THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING

Environmental life cycle impacts of lithium-sulfur and sodium-ion batteries

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Trust the process.

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Abstract

Mitigating climate change and other environmental problems will require a transition away from fossil fuels. Batteries can be part of such a transition as they enable a cleaner energy system by providing energy storage for intermittent energy sources such as wind and solar power, as well as a cleaner transport system by replacing internal combustion engine vehicles with electric vehicles. Globally, battery demand is projected to increase 6-20 times in the coming 15 years. If batteries are to become sustainability enablers globally, a large-scale diffusion of these technologies must be possible. To achieve such a diffusion, batteries should preferably contain few metals and materials connected to resource availability issues to reduce the risk of resource-related bottlenecks. Furthermore, battery technologies should be as environmentally benign as possible. The lithium-ion battery (LIB) is currently the dominating rechargeable battery technology, and while having high technical performance, it contains metals and materials connected to resource availability issues. However, there are several next-generation batteries (NGBs) that might be able to outperform LIBs from a life cycle environmental and resource perspective. The aim of this thesis is therefore to investigate the environmental and resource impacts of two NGBs, lithium-sulfur (Li-S) batteries and sodium-ion batteries (SIBs), with the overall goal of providing technology guidance.

To fulfil this aim, three studies have been included in the thesis. Two of them address the life cycle environmental and resource impacts of Li-S and SIBs, respectively. Furthermore, as lithium is a key metal for Li-S batteries, it is important to understand the environmental implications of extracting lithium from various sources with different ore grades. Therefore, in the third study, several lithium sources and their corresponding lithium production routes were assessed. Life cycle assessment (LCA) was applied in all studies, as comparing environmental and resource impacts of products in a holistic manner requires a life cycle perspective. Additionally, as Li-S batteries and SIBs are emerging technologies and not yet produced at large scale, prospective LCA was applied. Prospective aspects that were considered include production scale-up and accounting for potential future changes to the batteries as well as some supplies of materials and energy.

The results show that SIBs are on par with LIBs regarding climate change and perform better regarding mineral resource scarcity. Li-S batteries can perform similarly to LIBs for the same impact categories, but the results are uncertain as the future values of several Li-S design parameters are based on estimations. Furthermore, the environmental and resource performance of Li-S batteries is sensitive towards the lithium source and grade. Several lessons have been learned regarding Li-S battery and SIB impacts as well as the methodology applied. It is concluded that of the investigated NGBs, SIBs show the largest potential from an environmental and resource perspective. Furthermore, due to uncertainties inherent to prospective LCA, results should be seen as indicative rather than absolute. Additionally, involving a technology expert in prospective LCA projects can enhance the understanding of the future technical NGB systems.

Keywords: prospective LCA, next-generation batteries, lithium-sulfur batteries, sodium-ion batteries

List of appended papers

Paper I
Wickerts, S., Arvidsson, R., Nordelöf, A., Svanström, M. & Johansson, P. 2023. Prospective Life Cycle Assessment of Lithium-Sulfur Batteries for Stationary Energy Storage.
ACS Sustainable Chemistry and Engineering, 11:9555-9563.
DOI: 10.1021/acssuschemeng.3c00141

Wickerts, S., Arvidsson, R., Nordelöf, A., Svanström, M. & Johansson, P. 2024. Correction to "Prospective Life Cycle Assessment of Lithium-Sulfur Batteries for Stationary Energy Storage".
ACS Sustainable Chemistry and Engineering.
DOI: 10.1021/acssuschemeng.4c01782

Paper II
Chordia, M., Wickerts, S., Nordelöf, A. & Arvidsson, R. 2022. Life cycle environmental impacts of current and future battery-grade lithium supply from brine and spodumene.
Resources, Conservation & Recycling, 187, 106634.
DOI: 10.1016/j.resconrec.2022.106634

Paper III:
Wickerts, S., Arvidsson, R., Nordelöf, A., Svanström, M. & Johansson, P. 2024. Prospective life cycle assessment of sodium-ion batteries made from abundant elements.
Journal of Industrial Ecology, 28: 116-129.
DOI: 10.1111/jiec.13452

List of figures

List of tables

Table of contents

1. Introduction

It is evident that a large-scale societal transition is needed, as 2023 was the hottest year ever recorded and greenhouse gas emissions (GHGs), contributing to the warming of the Earth, continue to increase. Batteries are sustainability enablers as they open the door to a fossil-free energy system by providing energy storage for intermittent energy sources such as wind and solar power, as well as a cleaner transport system by replacing internal combustion engine vehicles with electric vehicles (Zhang et al., 2021). The world is therefore gearing up its battery production. 2,900-10,000 GWh of storage capacity is projected to be required in 2040 (Degen et al., 2023), depending on which socioeconomic pathway is considered, i.e., how well the environmental boundaries are respected (Riahi et al., 2017). This range can be compared to today's 500 GWh (Degen et al., 2023). That said, batteries themselves also need to be justifiable from a sustainability perspective (Edström et al., 2020).

If batteries are to become global sustainability enablers, battery technologies need to be diffused on a large scale. In turn, realizing such a large-scale battery diffusion requires batteries to possess several properties. Edström et al. (2020) point to safety and cost-efficiency as important aspects. Furthermore, batteries need to have technical performance that can meet application demands (Edström et al., 2020). Additionally, while facilitating a different energy system is the key sustainability characteristic of batteries, they should be as environmentally benign as possible. In addition, battery technologies should preferably be composed of materials accessible to such an extent that a large-scale diffusion of batteries is possible.

Aspects that influence the availability of a natural resource (in this case mineral resource) are manifold (André and Ljunggren, 2021). One of them is scarcity, meaning that the mineral resource has a natural rarity combined with a high societal demand. Scarcity, in turn, can lead to geopolitical issues, such as wars and trade conflicts (Dewulf et al., 2016). Mineral resources facing high supply risk (e.g. due to geopolitical issues) combined with high economic importance are classified as critical raw materials for certain regions (Schrijvers et al., 2020). Considering these challenges related to resource availability, batteries would benefit from being made from mineral resources that exhibit as few resource availability issues as possible.

The market of rechargeable batteries is dominated by lithium-ion batteries (LIBs), and more specifically the nickel-manganese-cobalt (NMC) based cathode chemistry and the graphite-based anode chemistry (IEA, 2023a). There are LIBs without cobalt and nickel as well, which instead contain elements such as iron and phosphorous ($LiFePO_4$-based cathodes) (Xu et al., 2020). Most LIBs possess several sought-after characteristics. They are safe, and their cost-efficiency is continuously improving (Armand et al., 2020). LIBs have relatively high specific energy density (Wh/kg) and power density (W/kg), as well as high volumetric energy density (Wh/L). However, LIBs also face several challenges. Current LIBs have specific energy densities limiting them from use in some applications (Demir-Cakan et al., 2017). NMC-based LIBs contain several materials that are linked to different sustainability concerns. One such example is the risk of scarcity, as the cumulative demand for lithium, nickel, and cobalt could exceed the currently known reserves in a not-too-distant future (Xu et al., 2020). The sources of these metals and their corresponding production are also concentrated to specific parts of the world (see Figure 1), entailing that the metals are more sensitive with regard to potentially becoming critical for other regions (Schrijvers et al., 2020). Lithium occurs in both brines and minerals, where the brine-based lithium can be connected to extensive freshwater withdrawal

(Harper et al., 2019). Cobalt is mostly mined in the Democratic Republic of the Congo (Watts, 2019), and is linked to issues such as child labor and unsafe working conditions (Sovacool, 2019). Nickel extraction, which is largely occurring in Indonesia (USGS, 2024), can be linked to water pollution (Firdaus and Levitt, 2022).

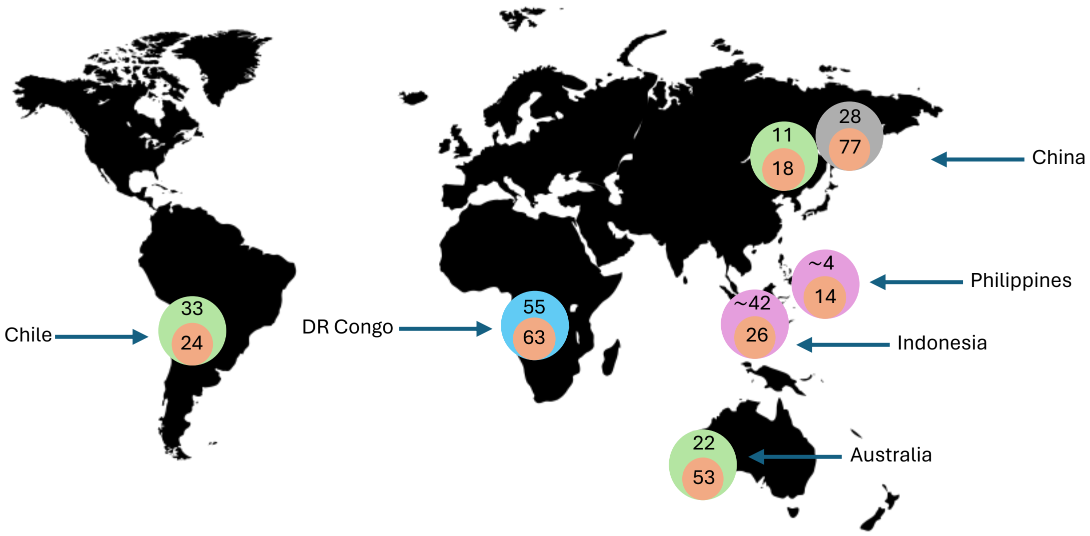

Figure 1. Certain countries' share of the global reserves for lithium (represented with green circles), cobalt (represented with a blue circle), nickel (represented with purple circles), and natural graphite (represented by a grey circle), as well as the country's share of the global production (represented by orange circles). All numbers represent percentages. Figure made from information obtained from SGU (2023) and USGS (2024).

Acknowledging that battery technologies are needed for the sustainability transition, combined with LIBs having several sustainability challenges, a search for new battery technologies is ongoing. Many upcoming battery technologies, or next-generation batteries (NGBs), exist, such as sodium-ion batteries (SIBs), magnesium batteries, lithium-sulfur (Li-S) batteries, lithium-air batteries, and solid-state batteries (Stephan et al., 2023). Of the many NGBs existing, Li-S batteries and SIBs represent two promising candidates, as they contain fewer mineral resources linked to resource availability issues than LIBs, and they have relatively high technical performance. Li-S batteries have particularly high specific energy density (Demir-Cakan et al., 2017). This could enable applications requiring high specific energy, and lead to lower environmental and resource impacts per unit of energy stored. However, lithium is a key metal for Li-S batteries and linked to resource availability issues (Xu et al., 2020). It is therefore relevant to understand how different lithium sources and grades affect the battery's environmental and resource impact. SIBs constitute another promising NGB technology. Most SIBs contain only abundant elements (Zhao et al., 2023), making their production potentially more robust from a resource availability point-of-view and could also lead to low environmental impacts as less energy might be required to extract the resources. That said, most of SIBs' technical performance does not level with NMC-based LIBs (Stephan et al., 2023). To understand whether Li-S batteries and SIBs can outperform LIBs from an environmental and resource point of view, assessments of impacts along the life cycles of these battery technologies are required.

2. Aim and thesis structure

The aim of this thesis is to evaluate if and how Li-S batteries and SIBs can be promising alternatives to LIBs in terms of life cycle environmental and resource performance, with the overall goal of providing technology guidance. Furthermore, as several current battery technologies and NGBs require lithium, a related aim is to understand how different lithium sources with different lithium grades influence the environmental and resource life cycle impacts of such batteries.

To answer these aims, four research questions are addressed, which in turn are answered by retrieving information from three studies that are presented in three separate papers (Paper I-III). Two research questions use information from an individual paper and two research questions utilize information from a combination of papers:

1. What are the environmental and resource life cycle impacts of Li-S batteries, what are the hotspots, and how can the impacts be reduced? (Paper I)
2. How do different lithium grades and sources affect the life cycle environmental and resource impact of lithium-containing battery materials, and in turn lithium-based battery technologies, in particular Li-S batteries? (Paper I and II)
3. What are the environmental and resource life cycle impacts of SIBs, what are the hotspots, and how can the impacts be reduced? (Paper III)
4. Which battery technology, Li-S, SIB, or LIB, shows the greatest promise from a life cycle environmental and resource point-of-view? (Paper I and III)

Chapter 1 has introduced the issues that this thesis attempts to address. Chapter 2 provides the aim and research questions formulated to fulfil the aim, as well as the thesis structure. In Chapter 3, a technical background to the NGBs assessed in this thesis is given, i.e., the basics of batteries are described followed by a brief explanation of Li-S batteries and SIBs. Chapter 4 provides a description of the methodological framework applied in the thesis. In Chapter 5, the papers are summarized and synthesized. Chapter 6 provides a concluding discussion of lessons learned regarding methodology as well as Li-S and SIB impacts.

3. Technical background

3.1 Battery basics

A battery consists of several electrochemical cells, which make use of chemical redox reactions to produce electricity on demand (Goodenough and Park, 2013). There are both “primary” cells, which are non-rechargeable and can only be discharged once, and “secondary” cells meaning that they are rechargeable, i.e., can be charged and discharged multiple times (Berg, 2015). An electrochemical cell is the same as a battery cell, and the latter term is used from now on. As rechargeable batteries are of focus in this thesis, only those are described further.

Rechargeable batteries can be categorized in many ways. Following Beard (2019), the categorization can be made based on the type of electrolyte. This is one common way of grouping. As can be seen in Figure 2, aqueous, non-aqueous, and other types of electrolytes such as solid-state electrolytes can be utilized. All liquid electrolyte battery cells consist of a positive electrode (cathode), a negative electrode (anode), and a liquid electrolyte separating the two electrodes (Berg, 2015). When the battery cell is discharged, ions move through the liquid electrolyte, from the anode to the cathode (inside of the battery) and electrons are lead through an electric circuit (outside of the battery). When the battery is charged, the ions and electrons move in the opposite direction.

Continuing the battery categorization, both aqueous and non-aqueous electrolytes can be divided further (Beard, 2019). Aqueous electrolytes are subdivided based on their pH: acid electrolytes into one group and alkaline and neutral electrolytes into another one. The lead-acid battery is one example of a battery technology utilizing acid electrolytes. Non-aqueous electrolytes can be divided into organic and inorganic ones. There are several battery technologies that make use of organic electrolytes, e.g., metal-ion batteries and metal-sulfur batteries (Beard, 2019, Stephan et al., 2023). Within these groups there are in turn different battery technologies, such as LIBs, Li-S batteries, and SIBs. Continuing, within the battery technology groups, there are cathode and anode chemistries, e.g. the NMC-based cathode chemistry and the graphite-based anode chemistry, utilized in many LIBs. While all groups depicted in Figure 2 can be categorized further, the battery technologies relevant for this thesis are highlighted. Furthermore, note that a certain battery technology can belong to multiple groups. For example, the Li-S battery can utilize a solid electrolyte instead of an organic liquid electrolyte, making it a Li-S solid state battery in such a case (Schmaltz et al., 2022). While not common, there are also LIBs that utilize aqueous electrolytes. These examples are however not shown in Figure 2.

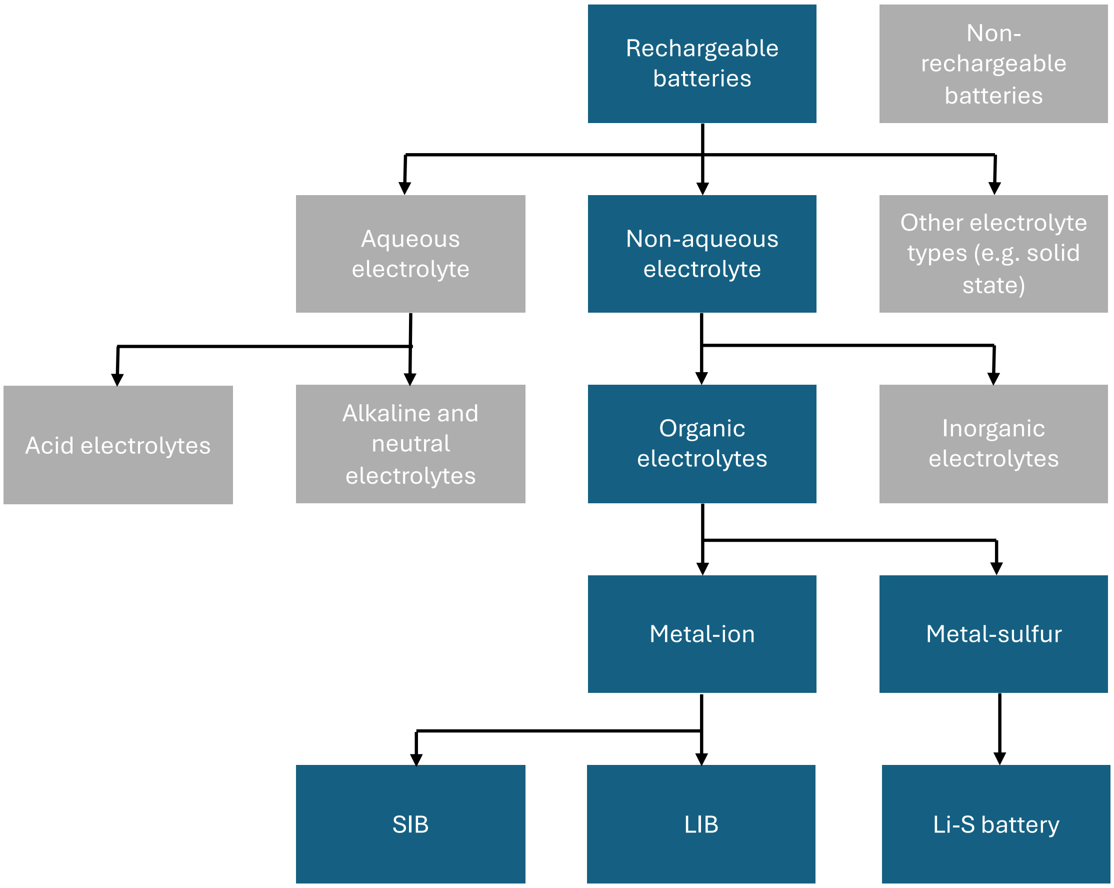

Figure 2. Battery categorization made based on common battery technologies. The blue color indicates battery groups relevant for this thesis. SIB=sodium-ion battery, LIB=lithium-ion battery, Li-S=lithium-sulfur.

3.2 Li-S batteries and SIBs

The Li-S battery, a metal-sulfur battery, generally consists of a lithium metal anode and a sulfur cathode with a liquid electrolyte in between, given the focus on liquid electrolyte batteries (Demir-Cakan et al., 2017). There are however many materials being tested for this battery technology. For example, composites consisting of elemental sulfur and carbonaceous additives are tested in terms of cathode materials. The exact composition of the Li-S chemistries assessed within this thesis can be found in Paper I. Li-S batteries have high specific energy densities, theoretically, with the expectation of reaching a specific energy density of 550 Wh/kg in 2035, compared to the expected specific energy density of LIBs ~ 360 Wh/kg the same year (Stephan et al., 2023). Still, LIBs will still be superior regarding volumetric energy density (Wh/L), implying that Li-S batteries might foremost be used in applications where weight is more important than size. Li-S batteries and LIBs differ regarding other key performance indicators (KPIs) as well, as can be seen in Table 1. Considering the characteristics of Li-S batteries, some applications are more likely than others. According to Volta foundation (2023), examples include aerospace applications, heavy duty trucks, and E-bikes. Li et al. (2018) also mention stationary energy storage in grids as a possible application for Li-S batteries.

The SIB, a metal-ion battery, often utilize a hard carbon anode and a sodium-containing cathode combined with a sodium-containing liquid electrolyte (Tapia-Ruiz et al., 2021). There are several cathode materials being tested, including layered oxide materials, polyanions and Prussian blue analogues (Zhao et al., 2023). The exact composition of the SIBs assessed within this thesis can be found in Paper III. Two of the main selling points of these batteries are their use of abundant materials, as well as being a drop-in technology to LIB cell production. Nonetheless, lower specific energy density and volumetric energy density are to be expected for SIBs, due to that sodium does not level with lithium in terms of electrochemical potential (Stephan et al., 2023). That said, roughly 200 Wh/kg and 400 Wh/L are expected in 2035 (Stephan et al., 2023). The remaining KPIs for SIBs can be found in Table 1. Grid applications and some consumer electronic applications, such as E-bikes, are seen as possible applications for SIBs (Volta foundation, 2023). Stephan et al. (2023) complement the already mentioned applications with EVs.

Table 1. Comparison of some KPIs for Li-S batteries, SIBs, and LIBs. Note that the ranges shown in certain columns are due to, e.g., that multiple battery chemistries (having different KPIs) are included for the battery technology.

Battery technology	Specific energy density, current/ future (Wh/kg)	Volumetric energy density, current/future (Wh/L)	Future production cost (€/kWh)	Safety	Cycle life, current/future
Li-S	300*/550-700*, **	300-450*/700*	50*	Higher than LIBs but lower than SIBs**	>200/>400****
SIB	140-190*, ***/>200*, ***	230-380*, ***/>400*	<40*	Higher than both Li-S and LIBs**	2000/6000****
LIB	140-300*, ***/320-360*	240-750/800-960*, ***	45-90*	Lower than both Li-S and SIBs**	1000-3000/2000-10000****

*Stephan et al. (2023), **Robinson et al. (2021), ***Tapia-Ruiz et al. (2021), ****BEPA and Batteries Europe (2024).

4. *Methodological framework*

To obtain a broad understanding of a battery's or a battery material's life cycle impacts on the environment, it is beneficial to apply a method that accounts for the life cycle perspective, addresses a range of environmental concerns, and has a product focus. As can be seen in, e.g., Finnveden and Moberg (2005) or Bjørn et al. (2018a), life cycle assessment (LCA) is the method that showcases these characteristics.

4.1 The LCA framework

The environmental LCA methodology aims to protect areas categorized as resource use, human health, and ecological consequences. These areas are often called safeguard objects or areas of protection (AoP) (Baumann and Tillman, 2004). LCA quantifies potential environmental impacts caused by a product system, that might damage the AoP at the so-called endpoint level. Examples of such environmental issues include climate change, eutrophication, and mineral resource use, which can be used as indicators at the midpoint level. LCA can consider all life cycle stages from raw material extraction to the end-of-life (EoL) treatment, or specific parts of the life cycle (Curran, 2017).

Every LCA has a functional unit (FU), which describes the function that the assessment object (i.e., the product) provides, in quantitative terms (Bjørn et al., 2018b). The FU is connected to a reference flow, which represents the amount of product needed to achieve the FU. LCA can be used for descriptive purposes, or for serving as a basis for decision-making (Baumann and Tillman, 2004). A life cycle perspective is crucial in some contexts as it enables the identification of burden-shifting between life cycle stages and/or between environmental impacts (Bjørn et al., 2018a). When such burden-shifts have been identified, they can also be addressed.

The international organization for standardization (ISO) has developed a standardized LCA procedure (ISO, 2006). In this procedure, the goal and scope definition step is conducted first. The goal of the study is decided, followed by a description of the scope characteristics. Aspects addressed in the scope definition are, e.g., the FU and system boundaries (Curran, 2017). Other aspects of the scope definition include how to handle multifunctionality (i.e., how to handle processes that produce more than one product and where all products cannot be linked to the study's reference flow) (Bjørn et al., 2018c) and what data to use, as well as the selection of impact categories. In the next step, called the inventory analysis, a model of the system under study is constructed and data is collected, followed by calculations to obtain mass and energy flows (Arvidsson and Ciroth, 2021). The outcome of the inventory analysis is a table with elementary flows. These flows are then, via cause-effect models, converted into potential environmental impacts in the impact assessment step (Hauschild and Huijbregts, 2015). In parallel, an interpretation step is performed, where the other steps in the procedure are evaluated in terms of, e.g., uncertainties and completeness (Curran, 2023). As can be seen in Figure 3, the LCA procedure is iterative.

There are different system boundaries that are of relevance in an LCA study (Baumann and Tillman, 2004). Studies can stop after the raw material extraction and production, making them cradle-to-gate studies. Other studies might encompass the whole life cycle, i.e., a cradle-to-grave study, meaning that raw material extraction, production, use, and the end of life are included. In addition, the geographical boundaries of the studied system describe where in the world different parts of the studied system occur. The temporal boundary describes when the included processes occur in time, e.g., at the current time or in the future. The latter is often considered in assessments of emerging technologies, which are described in Chapter 4.3. Furthermore, the temporal boundary also indicates the study's time validity (Bjørn et al., 2018b).

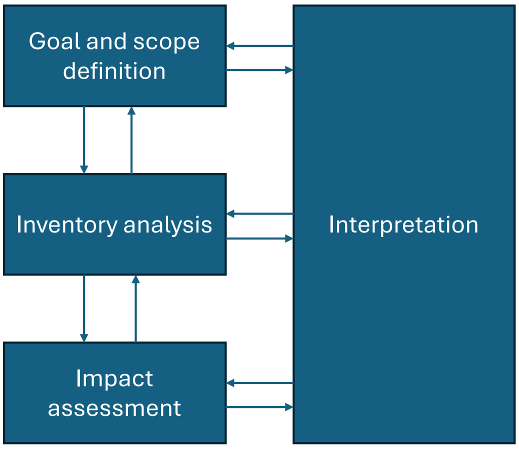

Figure 3. A depiction of the LCA procedure (ISO, 2006).

When doing the life cycle impact assessment (LCIA), the environmental flows linked to the studied product system are converted into potential environmental impacts (per FU) (Baumann and Tillman, 2004). This is done by using impact assessment methods, which all utilize cause-effect models to convert a certain flow to an impact. The impacts can be estimated using either midpoint indicators, i.e., going through the cause-effect chain to some extent, or using endpoint indicators, going through the whole cause-effect chain, ending up close to or at the AoP (Rosenbaum et al., 2018). Compared to midpoint indicators, endpoint indicators focus directly on the AoP. Therefore, the endpoint indicators can give a better understanding of the characterized flows' impact on the AoP (Hauschild and Huijbregts, 2015). However, endpoint indicators include additional mechanisms for quantifying the link between the midpoint and endpoint level (e.g., the damage on human health from climate change), making endpoint indicators more uncertain.

Including an extensive list of impact categories in an LCA study might lead to confusion of which impacts should be regarded as more relevant, especially if there is no motivation to why the categories are included (Porzio and Scown, 2021). This is especially true for prospective LCAs, considering the higher uncertainties that are intrinsic to future-oriented studies. On the other hand, some argue that a substantial number of impact categories need to be addressed for the study to be categorized as an LCA study (Thonemann et al., 2020). Additionally, finding potential trade-offs between impacts categories is difficult when including too few impact categories.

4.2 Attributional and consequential LCA

There are two types of LCA, called attributional and consequential, which correspond to different goals (Ekvall, 2020). While there are different definitions of the two types, similar characteristics can be seen in different definitions (Ekvall et al., 2016). The purpose of attributional LCA can be described as quantifying existing environmental flows, and thus impacts, that can be linked to the product system. This implies that average data of the processes is used. Multifunctional processes are handled by partitioning the environmental burden between the products. Consequential LCA instead aims to quantify the environmental flows of the system that might change due to a certain decision (Ekvall, 2020). In terms of data, it should reflect the changed flows and therefore marginal data should be used. Multifunctional processes are dealt with by substitution. Both attributional and consequential studies can be retrospective and prospective (Arvidsson et al., 2018).

If open-loop recycling is included in an LCA study, then there is an issue of how to allocate the burden of recycling between two lifecycles (Ekvall et al., 2020). This is because recycled material coming from the first life cycle will be used in another product, i.e., in a second life cycle. There are various allocation approaches, which fit with either attributional LCA or consequential LCA, including the cutoff-approach and the circular footprint formula.

4.3 Prospective LCA

Emerging technologies are fast-growing and uncertain (Rotolo et al., 2015). There is a great opportunity in guiding development of emerging technologies, because improvements can then be made to the technology without major impediments (Collingridge, 1980). However, large uncertainties inherently exist for emerging technologies. On the contrary, when the technology is well understood, the opportunity to make improvements is limited. This paradox of knowledge versus control can be referred to as the Collingridge dilemma.

The high uncertainty of emerging technologies warrants specific consideration in LCA. This has been acknowledged by the LCA community, and a subcategory of LCA has become popular, namely prospective LCA (Arvidsson et al., 2023). Prospective LCA can be defined as: "An LCA is prospective when the (emerging) technology studied is in an early phase of development (e.g., small-scale production), but the technology is modeled at a future, more-developed phase (e.g., large-scale production)" (Arvidsson et al., 2018). However, recent discussions between researchers working with prospective LCA resulted in a new definition: "LCA that models the product system at a future point in time relative to the time at which the study is conducted" (Arvidsson et al., 2023). This latter definition does not take technology maturity into account, however the authors categorize "ex-ante LCA" as a type of prospective LCA that does include this aspect. Following the definition by Arvidsson et al. (2023), prospective LCA involves all studies that apply a future time horizon, whereas ex-ante LCA is a prospective LCA that also includes a scale up of technology maturity. The more general term of prospective LCA is used throughout this thesis.

When assessing an emerging technology in LCA, it can be relevant to evaluate its current maturity. Technology readiness levels (TRLs) as well as manufacturing readiness levels (MRLs) can be used for this purpose, where 10 is the highest level for technology readiness and 9 is the highest for manufacturing readiness (van der Hulst et al., 2020). For both scales, 1 is the lowest level. The TRL scale refers to the maturity of technical design and functionality whereas the MRL scale instead refers to the maturity of related production processes. For emerging technologies, there is a temporal difference between the current TRL/MRL (early phase of development) and the future TRL/MRL (more developed phase). The time corresponding to the future TRL/MRL can be defined as the temporal boundary in a prospective LCA. Since the emerging technology is not yet produced at large scale or industrial scale, there are three distinct aspects that could be considered in a prospective LCA study (Cucurachi et al., 2018). First, the technology's design and performance at large scale are to be decided, considering the TRL of interest. Second, the production processes are scaled up, so they correspond to the MRL of interest. To determine aspects such as technology and manufacturing design for the TRL/MRL of interest, technology experts can be involved in LCA studies (Tsoy et al., 2020). Third, as the higher TRLs and MRLs will occur in the future, possible changes to the surrounding infrastructure are to be accounted for. As the future is inherently uncertain, multiple future developments in the form of different scenarios are useful.

Scenarios, in the context of prospective studies, can be interpreted as representations of different futures, which are, e.g., possible, probable and/or preferable (Börjesson et al., 2006). In the case of prospective LCAs, Arvidsson et al. (2018) recommend using either predictive scenarios, where the status quo can be included, or scenarios that reflect possible futures by using scenario ranges. Also Cucurachi et al. (2018) mention that different types of scenarios can be included when assessing emerging technologies. Scenarios can be applied to both the foreground and background systems. The foreground system consists of processes central to the product assessed, which a certain actor can influence (Arvidsson and Ciroth, 2021). The background system then contains the remaining parts of the product system, and it is important to match the foreground and background systems temporally (Arvidsson et al., 2018). There are LCA software that enable easier implementation of prospective background scenarios, such as Futura (Joyce and Björklund, 2021). There are also prospective background databases, such as Premise (Sacchi et al., 2022).

5. *Summary and synthesis of papers*

Three studies have been included in this thesis. Papers I and III evaluated the life cycle environmental and resource impacts of NGBs, which are not produced at large scale yet. Paper I evaluated the whole life cycle, including a battery application, while Paper III focused on the battery cell production. Paper II instead focused on how lithium sources and grades influence the environmental and resource impacts of upstream lithium supply. This paper therefore reviewed the life cycle environmental and resource impact of different lithium sources and their corresponding lithium production routes, both in already published studies but also based on own primary data collection and modelling. The methodological choices for all papers are stated in the coming subchapters, and at the end of the chapter, a summary of all choices is provided (see Table 6).

5.1 Objects of study

The assessment objects in Papers I and III were considered to be emerging technologies. This consideration was made based on the type of information found in the literature. When searching the NGB literature, several battery roadmaps containing information on Li-S batteries and SIBs could be found. These roadmaps highlighted strengths and challenges for each battery technology to become commercially available (Robinson et al., 2021, Tapia-Ruiz et al., 2021, Stephan et al., 2023, BEPA and Batteries Europe, 2024). This confirmed that they are still considered as emerging technologies. The Li-S battery technology assessed in Paper I had an estimated MRL of 4-5. Although not defined in Paper I, reaching MRL 10 seems unlikely to happen before 2030, considering the current state and speed of Li-S battery development. The SIB technology assessed in Paper III was estimated to have TRLs/MRLs of 7-8, and the temporal boundary (at which TRL 9 and MRL 10 seem likely to be achieved) was estimated to be around 2025-2030. Paper II considered a lithium containing battery material, in particular lithium hydroxide monohydrate (LHM). To account for geological circumstances of different lithium sources with different lithium grades and differences in LHM production processes, eight LHM production routes were assessed. As Paper II considered mature technologies and production processes, the TRL/MRL scales were not applied.

5.2 System boundaries

In terms of technical boundaries, Paper I considered a cradle-to-gate scope as well as a cradle-to-grave scope. These boundaries were selected to facilitate comparisons on both levels. The battery application modelled in that study was an installation for large-scale energy storage of wind power. Both Paper II and Paper III considered cradle-to-gate boundaries, stopping at the factory gate of LHM and SIB cells, respectively. One argument for selecting the cradle-to-gate boundary in Paper III was that the use and EoL phases lacked data. For paper I, on the other hand, pilot scale data for battery operation characteristics (Ainsworth, 2016), as well as a study describing a hydrometallurgical recycling process specific to Li-S batteries were found (Schwich et al., 2020). Therefore, it was decided to evaluate both scopes, as stated above. For Paper II, the more limited system boundary was selected due to the aim of evaluating the production of LHM.

Regarding temporal boundary, Papers I and III are prospective studies with a future time horizon. For Paper II, both current and future production routes of the battery material were included, where the future production represents upcoming mines that will be operational in 5-10 years. However, note that in both cases, mature technologies and production processes were assessed. Following the prospective LCA definition suggested by Arvidsson et al. (2023), the assessment of future production routes in Paper II would be classified as prospective.

The geographical boundaries differ in the studies. Papers I and III attempted to evaluate the life cycle impacts of the respective NGB generally, which is why global datasets were applied in both papers. Paper II on the other hand, assessed whether the lithium source and grade affect the environmental and resource impacts of the LHM production and in extension of Li-S batteries. Therefore, Paper II reviewed several LHM production routes, having different lithium sources located in Chile, Argentina, Australia, Canada, and Finland. In Chile and Argentina, the lithium occurs in brines, while the metal occurs in the mineral spodumene in the other countries.

5.3 Upscaling

In Papers I and III, upscaling of processes to MRL 10 was conducted within the respective product system. In both papers, a gigascale factory model by Chordia et al. (2021) was applied to upscale the battery cell production. The model was developed for NMC 811-based LIB cylindrical cells and is based on data from environmental permit applications for a Swedish cell producer. The "gigascale" refers to the factory's annual production capacity, which is equal to 16 GWh (Chordia et al., 2021). The model was applied to the respective NGB study by identifying which processes in the gigascale factory model that could be applied to the cell production of the respective battery technology. An illustration of how the original model was modified to represent Li-S battery and SIB cell production is shown in Figure 4. All inputs and outputs were modified to align with the battery technology under study. As Li-S batteries contain lithium metal anodes, the gigascale factory process for anode production could not be applied fully. Instead, a separate production process based on extrusion of liquid metallic lithium was modelled (Deng et al., 2017, Heimes et al., 2018). However, data regarding anode cutting/slitting and dry room facilities were still obtained from the gigascale factory model. Furthermore, the gigascale factory model is based on production of cylindrical cells, but pouch cells were modelled in both Papers I and III. For pouch cells, stacking was applied instead of winding and packaging was applied instead of inserting. However, data for winding and inserting were still applied as proxies for the pouch cells.

For production of upstream battery chemicals, the approach by Piccinno et al. (2016) was applied. This framework is applicable when laboratory data is available but information regarding the process scale up is lacking. The framework, assuming batch production, builds on the following sequence: a reaction step followed by purification and isolation steps. Material inputs need to be known from the laboratory description or elsewhere, as such inputs are scaled up linearly. Solvents, while being material inputs, are scaled up using a 20% reduction, based on mass. Energy inputs for large-scale production can be obtained by using process equations provided in the framework. The process equations are not data intensive (see e.g., Eq.1). For example, the energy use for an up-scaled stirring process (using a reactor of 1000 L) can be obtained if the density of the reaction mixture (ρ_{mix}) as well as the reaction time (*t*) are known.

$$E_{stir(1000L)} = 0.018 \times \rho_{mix} \times t \qquad \text{Eq.1}$$

To obtain complete unit processes for the battery chemicals, a step-wise procedure was developed, which was refined and later published in Paper III (see Figure 2 in Paper III). Paper I included hydrometallurgical recycling in the two out of six cradle-to-grave scenarios (the scenarios are explained in Chapter 5.4). For the hydrometallurgical process, the framework by Piccinno et al. (2016) could be applied as a few materials, e.g., lithium carbonate, were modelled to be re-produced in a batch liquid reaction. For one battery material in Paper III, an upscaled production process could be obtained via a collaboration with a manufacturer.

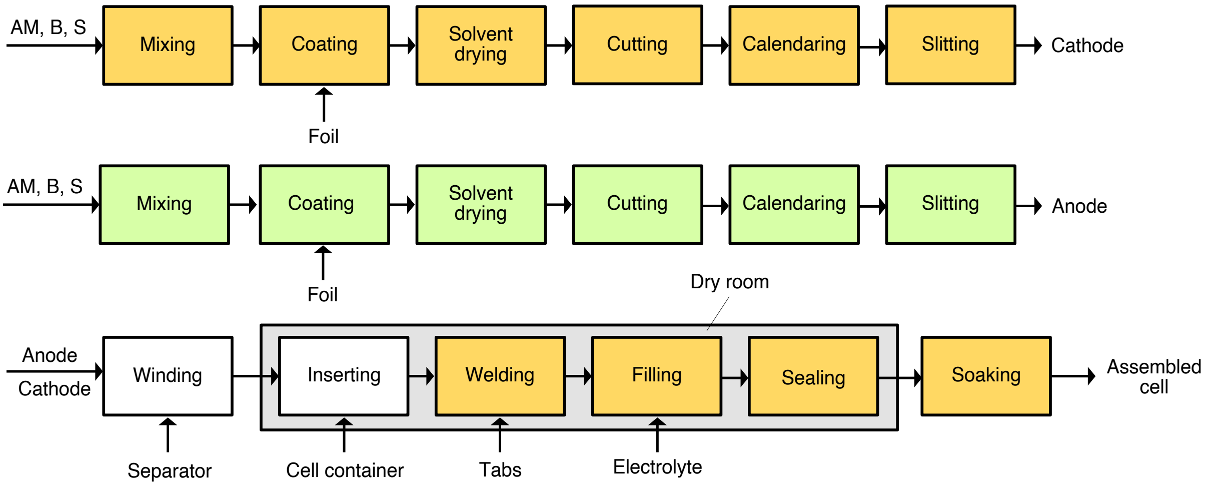

Figure 4. Processes for cathode and anode production as well as battery assembly included in the gigascale factory model (Chordia et al., 2021). Orange boxes represent processes included both in the Li-S and SIB production, whereas green boxes are only applicable to the SIB production. White boxes are not included for any of the battery technologies, as pouch cells were modelled in both papers. AM=active material, B=binder, S=solvent.

5.4 Scenario analysis

A scenario analysis was included in Papers I and III. Scenarios can be divided into foreground and background scenarios. For the foreground and background systems, “what-if” scenarios, representing predictive futures were included (Börjesson et al., 2006). The scenarios were structured in different ways in the papers, however they were either targeting characteristics of the battery technology, i.e., foreground scenarios, and/or addressing other parts of the product system, i.e., background scenarios.

In Paper I, scenario parameters were created to test both different bills of materials and technical performance, as both are uncertain (see Table 1 regarding technical performance). A change in cell materials was included, which focused on the electrolyte and the cathode. The technical performance of a battery cell on a cradle-to-gate level is linked to how much energy can be stored per unit mass. Therefore, the cradle-to-gate technical performance was varied by altering the specific energy density. Furthermore, as a higher technical performance implies a higher share of active material (Robinson et al., 2021), the cell composition for the cells with higher performance was adjusted. In addition, the electricity supply mix was varied to evaluate possible changes in the background system. Five scenarios, which included the above-mentioned scenario parameters, were created for the cradle-to-gate analysis: a base (B) scenario, a material selection (M) scenario, an energy system (E) scenario, a technical performance (T) scenario, and a combined (C) scenario. Additional performance parameters are of relevance for a cradle-to-gate scope (Peters et al., 2017, Baumann et al., 2017). Such performance parameters were varied in the cradle-to-grave T scenario, including the round-trip efficiency and the cycle life. For the cradle-to-grave analysis, a recycling scenario (R) was added. A summary of the scenarios is provided in Table 2. Some scenarios (B, M, T, and R) were modelled with a medium emission intense electricity supply mix (in the context of coal power having a high emission intensity) and others (E and C) with a low emission intense electricity supply mix. A global decarbonization is occurring (IEA, 2023b), and therefore, encompassing a high emission intense electricity supply mix, similar to coal power, was considered too conservative in a future-oriented study. These electricity supply mixes were modelled using proxies, where the current EU mix (ca. 400 g CO_2 eq/kWh) was used for the medium emission level and wind power (ca. 20 g CO_2 eq/kWh) for the low emission level. The scenario parameters were combined in different ways to understand the impact of one individual parameter.

Paper III included several scenario parameters, see Table 3. Two bills of materials for the SIB cells were assessed, and while not described as scenarios in the paper, the exploration of different SIB cells can be seen as a foreground scenario. The first cell contained materials from fossil-derived raw materials and a fluorine-containing electrolyte (Cell 1), and the other one contained materials from biobased raw materials as well as a fluorine-free electrolyte (Cell 2). The impact of supplying different kinds of electricity was, also explored in Paper III, with the same logic for the scenario range.

The SIB production system contained several by-products, where the future demand of these by-products is not clear. Therefore, a scenario range regarding allocation approaches was included in Paper III, see more in Chapter 5.7 addressing allocation for all papers. All scenario parameters included in Paper III were combined in different ways, categorized as S1, S2 and so on, to understand the impact of one individual parameter. Note that this scenario categorization was added in this thesis, and not used in Paper III.

Table 2. Scenarios in Paper I.

System boundary	Base scenario	Material selection scenario	Energy system scenario	Technical performance scenario	Recycling scenario*	Combined scenario
Cradle-to-gate	Base battery cell Base composition Base performance Current EU mix	Alternative battery cell Base composition Base performance Current EU mix	Base battery cell Base composition Base performance Wind power	Base battery cell Alternative composition High performance Current EU mix	Base battery cell Base composition Base performance Current EU mix	Alternative battery cell Alternative composition High performance Wind power
Gate-to-grave	Base battery operation Landfilling Current EU mix	Base battery operation Landfilling Current EU mix	Base battery operation Landfilling Wind power	Alternative battery operation Landfilling Current EU mix	Base battery operation Hydrometallurgical recycling Current EU mix	Alternative battery operation Hydrometallurgical recycling Wind power

*This scenario is only included in the cradle-to-grave analysis

Table 3. Scenarios in Paper III. MPBAB=main product bears all burden.

S1	S2	S3	S4	S5	S6	S7	S8
Cell 1 Current EU-mix Mass-based allocation	Cell 1 Wind power Mass-based allocation	Cell 1 Current EU mix MPBAB	Cell 1 Wind power MPBAB	Cell 2 Current EU mix Mass-based allocation	Cell 2 Wind power Mass-based allocation	Cell 2 Current EU mix MPBAB	Cell 2 Wind power MPBAB

5.5 The LIB benchmark

LIBs are currently the dominant rechargeable battery technology on the market, as mentioned in Chapter 1. When comparing LCIA results of emerging and incumbent technologies, it is preferable if LCA studies of the incumbent ones are based on primary data to avoid uncertainties related to re-production of LCA data. This should in theory be possible considering that the incumbents exist as mature technologies at the point in time when they are assessed. For the cradle-to-gate scope, there are three LIB studies that are based on primary data, whereas the LIB study applied for the cradle-to-grave comparison is based on secondary data.

For the cradle-to-gate comparison, the three LIB studies modelled gigascale production of NMC-based LIB cells, which were based on data from Chinese and Swedish manufacturers, respectively (Dai et al., 2019, Sun et al., 2020, Chordia et al., 2021). To understand potential disparities in the LCIA results of the NGBs and the LIB benchmark (presented in Chapter 5.13) due to modelling differences, the data sources as well as the electricity supply mix and background database for the LIB studies are provided (see Table 4). The studies by Dai et al. (2019), Sun et al. (2020), and Chordia et al. (2021) represent current large-scale LIB production. The comparison between the current large-scale LIB production and the future large-scale production of Li-S batteries and SIBs is thus done on equal TRL/MRL bases (see Figure 5).

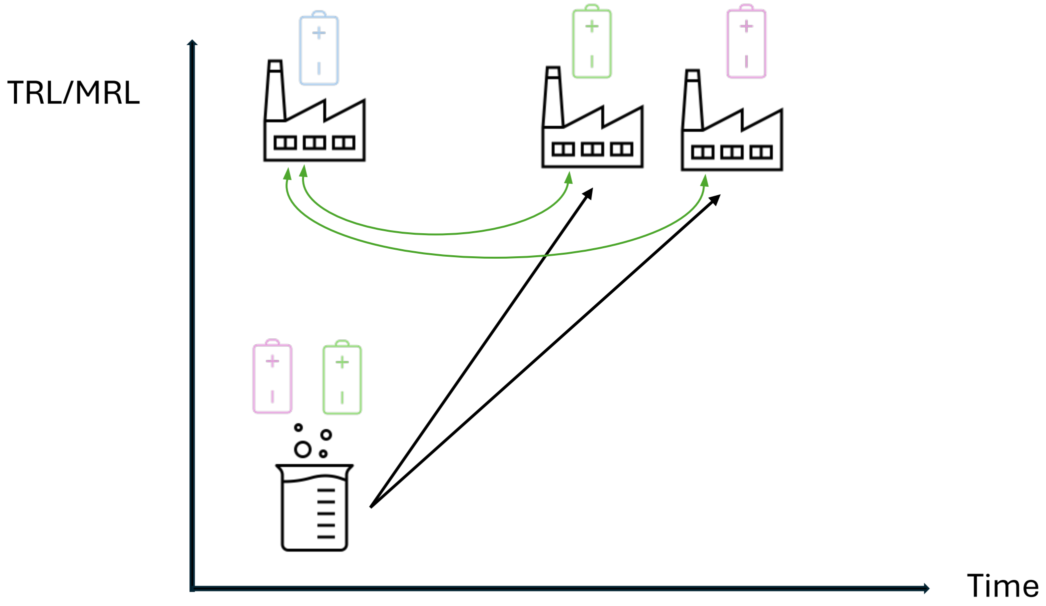

Figure 5. Depiction of how the Li-S battery and SIB upscaling relate to time as well as the time difference between the upscaled NGBs and the LIB benchmark. Purple batteries represent Li-S batteries, green batteries represent SIBs, and the blue battery represents LIBs. Black arrows represent upscaling whereas green arrows indicate the battery technology comparison in the respective paper.

Table 4. Electricity supply mix, background database and cell production data source for the LIB benchmarking studies. GREET=The Greenhouse gases, Regulated Emissions, and Energy use in Technologies Model, CALCD= Chinese Automotive Life Cycle Database.

Study	Electricity supply mix	Background database	Data source for cell production
Dai et al. (2019)	United States	GREET	Chinese manufacturer
Sun et al. (2020)	China	Ecoinvent 3.0 and CALCD	Several Chinese manufacturers
Chordia et al. (2021)	South Korea/Sweden	Ecoinvent 3.7.1	Environmental permit applications for a Swedish cell producer

5.6 Functional units

For batteries, the function is to store energy with the purpose of enabling energy delivery at a certain point in time. In cradle-to-gate studies, the most common FU is related to the theoretical storage capacity of the battery. Therefore, 1 kWh of theoretical storage capacity is often used as FU in case studies (Peters et al., 2021, Chordia et al., 2021, Dai et al., 2019). Several recent articles claim that FUs based on storage capacity can be misleading, however they also state that this type of FU can facilitate comparison between studies (Porzio and Scown, 2021, Peters, 2023). For the cradle-to-gate scopes in Papers I and III, a FU of 1 kWh of theoretical storage capacity was used. Regarding cradle-to-grave studies involving batteries, the FU depends on the battery application assessed. However, regardless of application, focus of the FU is on how much energy a battery can deliver in a certain amount of time, or how far an electric vehicle can drive (Peters, 2023). For the cradle-to-grave analysis in Paper I, a FU of 1 MWh of delivered electricity to the grid over the whole lifetime of the application was used, which has also been applied in, e.g., Peters and Weil (2017) and da Silva Lima et al. (2021). For Paper II, which applied a cradle-to-gate boundary, the FU was set to 1 ton of LHM.

5.7 Allocation

All studies included in the thesis are of the attributional type, as the aim is to determine what burdens can be attributed to these NGBs under certain scenarios, and not to answer questions such as "what would be the environmental consequences if A changed to B?". If the latter type of statement was considered, then consequential LCA could have been a better choice. The selection of attributional LCA implied that average data were used, and multifunctionality was handled by allocation. For the prospective LCAs, i.e., Papers I and III, mass-based allocation was used for multi-output processes. In Paper III, the mass-based allocation approach was complemented by a more conservative approach; the main product bears all burden (MPBAB). Applying the MPBAB approach, the environmental impact is attributed to a selected product of the system, whereas all other products are considered free of burden (Hermansson et al., 2020). This allocation approach was applied in the papers by designating all products linked to the studied SIB as main products although these products might currently be considered by-products. Economic allocation was not used in either Paper I or III, due to the difficulty to estimate future prices (Sander-Titgemeyer et al., 2023). In Paper II, the MPBAB approach was also applied. For the cradle-to-grave scope in Paper I, the cutoff approach was used for materials modelled to be sent to open-loop recycling.

5.8 Data sources

In all papers, the Ecoinvent database (version 3.7.1 for Paper I and version 3.8 for Paper II and III) was applied for modelling the respective background systems. In terms of the foreground system in Paper I, some processes were based on data obtained from LCA studies but modified to fit the system under study. Other processes had to be modelled from scratch. That procedure is described in a step-wise manner in Paper III. The procedure was helpful when developing unit processes that include production upscaling. In terms of data collection, the upscale modelling required synthesis descriptions with data on, e.g., yields and inputs (Piccinno et al., 2016). Such synthesis descriptions were found in, e.g., patents. Technical performance data was obtained from battery roadmaps, manufacturing data as well as expert judgements from a technology expert (Robinson et al., 2021, Ainsworth, 2016).

The foreground system for the current production routes in Paper II relied on data from the Ecoinvent database as well as an LCA study, i.e., the study by Kelly et al. (2021). The Ecoinvent production routes are based on several studies, e.g., Stamp et al. (2012). For the future production routes in the same paper, technical reports, and environmental impact assessment (EIA) reports from several upcoming lithium mines were used as input data. The existing product systems in Ecoinvent, which represented the current production routes for both brine- and spodumene-based LHM production were used as comparison objects to the production routes based on technical and EIA reports. Paper III relied on LCA studies, modified to fit the product system, as well as own modelling. Technical performance data was obtained from expert judgements. However, a collaboration with a manufacturer in the SIB life cycle enabled primary data for one of the foreground processes. This manufacturer could also bring insights about SIB cells in general, which was helpful for other aspects of the modelling.

5.9 Impact categories selected

For batteries, there are a few impact categories that can be considered more relevant to include in a study. Table 5 lists the impact categories included in each paper. As can be seen in the table, only midpoint indicators were applied in the papers. This is because midpoint indicators are easier to understand and interpret. In addition, as pointed out earlier, endpoint indicators result in higher uncertainty (Thonemann et al., 2020), which is why they were not considered.

In all papers, climate change and mineral resource use impact categories were included. Enabling an energy transition to renewables is the main advantage of batteries, however it is still important to assess the batteries' climate impact. Resource availability is a potential bottleneck for the widespread diffusion of batteries. This is why mineral resource use was included in all papers. Two different indicators of mineral resource use were addressed: the surplus ore potential (SOP) indicator and the crustal scarcity indicator (CSI). The SOP indicator characterizes resources based on the additional ore extracted to yield the same amount of resource, given declining ore grades (Huijbregts et al., 2016). This indicator is part of the ReCiPe package, which is commonly applied in LCA studies. However, the SOP includes time sensitive parameters, such as price-allocation for by-products, making it not optimal for use in future-oriented studies (Arvidsson et al., 2020). Therefore, the SOP indicator was complemented by the CSI. The CSI is an inclusive impact indicator in terms of resources characterized (Arvidsson et al., 2020). The indicator characterizes resources based on their crustal concentrations, making the indicator less time-sensitive and thereby applicable for future-oriented studies. These impact categories are seen as important in battery LCAs: when addressing traction batteries, Zackrisson (2021) ranks climate change impacts and mineral resource depletion as the two most important impact categories. These impact categories are also commonly used in battery LCAs: Picatoste et al. (2022) show that climate change is the most common impact category to assess in battery LCAs. Mineral resource use is also included in several battery LCAs (Picatoste et al., 2022).

Water use was included in Papers I and II. This impact indicator is pointed out as potentially important to address in battery LCAs in general (Porzio and Scown, 2021). In Paper II, two impact assessment methods for water use were included, where one of them accounts for the water consumption and the other one considers the consumption as well as the water availability in a certain region (Huijbregts et al., 2016, Boulay et al., 2018). The focus on water in Paper II is further justified by the arid settings of brine-based lithium extraction, e.g. in the Atacama Desert in Chile (Liu et al., 2019). As freshwater extraction is a focus point in Paper II, and water pollution can be linked to mining activities (Liu et al., 2019), freshwater toxicity was also included in Paper II.

In Paper III, fossil resource scarcity was included as one of the main impact categories. The reason for this is that two different SIB cells were assessed, where one of them contained fossil-derived battery materials whereas the other one contained battery materials derived from biobased raw materials.

There are slight differences in the papers considering the number of impact categories highlighted in the main manuscripts, the number of impact categories in the supporting information, and which actual impact assessment methods were applied (see Table 5). However, the overall approach of what to present in the LCIA step was the same in all papers: a focus on a selected number of impact categories, especially relevant to the system under study. The differences are essentially results of the review processes for each of the papers.

Table 5. Summary of modelling choices in the LCIA step. SI=supporting information, IPCC=international panel on climate change, CSI=crustal scarcity indicator, SOP=surplus ore potential, AWARE=Available water remaining, R= ReCiPe (hierarchist perspective).

Paper	Impact categories and impact assessment methods in the main paper	Impact categories and impact assessment methods in the SI
I	Climate change (IPCC 2013) Mineral resource use – CSI (CSI) Mineral resource use – SOP (R) Water consumption (R)	The impact categories highlighted in the main paper as well as: Acidification (R) Eutrophication (R) Ozone formation (R) Fine particulate matter (R) Stratospheric ozone depletion (R) Fossil resource scarcity (R)
II	Climate change (R) Mineral resource use – CSI (CSI) Mineral resource use – SOP (R) Water use (R) Water use (AWARE) Freshwater ecotoxicity (USEtox)	The impact categories highlighted in the main paper as well as: Freshwater ecotoxicity (R) Fine particulate matter (R) Fossil resource scarcity (R) Freshwater eutrophication (R) Ionizing radiation (R) Land use (R) Marine ecotoxicity (R) Ozone formation (R) Stratospheric ozone depletion (R) Terrestrial acidification (R) Human toxicity (R) Marine eutrophication (R)
III	Climate change (R) Mineral resource use – CSI (CSI) Mineral resource use – SOP (R) Fossil resource scarcity (R)	The impact categories highlighted in the main paper as well as: Water use (R) Freshwater ecotoxicity (R) Fine particulate matter (R) Freshwater eutrophication (R) Ionizing radiation (R) Land use (R) Marine ecotoxicity (R) Ozone formation (R) Stratospheric ozone depletion (R) Terrestrial acidification (R) Human toxicity (R) Marine eutrophication (R)

Table 6. Summary of methodological choices made in the studies included in the thesis. TRL=technology readiness level, MRL=manufacturing readiness level, FS=foreground scenario, BS=background scenario, LHM=lithium hydroxide monohydrate, MPBAB=main product bears all burden.

Paper	TRL/MRL of study object	Life cycle stages included	Functional unit	Temporal boundary	Geographical boundary	Allocation	Prospective modelling
Paper I	Current MRL: 4-5 Future MRL: 10	Cradle-to-gate/ cradle-to-grave	1 kWh of theoretical storage capacity/ 1 MWh of delivered electricity to the grid during the whole lifetime of the battery application	Future, beyond 2030	Global	Mass-based	FS: Upscaling battery materials, adjusted gigafactory model, technology improvements BS: Electricity supply mixes
Paper II	Already mature technologies	Cradle-to-gate	1 ton of LHM	Current/future (2027-2032)	Chile, Argentina, Australia, Finland, Canada	MPBAB	None – already mature technologies
Paper III	Current TRL/MRL:7-8 Future TRL/MRL: 9 (for TRL), 10 (for MRL)	Cradle-to-gate	1 kWh of theoretical storage capacity	Future, around 2025-2030	Global	Mass-based, MPBAB	FS: Adjusted gigafactory model, battery cell design variation BS: Upscaling battery materials, Electricity supply mixes

5.10 Paper I results

LCIA results for the main impact categories can be found in Figure 3 in Paper I. Regardless of impact category, scenario B has the highest impact for all impact categories, and scenario C yields the lowest impact. Climate change impacts range from 29-300 kg CO_2 eq/FU, water use from 0.42-3.9 m^3/FU, mineral resource impact using SOP from 2.9-5.8 kg Cu eq/FU and mineral resource impact using CSI from 1.7E4-6.3E4 kg Si eq/FU. For climate change impact and water use results, production of LiTFSI, a common electrolyte salt for Li-S batteries (Scheers et al., 2014), is the major hotspot in three out of five scenarios, as can be seen in Figure 6 (extracted from Figure 3 in Paper I). The two best ways of handling this hotspot is either to substitute LiTFSI by another electrolyte salt, which is done in the M scenario, or to increase the technical performance of the battery cell, as is done in the T scenario. Note that both these changes were made in the C scenario.

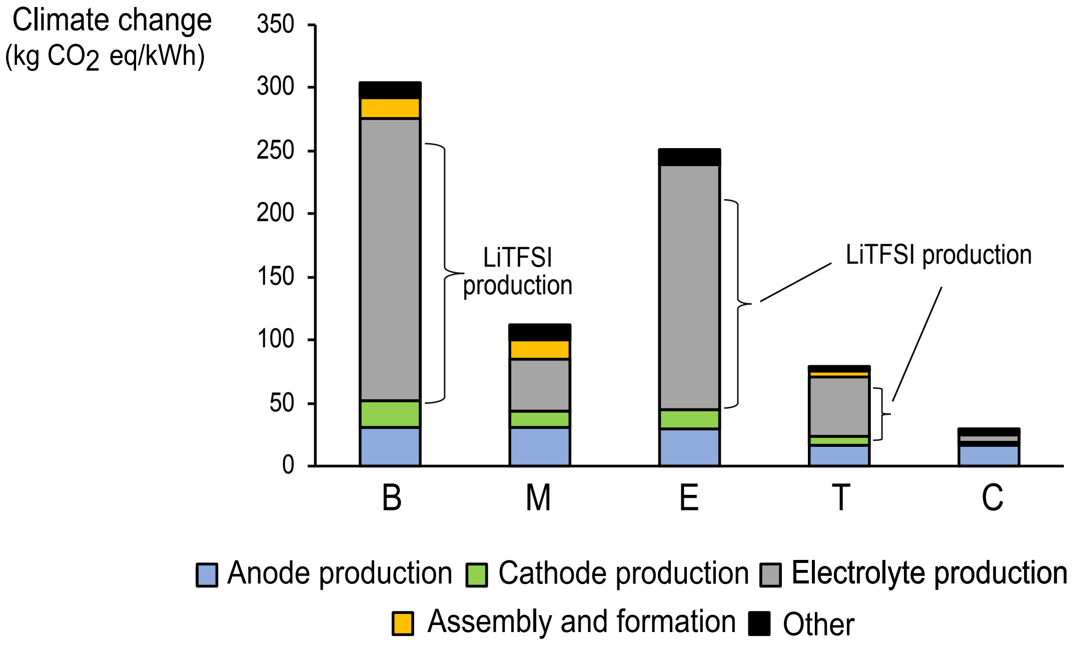

Figure 6. Climate change impacts for Li-S battery cells. B=Base scenario, M=Material selection scenario, E=Energy system scenario, T=Technical performance scenario, and C=Combined scenario.

Regarding mineral resource impacts, the result profiles differ between the impact indicators. For the CSI, rarer elements used in small amounts, e.g. lithium, make notable contributions as well as more abundant resources used in larger amounts, e.g. sodium chloride (see Figure 3 in Paper I). Measures that reduce the climate impact and water use also lower the CSI result. Lithium stands for the majority of the impact in the SOP-results for all scenarios. To reduce the SOP impacts, the technical performance needs to be increased.

Cradle-to-grave results are presented in Figure 4 of Paper I (please note the corrected results in Wickerts et al. (2024)). Climate change impacts and water use range between 42-530 kg CO_2 eq/FU and between 0.56-7.0 m^3/FU, respectively. The R scenario yields the highest impacts while the C scenario yields the lowest. The “cell production”, which includes the cell assembly plus its entire upstream production, is the most contributing phase in the scenarios that rely on the base cell characteristics (see Table 2). The reasons for the cell production being the major hotspot in the B, M, E, and R scenarios but not in the T and C scenarios are due to cradle-to-gate scenario characteristics as well as characteristics related to the battery operation. The use phase is another hotspot in most scenarios, which is partly due to that the large-scale battery installation requires electricity and partly due to losses occurring during the operation. The R scenario has a third hotspot, namely the EoL phase. This scenario indicates that, given the base characteristics for both battery cell production and battery operation, recycling of Li-S cells using hydrometallurgical processing is not beneficial. As for the cradle-to-gate level, increasing the technical performance is one way to significantly lower the results.

Mineral resource impacts using SOP range from 0.61-7.8 kg Cu eq/FU and using CSI from 1.6E4-1.2E5 kg Si eq/FU. The CSI results show a similar pattern as the climate change impacts and water use results. The R scenario models a closed loop for lithium, so it is not evident why this scenario has the highest CSI impact. The explanation lies in the chemical consumption of the hydrometallurgical recycling process. The SOP results provide a different pattern, where the B, M, and E show similar results, while the remaining scenarios yield significantly lower impacts. Using this indicator, hydrometallurgical recycling comes out as beneficial. For both the CSI and SOP results, increasing the technical performance is one way of reducing the mineral resource impacts.

Figure 4 in Paper I shows that recycling lithium carbonate, which is done in the R and C scenarios, is not done without adding an environmental burden. Therefore, a further analysis of key hotspots in the hydrometallurgical recycling was done. This analysis shows that sodium hydroxide production is the largest hotspot, followed by steam production. Sodium hydroxide was modelled as the leaching chemical in the hydrometallurgical process, which has an electricity intensive production process (Kurt and Bittner, 2006). As this chemical is primarily produced in China today (OEC, 2024), the impacts are largely related to the Chinese electricity mix.

5.11 Paper II results

Figure 7 shows the climate change impact for LHM production, both for brine-based and spodumene-based production routes. The figure also displays the geographical locations, lithium grades, and the data sources. The geographical locations of Cauchari and Maricunga (which correspond to future production) show the highest impacts, in terms of brine-based routes. The high impacts are partly due to the lower lithium concentration in these sources, implying that more brine must be extracted to yield the same amount of product as the ones with higher lithium concentrations. Furthermore, the two Atacama production routes, see Figure 7, show contrasting results, which indicate possible updates in the technical processes over time and/or which data is collected. In terms of the spodumene-based routes, the Ecoinvent process for the Australian source has the highest impact, even though this source has the highest lithium grade. Fossil energy is used for the extraction and processing operation, which is why the impact is high. Therefore, the climate change impact of infrastructure surrounding the production processes overshadow the benefit of having higher lithium grades. As the Atacama routes are termed as current production routes while the Cauchari and Maricunga locations correspond to future production, there is an indication of increased climate change impacts over time, given a decrease in lithium concentration. For spodumene-routes, the climate change impact of infrastructure surrounding the production processes overshadow the benefit of having higher lithium grades.

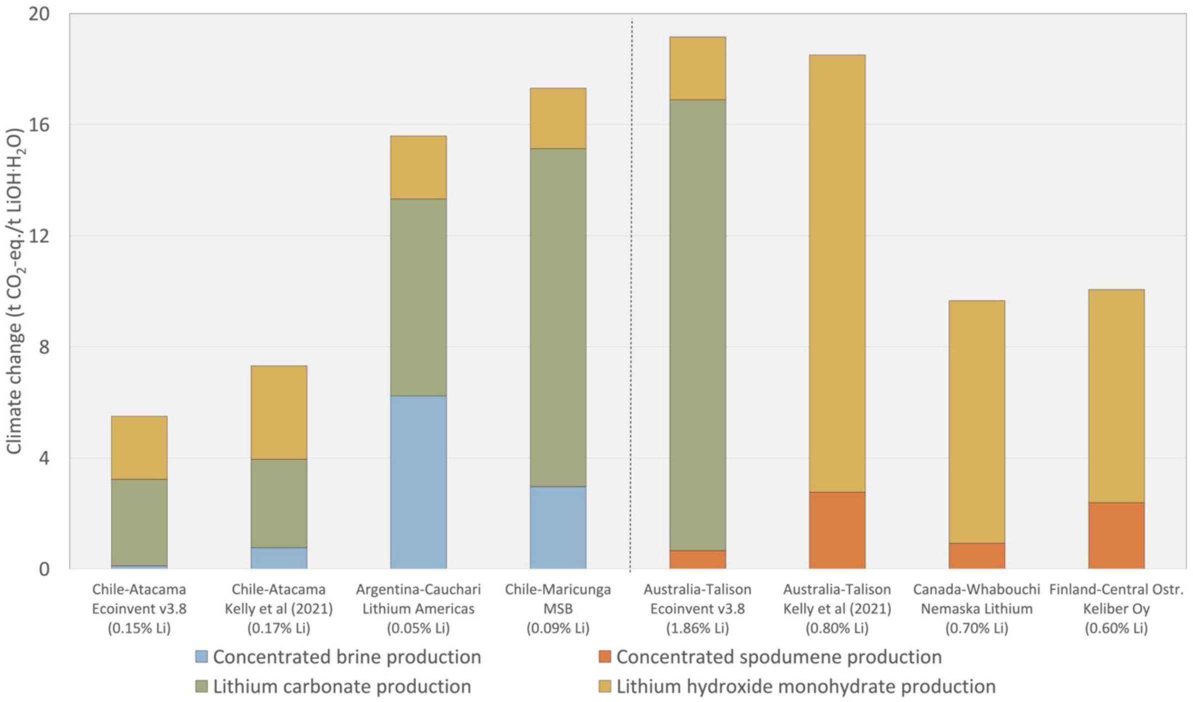

Figure 7. Climate change impacts for different LHM production routes, accounting for geographical locations of the lithium source, the underlying dataset, and the lithium grades.

The mineral resource impacts, for both the SOP and CSI method, can be found in Figure 2 in Paper II. Overall, brine-based production routes showcase significantly higher impacts than the spodumene-based ones. This is because various elements, which the brine consists of, are extracted along with lithium. When extracting spodumene, other elements than lithium are extracted as well, however not to the same extent as for the brine-based routes. In terms of elementary flow hotspots, chlorine is the largest contributor for most brine-based CSI results, while lithium is the largest CSI contributor for the remaining routes. Regarding SOP results, lithium is the hotspot for both brine and spodumene-based routes.

The water use and the freshwater ecotoxicity impacts can be found in Figures 3 and 4 in Paper II. For water use, the ReCiPe result (only accounting for water use at the inventory level) is highest for the production route with lithium extracted in Canada followed by the production routes utilizing the Maricunga and finish sources. In terms of AWARE results (accounting for the regionalized impact of water use), the Maricunga production route yields the highest result, implying higher characterization factors for Chile compared to the other locations assessed. In terms of total results, there is no indication of brine-based routes requiring more water than the spodumene-based ones, or vice versa. Note that water use linked to lithium extraction cannot be assessed without addressing an ongoing discussion related to water use in brines. The debate is linked to whether brine should be considered as water or a mineral (Bustos-Gallardo et al., 2021). Brines consist of water as well as non-metallic elements and metallic elements, and since brine is unfit for drinking as well as agricultural practices, the debate seem warranted. Ejeian et al. (2021) argue that brine should be considered as a type of water and not a mineral by pointing to the brine's water molecular structure. Pumping of brines is thought to potentially affect the freshwater volumes in the nearby region. If such a correlation between removal of brine and seepage of freshwater into brine aquifers exists, the brine use will likely influence the freshwater availability regardless if the brine is considered as water or a mineral (Bustos-Gallardo et al., 2021). Since the effect on freshwater availability due to brine extraction is not fully understood, the overall water use of brine extraction could be much higher than what is shown in Figure 3 in Paper II. Regarding freshwater ecotoxicity impacts, these are mainly related to the background system.

5.12 Paper III results

Figure 3 in Paper III shows the results for impacts on climate change, fossil resource scarcity, and mineral resources using both the SOP and CSI methods. The total results range from 58-130 kg CO_2 eq/FU for climate change impacts, 16-39 kg oil eq/FU for fossil resource scarcity, 0.47-0.72 kg Cu eq/FU for mineral resource scarcity using SOP, and from 8.9E3-2.1E4 kg Si eq/FU for mineral resource scarcity using CSI. Overall, Cell 1 and Cell 2 obtain almost the same results, as can be seen in, e.g., Figure 8 below (extracted from Figure 3 in Paper III). In fact, the biobased cell (Cell 2) does not appear to have an advantage over the fossil-based cell (Cell 1) in any of the included impact categories (in Figure 3). All impact categories are sensitive to the allocation approach and all except the SOP indicator are sensitive to the change in electricity supply mix. In terms of allocation, the product system of Cell 2 consists of more by-products than that of Cell 1, which is why the allocation method affects Cell 2 more than Cell 1 (compare e.g. S1 and S3 for Cell 1, with S5 and S7 for Cell 2 in Figure 8). There might be products that are today considered by-products but will be considered main products in a future where SIB cells are produced at large scale. In such a future, the MPBAB approach might be the more appropriate way of dealing with by-products in the SIB product system.

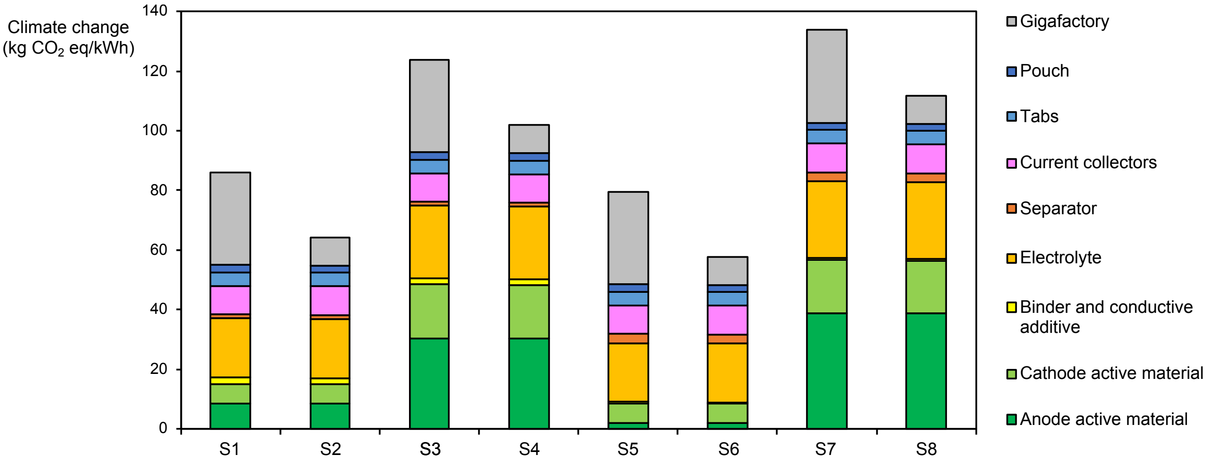

Figure 8. Climate change impacts for SIB cells, given the different scenario combinations (see Table 3).

The hotspots differ depending on the impact category and the specific scenario. One hotspot apparent for all impact categories is the electrolyte production. Cell 1 and Cell 2 have different electrolytes; however, they seem to have equal impacts for all impact categories (besides SOP). The production of electrolyte materials was not part of the foreground system (the foreground processes are stated in Section 2.2. in Paper III), and therefore the change in electricity supply mix was not applied to those production processes. However, one way of reducing the impacts of the electrolyte production might be to utilize electricity from renewable sources, as this electricity switch has shown to be beneficial in the foreground system when climate, fossil resources and mineral resources (regarding CSI) are considered. Another hotspot, particularly evident for climate change impacts and fossil resource scarcity impacts, is the anode active material production (with regard to the MPBAB approach). Therefore, measures to decrease emissions in the production of precursors for the anode should be taken.

5.13 Synthesized results

The thesis contains two research questions requiring a synthesis of results to be answered. More specifically, the part of research question two specific to Li-S batteries ("How do different lithium grades and sources affect the life cycle environmental and resource impact...in particular Li-S batteries?") as well as research question four ("Which battery technology, Li-S, SIB, or LIB, shows the greatest promise from a life cycle environmental and resource point-of-view?") need the synthesis. To answer the latter part of research question two, additional modelling had to be done. In Paper I, the lithium-containing compound required to produce different battery cell materials is lithium carbonate. However, for three of the production routes included in Paper II, LHM is directly produced from concentrated spodumene, and no lithium carbonate is produced as an intermediate product. Only the production routes that included lithium carbonate as an intermediate product could be applied to the Li-S product system. Therefore, only these production routes were evaluated for the cradle-to-gate boundary and for two of the scenarios, the B scenario, and the C scenario. This choice was made since the scenarios represent a worst-case scenario and a best-case scenario, respectively. Furthermore, only climate change and mineral resource impacts were evaluated, as these were considered most relevant. For research question four, cradle-to-gate results regarding climate change and mineral resource impacts were compared.

In Figure 9, climate change impacts of varying the lithium source, thus varying lithium carbonate production routes, for Li-S batteries are shown. Note that only the geographical locations of the lithium sources are stated in Figure 9 (see e.g. Table 1 in Paper II for the corresponding lithium grades and data sources). The B scenario showcases a minor decrease for the lithium carbonate produced from lithium extracted in "Chile Atacama 1", followed by an increase of 2-11% per FU, depending on the lithium source (Chile Atacama 1 is the route based on Ecoinvent). For the C scenario, there is again a decrease in impacts for the lithium extracted in "Chile Atacama 1", accompanied with an increase between 11-59% per FU, depending on the lithium source. The contrasting results between the scenarios are due to the cell composition. In the B scenario, a cell with a rather conservative specific energy density was modelled, whereas in the C scenario, a cell with higher specific energy density was modelled. To account for this higher specific energy density, the cell composition in the C scenario was modified to contain a larger share of active material. As the cell in the C scenario contained a higher share of lithium, results for this scenario are more sensitive to the change of lithium source.

The two resource use indicators show different result patterns (Figures 10 and 11), which were seen in Papers I and III as well. The CSI results range between 63,000 and 970,000 kg Si eq per FU in the B scenario, and 18,000 and 480,000 kg Si eq per FU in the C scenario (note the logarithmic scales). Figure 10 shows that the C scenario is more sensitive to a change in lithium source since the C scenario cell contains more lithium than the B scenario cell. However, other parts of the life cycle are still contributing more to the total impact.

The SOP results, shown in Figure 11, range from 0.37 to 60 kg Cu eq per FU for the B scenario, and from 0.1 to 31 kg Cu eq per FU for the C scenario. The contribution of lithium carbonate is similar and high (close to 100%) in both scenarios. The "Chile Atacama 2" route yields significantly higher impacts than the other lithium sources (Chile Atacama 2 is the production route based on Kelly et al. (2021)). The high result can be linked to the brine composition of that specific lithium source, combined with that the SOP method including characterization factors for both lithium and magnesium (elements that are present in the specific brine). However, chlorine which contributes notably to most brine-based CSI results is not characterized in the SOP method. Furthermore, the only spodumene-based route (with lithium extracted from the Australian source) obtains so low results in both scenarios that they are not visible in Figure 11.

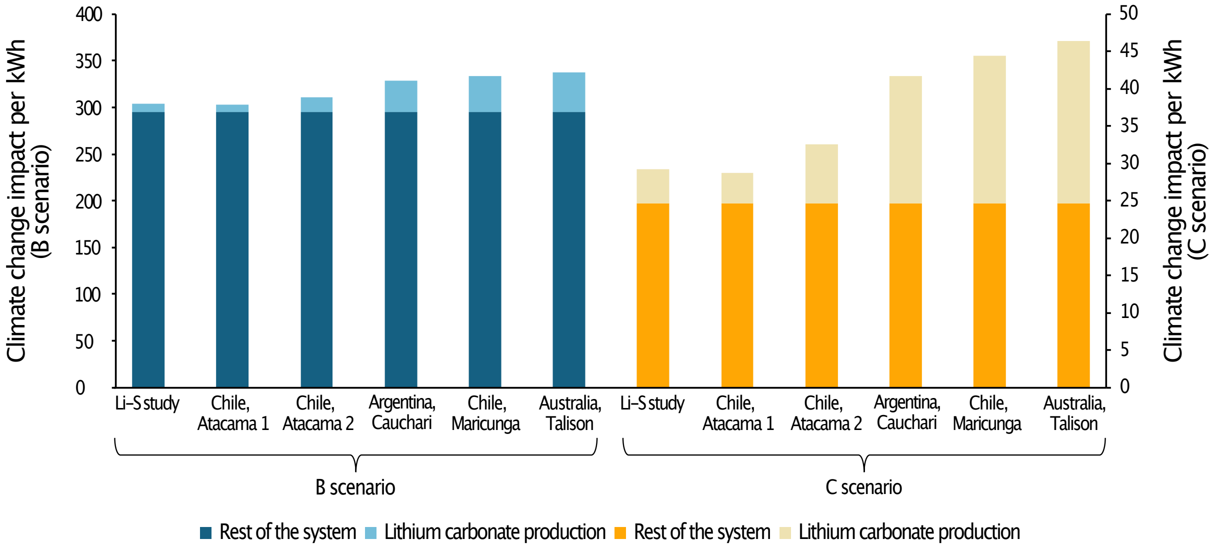

Figure 9. Climate change impact for Li-S batteries (in kg CO_2 eq per kWh of theoretical storage capacity), considering different lithium carbonate production routes.

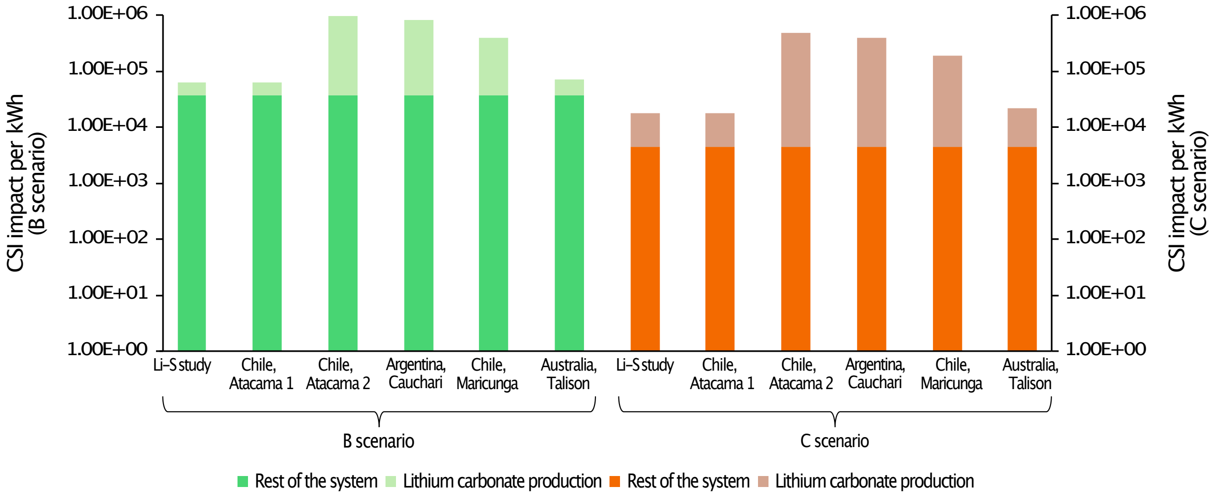

Figure 10. CSI results for Li-S batteries (in kg Si eq per kWh of theoretical storage capacity), considering different lithium carbonate production routes.

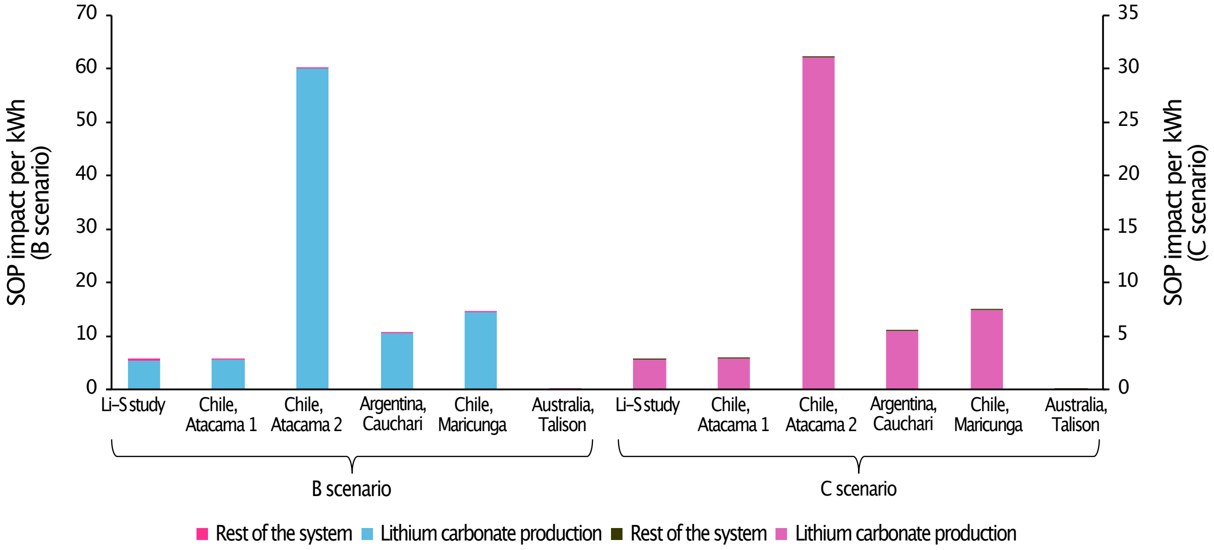

Figure 11. SOP results (in kg Cu eq per kWh of theoretical storage capacity) for Li-S batteries, considering different lithium carbonate production routes.

Comparison of cradle-to-gate climate impacts of Li-S batteries, SIBs, and LIBs, shows that the first-mentioned battery technology has both the highest (i.e., the B scenario) and lowest (i.e., the C scenario) impact (see Figure 12). Explanations for the high Li-S results could include possible over-estimations in inputs for some of the upscaled processes, while the high specific energy density is an explanation for the low impact. Comparing the impacts of SIBs and LIBs, they perform roughly the same. The fact that SIB cells consist of more abundant materials than LIB cells does not matter from a climate point of view, according to these results. Note that only mass-based allocation was applied in Paper I. If the MPBAB would have been applied in Paper I, the results would have increased. This would affect the B, E, R, and T scenarios more than the M and C scenarios, as they included more by-products.

SIBs are superior to both Li-S batteries and LIBs, regardless of the indicator when considering the mineral resource impacts (see Figure 13). Comparing the cradle-to-gate CSI results of Li-S batteries and LIBs, the B scenario is in line with LIBs while the C scenario yields much lower results than LIBs. For the cradle-to-gate SOP results, Li-S batteries obtain lower impacts than LIBs, regardless of scenario.

For comparison of cradle-to-grave scopes, there are very few studies of large-scale energy storage for renewable energy integration using LIBs. The study by da Silva Lima et al. (2021) was used to benchmark the cradle-to-grave Li-S results to the ones of LIBs, as it and Paper I model the same type of battery application and use the same FU. Regarding climate change impacts, the LIB has an impact of 72-95 kg CO_2 eq/FU, depending on the electricity type stored. The Li-S battery's impact varies between 42-530 kg CO_2 eq/FU, depending on the scenario. There are many possible reasons, in terms of modelling choices, for the contrasting results. The battery cell production's share in da Silva Lima et al. (2021) differs from the one in Paper I. In da Silva Lima et al. (2021), battery cell production stands for 40-50% of the total impact, whereas the share for Li-S batteries in Paper I ranges between 30-72%. Therefore, differences in the upstream system as well as the battery cell production modelling could be reasons for the contrasting results. Regarding mineral resource use, only the SOP indicator could be used for the comparison. Li-S batteries once again show the highest (i.e., the B scenario) and lowest (i.e., the C scenario) impact. LIBs have an impact of 5.5-5.9 kg Cu eq/FU, depending on the electricity type stored, while the Li-S battery has varying impacts between 0.61-7.8 kg Cu eq/FU. Reasons for the differing results are the same as the ones addressed above, i.e., differences in the upstream system as well as in the battery cell production modelling.

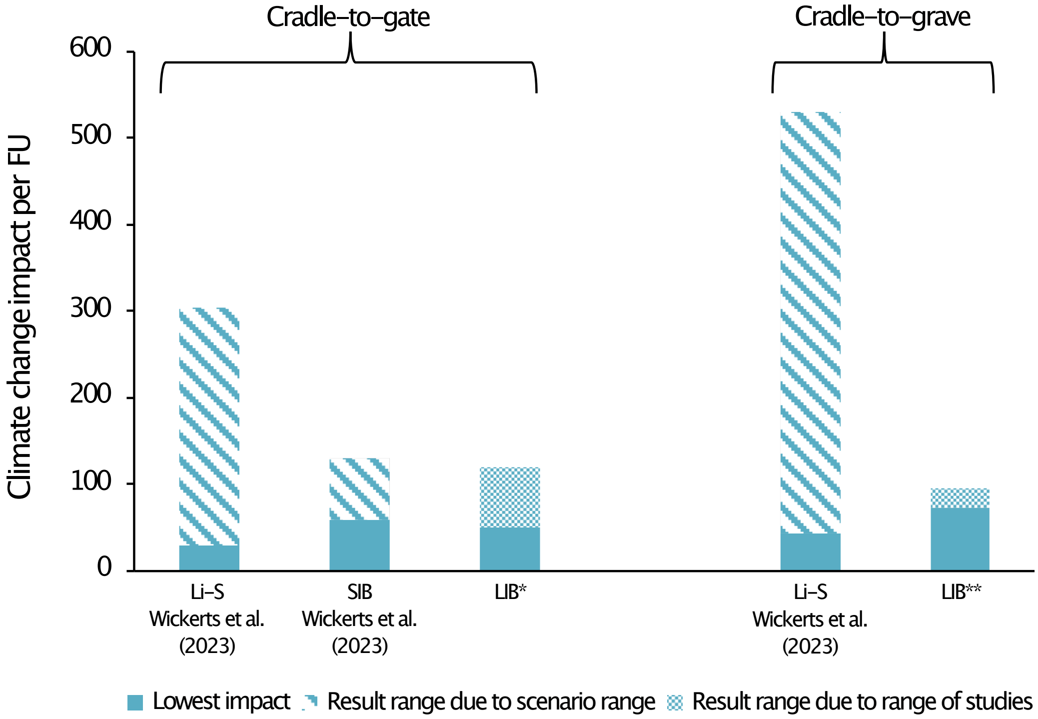

Figure 12. Climate change impact for Li-S batteries, SIBs, and LIBs (in kg CO_2 eq per FU). "Result range due to scenario range" refers to variation in results because of the scenario analyses included in Papers I and II. "Result range due to range of studies" refers to variation in results due to inclusion of several LIB studies. *Studies include Chordia et al. (2021), Dai et al. (2019) and Sun et al. (2020). **Studies include: da Silva Lima et al. (2021).

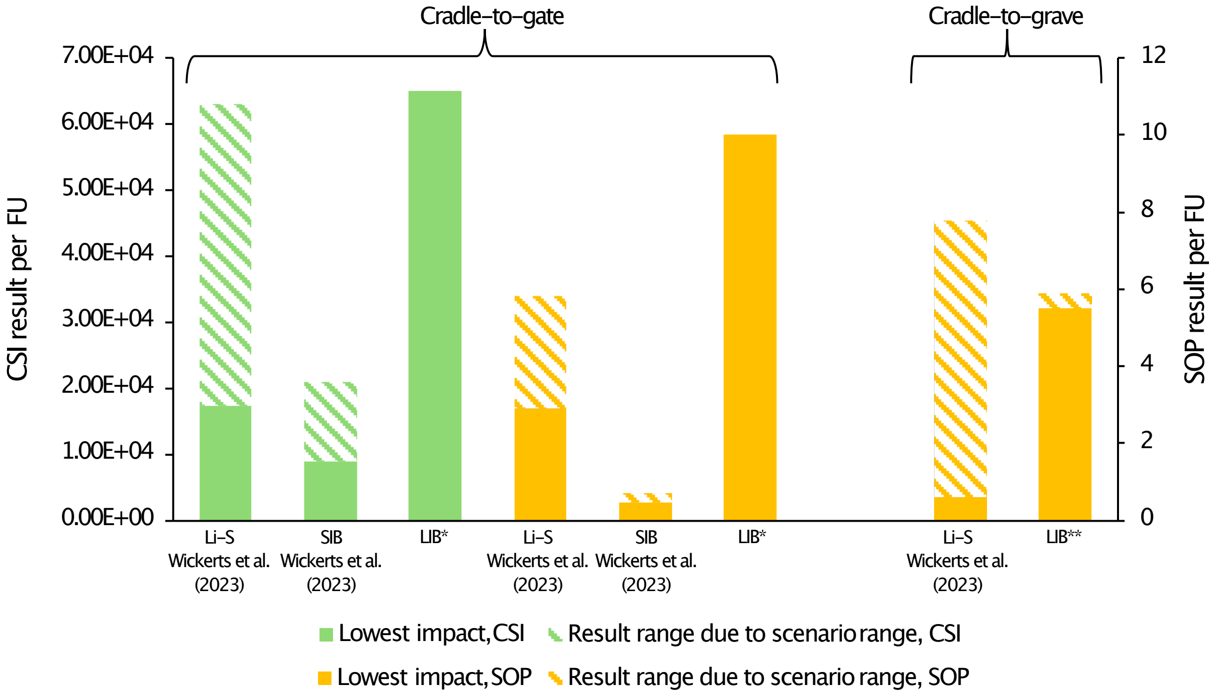

Figure 13. Mineral resource impacts for Li-S batteries, SIBs, and LIBs (in kg Si eq per FU for the CSI and in kg Cu eq per FU for the SOP indicator). “Result range due to scenario range” refers to variation in results because of the scenario analyses included in Papers I and II. “Result range due to range of studies” refers to variation in results due to inclusion of several LIB studies. *Studies include: Chordia et al. (2021). **Studies include: da Silva Lima et al. (2021).

6. Concluding discussion

Writing this thesis has resulted in several lessons learned, which can be related to the research questions stated in Chapter 2. However, multiple lessons have been learned regarding the applied methodology as well, which are important to summarize as they can be utilized for the remaining studies of the doctoral education. First, these methodological lessons are summarized in Chapter 6.1, followed by lessons learned regarding Li-S battery and SIB impacts in Chapter 6.2.

6.1 Lessons learned regarding methodology

There are aspects related to future-oriented studies, which need consideration when comparing emerging and incumbent battery technologies. First, there are uncertainties related to the performance of a battery technology entering the market (related to the TRL) but also to the production processes of the battery technology (related to the MRL). In terms of TRLs, though not considered in Paper I, the performance of the Li-S batteries for the T and C scenarios was partly based on projections while the same parameters were based on actual achievements for the SIBs. One of the scenario parameters, the specific energy density, might have been too conservative in the B, M, E, and R scenarios. This conservative specific energy density assumption was based on achieved pilot scale results (Ainsworth, 2016).

Regarding uncertainties related to the MRLs, the battery cell production is one example, where a gigascale factory model based on production of NMC 811-based LIBs was used. This choice entailed a mismatch between the battery technologies studied in Papers I and III (Li-S and SIBs, respectively) and the technology for which the model was developed (LIBs). It is known that production characteristics differ between NMC-based LIBs and Li-S batteries as well as SIBs. However, the difference is likely smaller for SIBs as they are considered a drop-in substitute technology to LIBs regarding production (Tapia-Ruiz et al., 2021). The granularity of the gigascale factory model is not on such a level that all differences could be accounted for. One example is that the cathode production for LIBs requires recovery of a solvent (N-Methyl-2-pyrrolidone) (Chordia et al., 2021), but the SIBs have water as solvent for both anode and cathode production. Therefore, it is unlikely that the same solvent recovery will be used in the SIB production process since water is much less valuable than the organic pyrrolidone solvent. This model is still a reasonable proxy as there are no existing gigascale factories for the battery technologies assessed in Paper I or III.

The application of the gigascale factory model represents top-down modelling, however another approach to handle the mismatch between a mature and an emerging technology is to apply bottom-up upscaling. For example, data on a lower MRL could be gathered, which is more specific to the emerging technology. The same type of production equipment could be assumed to be used at large scale. If this is done, there is a risk of instead quantifying impacts for production equipment used on low MRLs, which might not be used for large-scale production. A better bottom-up approach could be to perform the upscaling using frameworks, specific to certain materials, as the one by Piccinno et al. (2016). This framework was used in Papers I and III for upscaling upstream battery chemicals based on experimental and/or patent data specific to the production process of interest. In this way, the framework enables a more tailored and step-wise unit process development for proven large-scale equipment.

Yet another aspect to consider when assessing emerging technologies is the potential mismatch between the foreground and the background system. A large share of the impacts in Papers I and III could be attributed to the background system, which was modelled as status quo except for the electricity supply. Therefore, the environmental profiles of Li-S batteries and SIBs were largely dependent on the current production system for common commodities. This was clearly seen in the hydrometallurgical recycling process in Paper I (Figure 4 in Wickerts et al. (2024)). Considering the effect of the background system, it is imperative to understand the battery technologies' environmental performance in a future, e.g., decarbonized future without fossil fuels. Such a shift will also have implications regarding how some materials are produced. For example, the sulfur required to produce Li-S batteries is currently a by-product of fossil fuel production (USGS, 2024), but will need to be produced in other ways in the future. The prospective database Premise is trying to address this by providing prospective LCA data for an increasing number of commodities, currently including, e.g., electricity, transport, and cement (Sacchi et al., 2022).

In Papers I and III, one or more technology experts were involved. LCA studies aimed at providing technology guidance can benefit from including technology experts in technical process discussions, as such discussions facilitate the LCA practitioner's understanding of, e.g., which product and manufacturing properties are important to consider. This is particularly relevant for assessing emerging technologies, as documented technology knowledge and standardized solutions are then typically more limited. Figure 14 shows how the process of involving a technical expert can facilitate modelling of the technical system as well as result in more accurate guidance. In addition to insights about possible technical design solutions and manufacturing processes, expert judgements can also be used as a direct data source. This facilitates the LCA practitioner's understanding of the processes, which in turn enables the LCA practitioner to have a more in-depth understanding of what questions to ask the technology expert. Reciprocally, the technology expert receives an increased understanding of what type of knowledge the LCA practitioner needs. Furthermore, the technology expert could feel more motivated in doing the changes that lead to reduced impacts. As can be seen in Figure 14, this is an iterative loop, which yields an increasingly better understanding. This dynamic will manifest itself in a more relevant technical system, which in turn will yield more relevant LCIA results. The importance of connecting technology developers and sustainability assessors have been demonstrated by Clancy et al. (2013) and proposed by Tsoy et al. (2020).

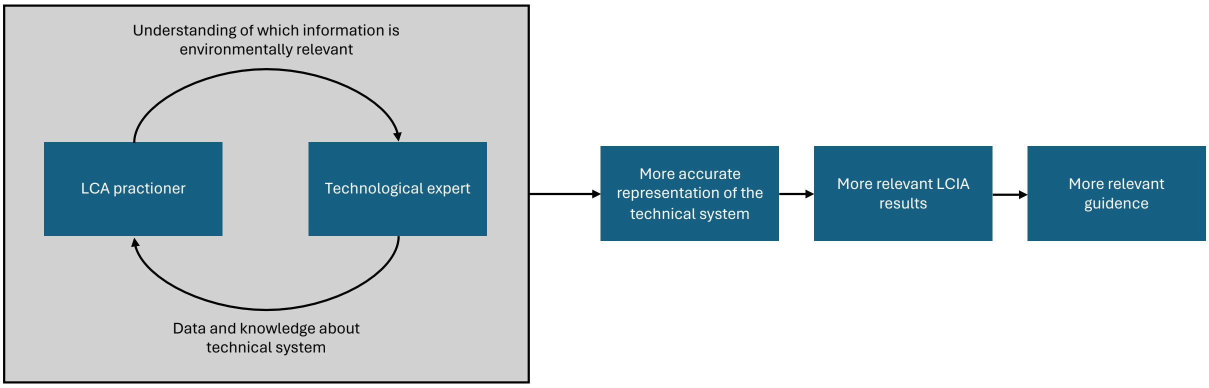

Figure 14. Dynamic between an LCA practitioner and a technology expert, enhancing the LCA study.

Based on the aspects brought up in this chapter, results of prospective LCAs should be interpreted as indicative rather than absolute. Still, these assessments of emerging technologies are required if society wants to find technologies that can assist in curtailing climate change and other environmental issues.

6.2 Lessons learned regarding Li-S battery and SIB impacts

Several lessons regarding the impacts of the two studied NGBs were learned from conducting the three studies. Regarding climate change, Li-S batteries, SIBs, and LIBs showcase impacts of the same order of magnitude. This was shown on a cradle-to-gate level for SIBs and both on a cradle-to-gate level and a cradle-to-grave level for Li-S batteries. Still, results for Li-S batteries span across a wider range than SIBs, making their actual climate impact more uncertain. Regardless, neither Li-S batteries nor SIBs have a clear advantage over LIBs regarding climate change, according to the studies' results. In terms of the mineral resource impact, another pattern is apparent: SIBs are clearly superior to both Li-S batteries and LIBs. As there is a risk of scarcity for, e.g., lithium, investing in battery technologies that contain abundant resources can be beneficial in a long-term perspective. However, considering the rapid scale-up rate of battery production, investing in battery technologies that contain abundant resources could be beneficial also in a short-term perspective, since geological abundance increases the likelihood of the resource being more distributed across the world and thus less likely to face phase constraints (i.e., less likely to become critical). Diversifying the battery technologies available on the market and thereby diversifying the material requirements could make the battery scale-up less sensitive to resource availability bottlenecks. Furthermore, utilising battery technologies that contain geologically abundant materials could lead to the avoidance of other sustainability concerns. In this context, SIBs represent a promising NBG containing almost exclusively abundant resources.

The lithium supply chain is related to the production of Li-S batteries. Paper II showed that the environmental and resource impacts of LHM is largely dependent on the geographical circumstances as well as technology choices for lithium processing. The impacts also depend on the temporal scope of datasets. The geographical circumstances include geological parameters such as grade and brine/mineral composition but also technology choices related to the surrounding infrastructure for example, e.g. the electricity supply. The results showed that while lithium might be more abundant in certain locations, there are other parameters that can counteract the benefit of extracting from more abundant sources, such as diesel-generated energy supply. Furthermore, the contrasting results of the two Atacama production routes indicate updates in the technical processes, showing the importance of using up-to-date datasets. The lithium production routes had implications for the environmental profile of Li-S batteries, and especially for the C scenario (the scenario including e.g. high technical performance and wind power). Therefore, a larger part of the environmental profile for high-performance Li-S batteries is related to the lithium supply than for low-performance Li-S batteries.

As both NGBs were compared to LIBs, there are a few things worth mentioning about the latter battery technology. While the LIB technology is mature, incremental advancements will be made also to its performance and manufacturing processes, which in turn could lead to reduced environmental and resource impacts (Buyle et al., 2019). However, as LIBs were not assessed in the papers, accounting for such advances was considered outside the thesis scope. Even so, the future environmental profile of the NGBs assessed in this thesis could benefit from such advancements as well, contributing to lower impacts for also them. This could be true especially for SIBs, as they are considered drop-in technologies to LIBs (Tapia-Ruiz et al., 2021). Furthermore, modelling choices made in the respective LIB study influence the LCIA results of those studies, and by extension the comparison made in this thesis. Inconsistencies between LCA studies will always exist, thus comparisons should be seen as indicative rather than absolute.

Based on the discussion above, SIBs represent the battery technology that shows the most promising environmental and resource characteristics in the nearby future. But, it is important to remember that different batteries will fulfil different needs, and since these needs have different requirements, there is no “one solution fits all” battery (Volta foundation, 2023). Considering the potential of SIBs, future research aims to understand the environmental and resource impacts of this NGB even better. Examples of modelling aspects that could be further explored include adjusting the cell production to be more specific to SIBs. Furthermore, the life cycle should be extended from the cradle-to-gate scope of Paper III to find showstoppers in both the use phase and the end of life, as well as exploring the environmental profile in a decarbonized background system, e.g., by using prospective databases such as Premise.

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