Non-toxic |

*Classif.* classification, *DRF* dose–response finding, *EC* effective concentration, *Precip.* precipitation

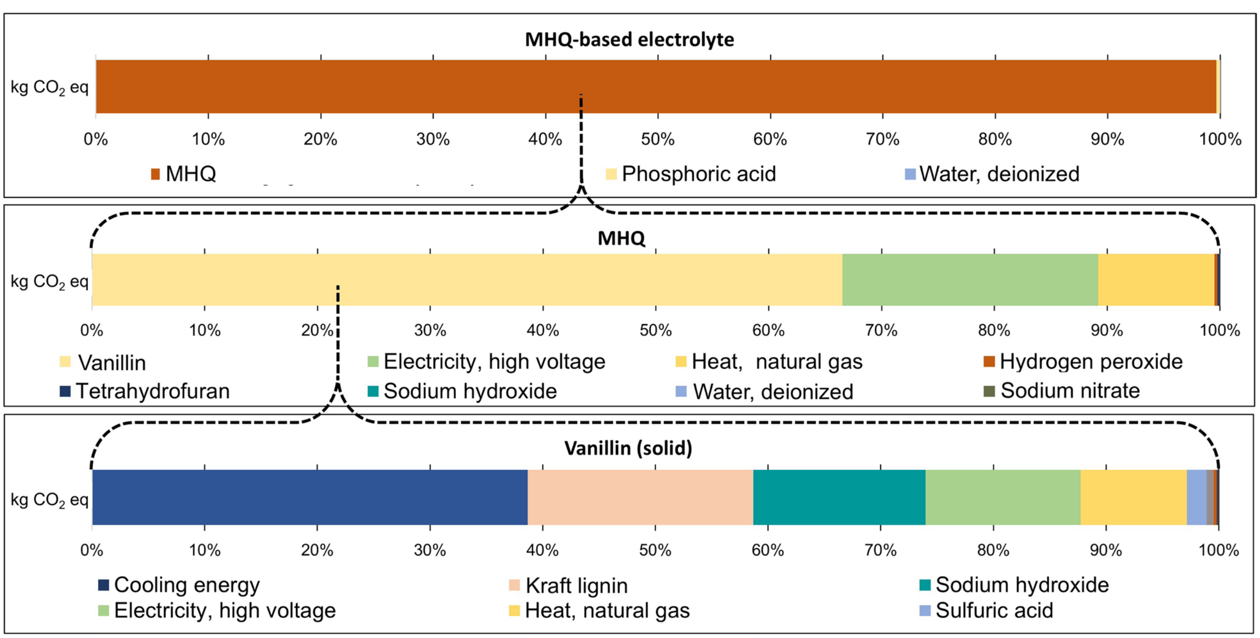


**Fig. 6** Environmental hotspots in terms of global warming potential (GWP) of the MHQ electrolyte. 100% represents the total impact, divided up in different categories according to their respective proportion of the full impact

the $EC_{50}$ ranges between these two groups are of seven orders of magnitude.

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

In Fig. 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.

Apart from the impacts related to energy demand, the progress in quinone development (Route B of MHQ synthesis, Fig. 7) 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. 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 for early phases of technology development (see [40]). 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.

### 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 Fig. 8. The results show that Brazil forms a hotspot in most indicators (8/10). Also, Canada and the United States indicate 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 [62]. The global rights index documents violations of internationally recognized collective labor rights by governments and employers [64]. 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 (Fig. 8A). Austria appeared as the country with the lowest risks for almost all investigated indicators (Fig. 8A–C).

## Discussion

The project-specific SSbD concept generated here served to assess a specific set of quinones derived from bio-based vanillin, which can be used in RFBs. The goal of this procedure was to consider materials performance and connect it to sustainability data, including

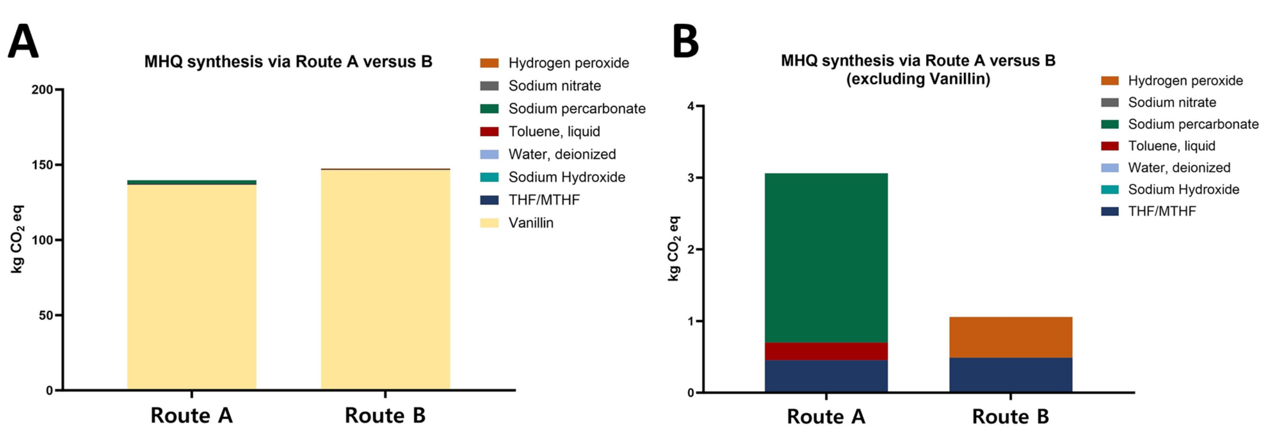


**Fig. 7** MHQ synthesis comparison of Route A and B based on kg $CO_2$ eq (**A**) and zoom in, disregarding vanillin (**B**). *eq* equivalents

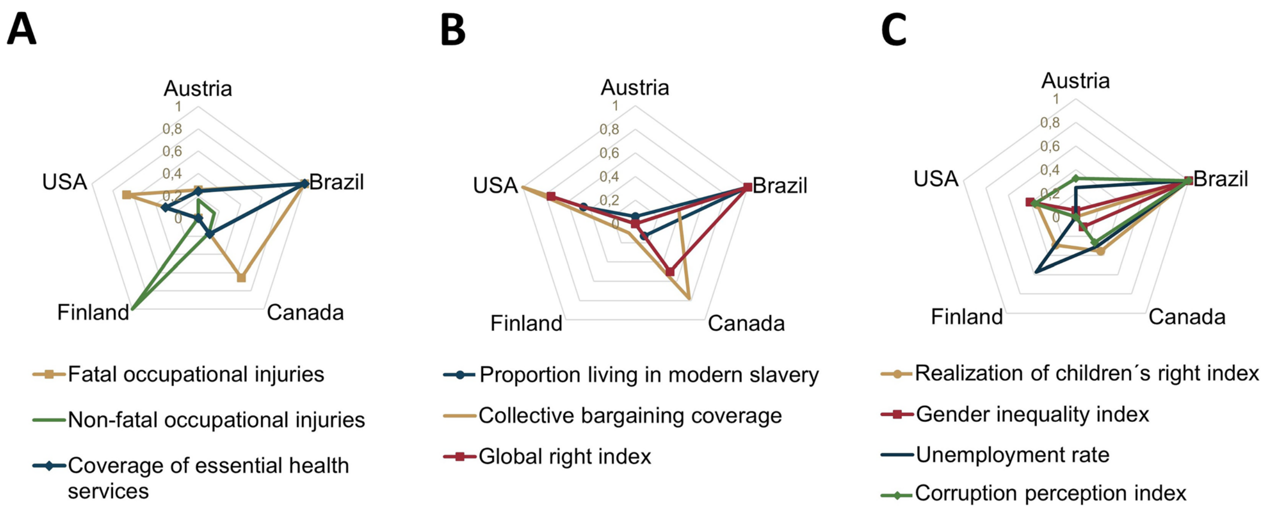


**Fig. 8** Social risks or opportunities in different indicators, highlighting hotspot countries (**A**–**C**). Normalized values from 0: lower to 1: higher social risks. Data extracted from [60–66]

ecotoxicity testing and putting it into the context of social and environmental performance.

### Safety and sustainability of quinone synthesis was improved by greener solvent choice, omission of toluene, and ultimately 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. To achieve phase separation for the recovery of solvent in the continuous process, $NaNO_3$ was used instead. $NaNO_3$ is well known as a process chemical with well manageable risk profiles. In addition to the listing of hazard potential provided here, tools such as VEGA QSAR [71] could improve the assessment and classification further. The starting point for this study was MHQ. Substitution of THF by MTHF provides not only similar yields of MHQ, but is less toxic [72] and a greener alternative, due to reduced emission (by 97%, [73]), as it can be sourced from renewable sources. Also, as a side-product, it is economically competitive for THF. 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 is an additional economic benefit, 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. However, it must be noted that the LCA used here 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 publication. Nonetheless, the possibility of employing ethanol as a solvent has been investigated; however, the authors reached the conclusion that the workup with other solvents is a main hindering issue and significantly reduces the yield of the process. Hence, the use of MTHF presents the optimal solution at the moment.

While this constitutes as acceptable improvement for the sustainability of the reaction itself, the toxicity of these compounds remains unknown. The newly synthesized quinones MGQ and MHQS are recommended for further use, as they presented with significantly superior ecotoxicity outcomes compared to their precursors and the state-of-the-art electrolytes used in RFBs, such as vanadium oxide [13].

### 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 [47, 74], 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 established vanadium electrolyte production. However, the results do give an indication, based on current knowledge, as to 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 indicate that these adaptations to the processing serve as convincing cases for implementing the SSbD approach, specifically for applying the re-design steps. 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 to the results regarding the GWP (Fig. 6) 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.

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

It should be noted that the results in Fig. 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 safe 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., Fig. 8A) on reporting of non-fatal occupational injuries, such as Finland, the data should be considered with caution, as Finland [75] has a much more rigorously enforced policy than other countries. The United States, for example, is underreporting workplace injuries and illnesses, which Pransky and colleagues have attributed to fear of repercussions (cf. other social aspects in the U.S. in Fig. 8, such as poor collective bargaining coverage) [76].

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

Batteries play 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. 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 SABATLE SSbD concept. 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.

### Relation to the recently published SSbD framework

The JRC recently published a review, a framework and methodological guidance for SSbD [25, 26, 77], which shall support the transition towards safer and more sustainable chemicals and materials, which has been further expanded by a recommendation by the EC [27]. The present study was conducted before the publication of the EC's documents, hence the exact stepwise approach described within them was not applied. However, specific steps of its implementation were already anticipated in the concept as shown in this publication. 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 terms of safety and sustainability tremendously.

## Conclusions

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 Fig. 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. Taken together, the implemented changes improved the RFBs in terms of sustainability

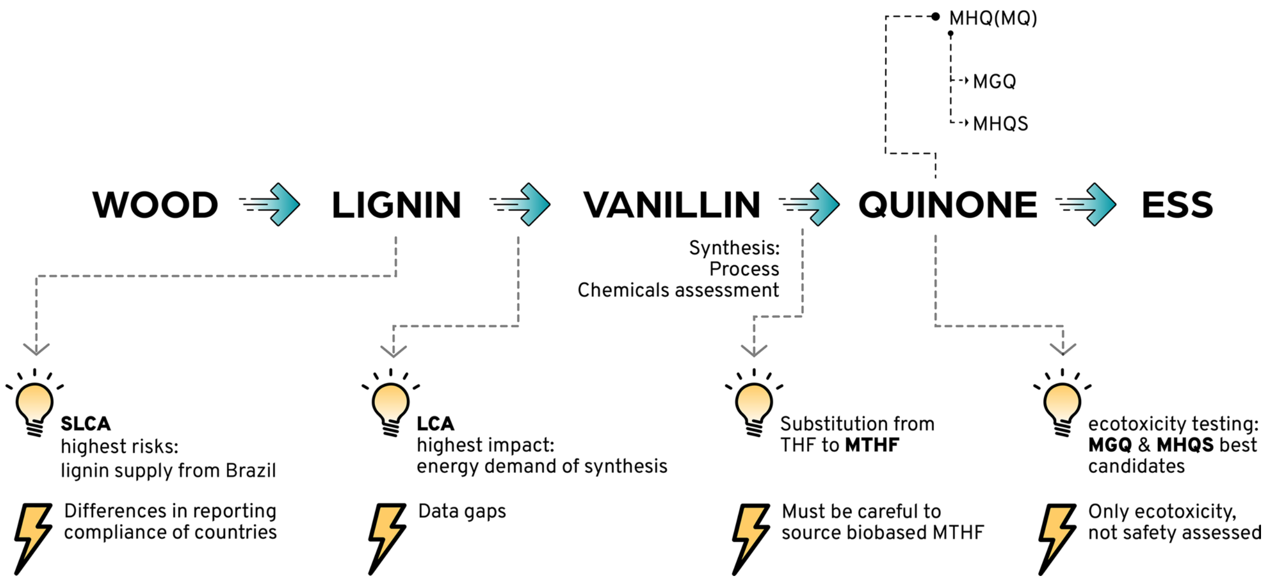


**Fig. 9** Schematic scheme of the process chain, highlighting the major findings and pitfalls

and the newly acquired knowledge for impact points in the process chain will improve control and development. It should be emphasized that the main objective of the study was to highlight a concept for implementing SSbD into battery development. The technology has continued to improve, and more sustainable processes are now available, which are being analyzed and will be published.

**Abbreviations**

| | |
|---|---|
| CID | Compound identification number |
| CLP | Classification, labeling and packaging |
| CRM | Critical raw material |
| DRF | Dose–response finding |
| EC | European Commission |
| ECHA | European Chemicals Agency |
| EF | Environmental footprint |
| ESS | Energy storage system |
| EU | European Union |
| GHG | Greenhouse gas |
| GWP | Global warming potential |
| ILO | International Labor Organization |
| JRC | Joint Research Centre |
| LCA | Life cycle assessment |
| LCI | Life cycle inventory |
| LCIA | Life cycle impact assessment |
| LIB | Lithium-ion battery |
| MGQ | 2,5-Bis(*N*-methylethanolamino) cyclohexa-2,5-diene-1,4-dione |
| MHQ | 2-Methoxyhydroquinone |
| MHQS | Sodium 3,3′,3″,3‴-((3,6-dihydroxybenzene-1,2,4,5 tetrayl) tetrakis(sulfanediyl))tetrakis(propane-1-sulfonate) |
| MPSNa | Sodium 3-mercaptopropylsulfonate |
| MQ | 2-Methoxy-1,4-benzoquinone |
| MTBE | Tert-butylmethylether |
| MTHF | 2-Methyltetrahydrofuran |
| NMEA | *N*-Methylethanolamine |
| REACH | Evaluation, authorization and restriction of chemicals |
| RFB | Redox flow battery |
| rpm | Rounds per minute |
| RVC | Reticulated vitreous carbon |
| SbD | Safe-by-design |
| SLCA | Social life cycle assessment |
| SSbD | Safe-and-sustainable-by-design |
| THF | Tetrahydrofuran |
| TLC | Thin layer chromatography |

## Supplementary Information

The online version contains supplementary material available at https://doi.org/10.1186/s13705-024-00503-x.

Additional file 1.

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**Author contributions**
CW conceptualized the study, contributed to the methodological design, critiqued data collection and wrote parts of the manuscript and revised the manuscript. JM carried out experiments, collected and analyzed data and wrote parts of the manuscript. JW carried out assessments, collected and analyzed data and wrote parts of the manuscript. GR, CL and SL carried out experiments, collected and analyzed data. JVH wrote parts of the manuscript, contributed to revising and graphical visualization. MR wrote parts of the manuscript and contributed to revising the manuscript and graphical visualization. AW carried out experiments, collected and analyzed data. AM carried out experiments, collected and analyzed data and wrote parts of the manuscript. CMB carried out assessments, collected and analyzed data and wrote parts of the manuscript. AF revised the manuscript and made suggestions for improvement. SS conceptualized the study, supervised, wrote parts of the manuscript, revised the manuscript and made suggestions for improvement. All authors read and approved the final manuscript.

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**Availability of data and materials**
No datasets were generated or analyzed during the current study.

## Declarations

**Ethics approval and consent to participate**
Not applicable.

**Consent for publication**
Not applicable.

**Competing interests**
SS is CEO of the company Ecolyte GmbH. GR is shareholder of the company Ecolyte GmbH.

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