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Closing gaps in LCA of lithium-ion batteries: LCA of lab-scale cell production with new primary data

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A B S T R A C T

Battery storage systems have become an important pillar in the transformation of the energy and transportation sector over the last decades. Lithium-ion batteries (LIBs) are the dominating technology in this process making them a constant subject of analysis regarding their sustainability. To assess their environmental performance, several Life Cycle Assessments (LCA) of LIBs have been performed over the last years. Yet, the amount of available primary data on their production remains low, leading to recurrent reliance on a few disclosed datasets, mostly at industrial scale. Thus, there is a need for new LCA studies at different scales (lab, pilot, industrial) using transparent datasets to facilitate more reliable and robust assessments. This work presents a screening of recent environmental assessments for LIBs at different production scales aiming at identifying remaining gaps and challenges, and deriving a detailed LCA of a lab-scale battery cell production. For the first time the environmental impact of a lab-scale battery production based on process-oriented primary data is investigated. The results are flanked by sensitivity analyses and scenarios and compared with literature values. The hotspots identified in this study, cathode slurry, anode current collector, as well as the energy demand of the dry room and coating process, are consistent with the literature, although the absolute values are an order of magnitude larger. The main reason for this are the inefficiencies inherent in lab-scale production. In order to analyze the effects of production scale, an upscaling to the pilot scale is performed.

1. Introduction

Lithium-ion batteries (LIBs) have become a prevalent power source for small electronic devices, electric vehicles, and stationary energy storage systems, owing to their superior performance among other types of batteries in terms of energy density, efficiency and cost (Baumann et al., 2017; Weil et al., 2015; Weil and Tübke, 2015; Zhang et al., 2020). In particular, the significant increase of electric vehicles lead into a worldwide increase of LIB sales from 3 GWh in 2000 to 160 GWh in 2018 (Stampatori et al., 2020; Thomitzek et al., 2019a; Pillot, 2019) while global production capacity of LIBs forecasts to reach up to 1211 GWh by 2025 (Stampatori et al., 2020). Yet, this rapidly growing market demand driven by the increasing electrification of today's society also raises concerns and challenges related to energy demand (Thomitzek et al., 2019a), emissions (Baumann et al., 2017; Emilsson and Dahllöf, 2019; Weil et al., 2020) and consumption of critical resources (Weil et al., 2018). Consequently, several studies have evaluated the sustainable character of LIBs, providing details of their manufacture (Chordia et al., 2021; Dai et al., 2019), recycling (Peters et al., 2018; Nordelöf et al., 2019; Mohr et al., 2020a; Rajaeifar et al., 2021) and general considerations over their life cycle (Emilsson and Dahllöf, 2019; Aichberger and Jungmeier, 2020; Peters et al., 2017). Particularly, energy-intensiveness

Abbreviations: AGEB, AG Energiebilanzen e.V.; BMS, Battery Management System; BTC, Battery Technology Center; B-U, Bottom-up; EFA, Energy Flow Analysis; EoL, End-of-Life; ILCD, International Reference Life Cycle Data System; KIT, Karlsruhe Institute of Technology; LCA, Life Cycle Assessmet; LCC, Life Cycle Costing; LCI, Life Cycle Inventory; LCIA, Life Cycle Impact Assessment; LIB, Lithium-ion battery; MEFA, Material and Energy Flow Analysis; PV, Photovoltaic; T-D, Top-down.

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during cell production and the use of critical resources have been found among the most concerning aspects related to LIB manufacturing. The standardized Life Cycle Assessment (LCA) method is often used to quantify the environmental impacts of LIBs, leading, however, to a broad range of results and large differences between studies. This heterogeneous picture is partly fostered by the use of varying system boundaries and baseline assumptions hampering comparability. Also traceability of results is often difficult given the lack of transparency and little provision of details related to the data acquisition process (bottom-up or top-down), especially critical when analyzing energy flows and corresponding modeling approach. In addition, Life Cycle Inventories (LCIs) are frequently built using secondary data extracted from a small amount of sources inhibiting both, the reliability and robustness of the analysis and potentially leading in error propagation (Bauer et al., 2022). An insightful assessment of the environmental footprint of LIBs requires transparent studies in which assumptions and limitations are understandable and plausible and the data origin is clear. Of particular interest are open and comprehensive studies performed with a large share of primary data in their inventories, revealing data in an easily reusable way on which further studies can be based on (Peters et al., 2017; Bauer et al., 2022). Another contributing factor influencing the environmental profile of LIB's is the scale of their manufacturing processes (Chordia et al., 2021; Degen and Schütte, 2022; Porzio and Scown, 2021; Jinasena et al., 2021). Most studies are associated to industrial production of batteries, but such classification may lead to ambiguity if the production volumes are not clearly indicated. This situation hinders the understanding of the relationship and dynamics between production scales and environmental performance of a battery system. Such dynamics become specifically intriguing when conducting prospective assessments for novel battery technologies as their production related data is often available at laboratory level only. The extent to which these lab-scale results could be valuable but also scaled-up to represent higher production scales remains to be investigated. Consequently, this study seeks to provide a comprehensive overview of the state of the art in environmental assessment of LIBs, comparing key characteristics, identifying discrepancies and research gaps, followed by a LCA facilitated by primary data collected at the laboratory level, aiming at filling the gaps identified in the literature review. The main novelties in this work can be summarized as follows:

- Extensive and detailed review of recent and relevant studies on environmental assessment of LIB manufacturing, with special respect to production scale.
- First (to the author's knowledge) LCA for LIB cell manufacturing at laboratory stage, compiling fully transparent primary data modeled with a bottom-up approach.
- Comprehensive comparison of own results with findings in literature.
- Analysis of the dynamics between production scale and environmental footprint through theoretical scale up.

2. Review of previous studies on LIBs

An extensive review of environmental assessments for LIBs has been carried out to characterize and identify research gaps that remain open in the subject. The screening is focused on literature published between the years 2010–2021, with the yearly distribution seen in Fig. 1 that evidences the increased interest in the field over the last years. Specific sources predating this period are included in the SI due to their perceived significance in this field. For this purpose, different study types, such as Material and/or Energy Flow Analysis (MEFA/EFA), Life Cycle Inventories (LCI), Life Cycle Costings (LCC) and LCA of battery pack and battery cell production, were considered. Overall, 64 studies were identified within these categories, which have been described in the corresponding Table S1 of the Supplemental Information (SI). A distinction between study type, cell geometry, cell chemistry, inventory

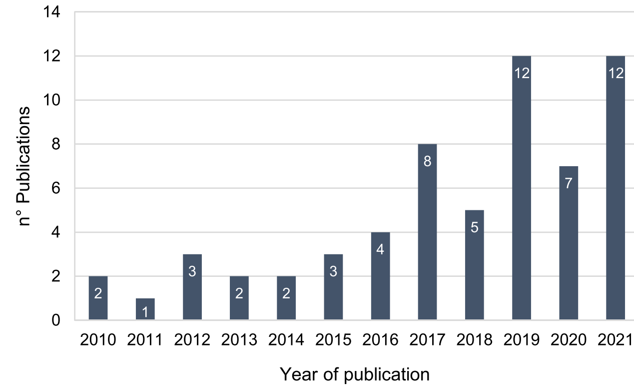

Fig. 1. Number of studies reviewed by publication year.

source, data type, the respective energy analysis approach as well as the indicated production scale and volume of each publication is made. In the following, the literature review results are discussed in detail concerning sources of inventory data, energy modeling approach, and production scale followed by a brief analysis of their system boundaries and the environmental potential of currently existing End-of-Life (EoL) strategies for LIBs.

2.1. Source of inventory data

Depending on the system boundaries defined in line with the goal and scope of a sustainability assessment, different foreground and background processes, comprising different life cycle stages, need to be considered. Foreground processes are directly characterized by the LCA practitioner by means of primary or secondary data that define inputs and outputs to the model, whereas background processes are addressed by using open-access or commercial databases that fill-in the gaps that would otherwise be time- and resource-consuming to estimate. Previous reviews have identified, among other issues, lack of transparency and an extensive use of secondary data in the characterization of foreground processes, with few primary data sources constantly replicated in more recent assessments (Aichberger and Jungmeier, 2020; Peters et al., 2017; Lai et al., 2022; Arshad et al., 2022). Considering that the quality of the foreground data is critical for the soundness of any sustainability assessment, transparency and traceability become crucial aspects in this respect. Valuable advances in the generation of primary data have been made recently (Chordia et al., 2021), but the reliance on outdated sources and the consequent need for more original data to construct LCIs remain. This is justified in Figs. 2 and 3, with Fig. 2displaying the percentage distribution of data sources used to build the foreground inventories among the 64 publications hereby reviewed. It can be seen that almost half of them (46%) rely on secondary sources such as other studies and/or databases and only 21% of the examined studies are fully based on original primary data, obtained either in cooperation with

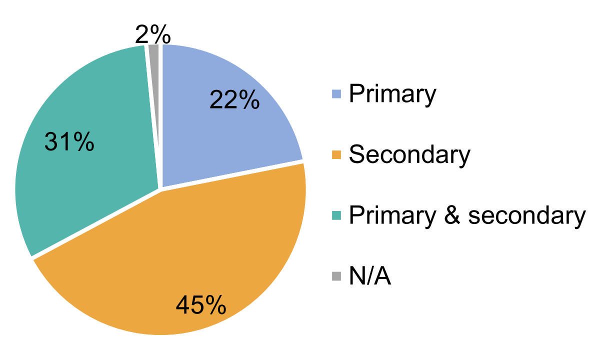

Fig. 2. Data types for foreground inventories among studies reviewed.

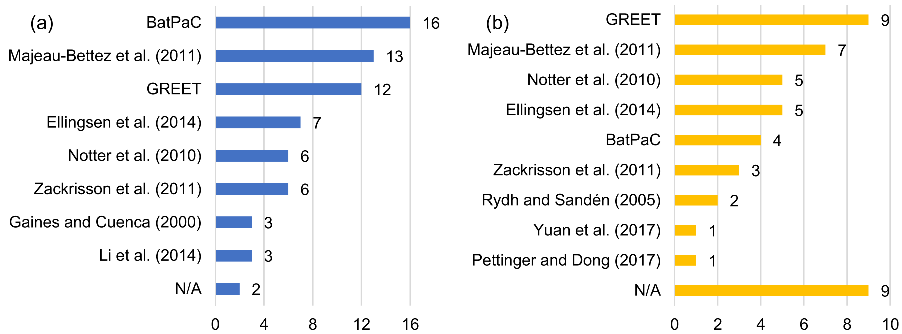

Fig. 3. Frequently referred publications as (a) data source for material inventory and (b) data source for energy inventory.

industry partners or with own measurements. In 32% of the studies a mixture of primary and secondary data sources was identified. Only in 2% of the studies (Gaines and Cuenca, 2000), the type of inventory data used was not comprehensible.

Fig. 3 displays the most frequently used secondary sources for material and energy data respectively. The outstanding significance of Dai et al. (2019) (GREET), Majeau-Bettez et al. (2011), Ellingsen et al. (2014), Notter et al. (2010) and Zackrisson et al. (2010) remains clear. The data sources used are mostly the same for both material and energy flows, though with slightly different distributions. The reason for this lies in the detailed information of the inventory provided by the identified sources and the fact that they are mainly based on transparent and comprehensible primary data. It should be noted that in many cases the inventories are built with data from more than one single source. Besides the fact that some literature sources are considerably outdated, the source of material and energy data was not apparent in nine publications (Gaines and Cuenca, 2000; da Silva Lima et al., 2021; Le Varlet et al., 2020; Liang et al., 2017; McManus, 2012; Tao and You, 2020; Vandepaer et al., 2017; Wang et al., 2019; Wang and Yu, 2021). The lack of this information severely hinders traceability of data, which compromises the transparency and reliability of these studies. This is due to the fact that energy consumption in cell manufacturing is a critical factor when determining the environmental profile of LIBs (Emilsson and Dahllöf, 2019; Dai et al., 2019; Ellingsen et al., 2014; Davidsson Kurland, 2019; Erakca et al., 2021; Yuan et al., 2017).

2.2. Modeling approaches and energy demand

Two different approaches are commonly employed to calculate the energy demand for LIB production, namely top-down (T-D) and bottom-up (B–U). In the former, the specific energy consumption is calculated from the gross energy demand of the complete manufacturing plant and later divided by its total throughput (or allocated according to the economic value of the outputs in case the plant manufactures multiple products). In the latter, the energy consumption data acquired is estimated for individual processes (sub-steps) within the production line and the complete manufacturing plant's energy demand is extrapolated on this basis. It has been documented that the calculated magnitude of total energy demand may deviate significantly between both approaches (Peters et al., 2017). Especially, when using a T-D approach, the estimated manufacturing energy demand tends to be higher than that determined with a B–U approach for the same system. This is due to the fact that T-D may encompass additional activities or flows not directly connected to the studied system (e.g. electricity used in the administrative department of a factory) that could be neglected in B–U modeling.

As indicated in Fig. 4, it was not possible to identify the modeling approach clearly for 31% of the studies herein reviewed. The T-D approach was used in 30% and the B–U approach in 30% of the studies examined. In a minor amount of studies (9%) a mixture of both

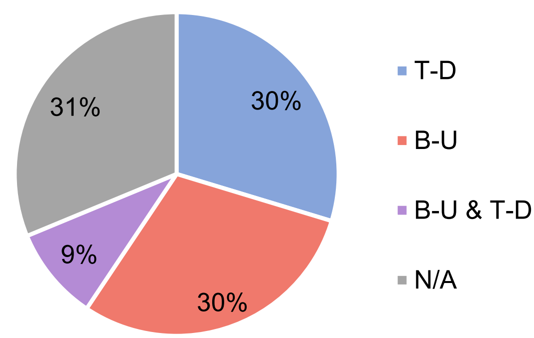

Fig. 4. Manufacturing energy modeling approach among reviewed studies.

approaches was applied. The selection of a specific approach should be clearly announced since its potential effects should be accounted for when interpreting the results and making comparisons between different studies. The suitability and selection of a specific approach shall be defined by the goal and scope of the study. Yet, when a detailed characterization and analysis of critical processes in battery production is required, the B–U modeling approach might result more adequate as the high granularity encountered in B–U results could provide a better understanding of the processes involved and their interconnections. This understanding could be particularly necessary e.g. in the identification of environmental or financial hotspots or when analyzing the environmental impact of emerging battery technologies. Mature models with B–U perspective also provide a breakdown of individual processes and respective material and energy flows that could potentially be adapted and used in the analysis of emerging/concept systems (e.g. Sodium-ion batteries).

2.3. Influence of production scale

Historically, most sustainability assessments have been performed on systems extracted from pilot and industrial production lines, or on theoretical models reflecting such conditions. Fig. 5, illustrates the research interest per production scale, namely lab-, pilot-, industrial- and Giga-scale. Note that the total amount of results (70) is higher than

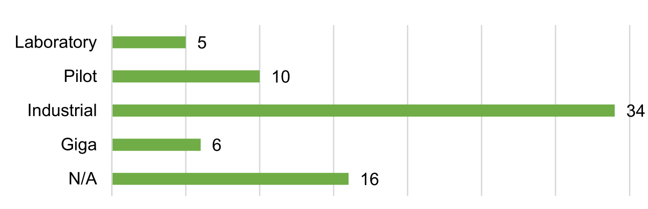

Fig. 5. Amount of study results for different production scales.

the total amount of studies (64) as some studies analyze scenarios at different scales.

For a total of 16 results (Gaines and Cuenca, 2000; Majeau-Bettez et al., 2011; Notter et al., 2010; Zackrisson et al., 2010; McManus, 2012; Vandepaer et al., 2017; Ahmadi et al., 2017; Amarakoon et al., 2013; Hammond and Hazeldine, 2015; Hischier et al., 2007; Ioakimidis et al., 2019; Kelly et al., 2020; Richa et al., 2017; Rydh and Sandén, 2005a, 2005b; Simon and Weil, 2013; Yang et al., 2020) the corresponding production scale is not evident. However, this information is crucial for the analysis and comparability of these studies. Whenever the production scale has been labelled as 'mass production', 'large scale', 'medium scale', or 'small scale' within the studies, the results have been allocated to industrial scale. With a total amount of 34, most results are available on an industrial scale. Six results were found labelled as Giga-scale in the respective studies, which is why they have been listed separately. This can nevertheless be considered as an extension of the industrial scale. Ten results were reported in the pilot scale and only five in the laboratory scale, of which only four correspond to LCAs (Liang et al., 2017; Troy et al., 2016; Wang et al., 2017; Zackrisson, 2016). Yet, only the availability of sufficient data from lab- and pilot scale systems, enable the determination of scaling methods and more reliable scaling factors as well as extrapolation methods for the LCI of prospective assessments, often analyzing theoretical industrial models when only lab- or pilot scale data is available. To better understand the effect of different production levels on the energy demand of cell manufacturing, Fig. 6 depicts the specific energy demand during battery cell production, expressed in Wh per Wh of cell storage capacity, at different scales as found in the literature.

Values represented with a triangle (Thomitzek et al., 2019a; Jinasena et al., 2021; Erakca et al., 2021; Yuan et al., 2017; Deng et al., 2019; Pettinger and Dong, 2017; Thomitzek et al., 2019b; von Drachenfels et al., 2021; Wessel et al., 2021) were determined using B–U approach, values symbolized with a square (Chordia et al., 2021; Dai et al., 2019; Ellingsen et al., 2014; Davidsson Kurland, 2019; Philippot et al., 2019; Sun et al., 2020) relate to a T-D approach. Whenever the modeling approach was not clearly identifiable, the values were symbolized with a diamond (Philippot et al., 2019). Studies marked with a star are LCAs, whereas the other studies are either MEFAs, EFAs or LCIs. Overall, 19 energy demand values have been identified. Only one study (Erakca et al., 2021) revealed the energy demand for LIB cell production on lab-scale and seven studies (Thomitzek et al., 2019a; Erakca et al., 2021; Yuan et al., 2017; Deng et al., 2019; Thomitzek et al., 2019b; von Drachenfels et al., 2021; Wessel et al., 2021) are related to pilot scale. Accounting for 11 values (Chordia et al., 2021; Dai et al., 2019; Jinasena et al., 2021; Ellingsen et al., 2014; Davidsson Kurland, 2019; Pettinger and Dong, 2017; Philippot et al., 2019; Sun et al., 2020), the majority of literature sources relate to production on industrial scale. Additionally, the annual production volume associated to each source is displayed in descending order on the vertical axis whenever identifiable. Although the scale of production is given in some studies, an explicit mention of the production volume is not specified. An exact production volume could only be determined in 18 of the 64 studies examined. In cases where an exact production volume was not available (Thomitzek et al., 2019a; Erakca et al., 2021; von Drachenfels et al., 2021; Wessel et al., 2021), the values were sorted based on own analysis of the manuscripts. The average magnitudes for pilot and industrial scale have been represented with a cross. The highest value of 1470 Wh (Erakca et al., 2021) can be found on lab-scale, whereas the lowest value of 29 Wh (Sun et al., 2020) can be found on industrial scale.

A clear relationship between the production volume and the specific energy demand per cell storage capacity can be identified when considering the large deviations of the values displayed in Fig. 6. With larger production volumes, the average energy requirements tend to be lower, which goes in line with literature where the implications of the production scale have been discussed (Chordia et al., 2021; Degen and Schütte, 2022; Porzio and Scown, 2021). This effect is especially evident in the pilot scale level, where the largest deviation with increased production volumes can be observed. At larger production volumes, i.e. industrial scale, the deviations decrease. In general, the observed trend is explained by the increasing efficiencies of scaled-up production, caused, for example, by the use of existing synergy effects (i.e. heat recovery) or the automation of specific processes (Piccinno et al., 2016; Shibasaki et al., 2006). In addition, it is noticeable that only B–U approaches were used for values at laboratory and pilot scale, whereas values in the higher Gigawatt range were determined using T-D approaches. A reason for this is that, due to the confidentiality of intellectual property, industry actors tend to disclose aggregated data of the complete operation (T-D) instead of data at the individual process level (B–U), preventing traceability. In addition, lab and pilot scale production processes are often decoupled of each other, facilitating data

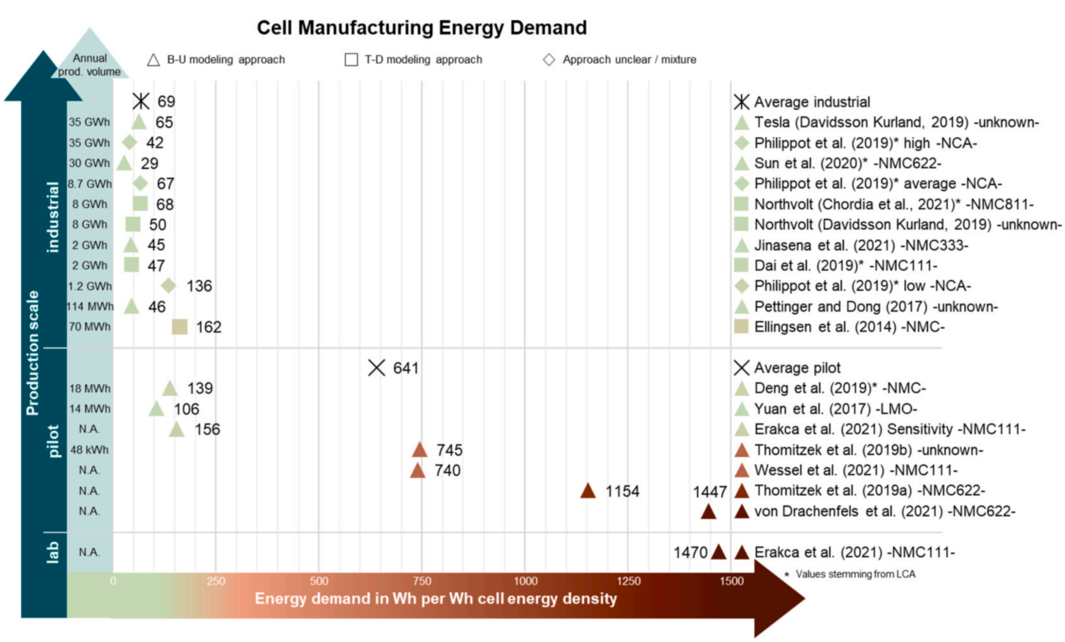

Fig. 6. Cell manufacturing energy demand in Wh per Wh cell energy storage capacities for different studies on varying production scales.

collection with a B–U approach (Piccinno et al., 2016; Shibasaki et al., 2006). Not only the energy consumption, but also the material consumption is affected significantly by the production volume. As production capacity increases and efficiency rises, material waste and thus material consumption decline. Ultimately, the production volume affects the whole LCI and consequently the assessed environmental impacts of a system.

It becomes clear that economies of scale have the potential to shape the results of an LCA and therefore should, on the one hand, be explicitly described during the assessment of any given product and, on the other, be also considered for the execution of sensitivity analysis in prospective assessments of emerging products.

2.4. End-of-Life phase

With regards to system boundaries, the cradle-to-gate and gate-to-gate perspectives are the most frequently employed. The EoL phase, which shall be considered either in a cradle-to-grave or a cradle-to-cradle perspective, has been often neglected, just gaining attention in recent years. This is likely due to the initial lack of available data surrounding the waste management of LIB, product of the premature state of specialized industry. Recycling of LIBs is currently performed via pyrometallurgical and hydrometallurgical main processes, in combination with different physical upstream and downstream treatment options, that seek to recover the valuable fraction of materials (e.g. Cobalt or Cobalt) within the batteries (Zheng et al., 2018; Mohr et al., 2020b; Velázquez-Martínez and Santasalo-AarnioReuter, 2019). In particular, newer developments, such as the battery directive, clearly point out recycling goals and the relevance for LIB and their corresponding materials (European Parliamentary Research Service, 2022). However, the environmental performance of these activities is largely dependent on the cell chemistry (Mohr et al., 2020a) and, in some cases, their specific and non-negligible burdens may outweigh their environmental benefits (Rajaeifar et al., 2021). Additionally, inconsistencies in the implementation of typical modeling approaches for LCA of waste management, namely cut-off and EoL recycling approach, have led to uncertainties regarding the true impacts of recycling, with potential over- and underestimations of results found in previous studies (Nordelöf et al., 2019). Techniques for recovery of electrode materials such as cathode recycling (Ciez and Whitacre, 2019; Iturrondobeitia et al., 2022) or graphite recycling (Rey et al., 2021) for direct reconditioning and reuse (Sloop et al., 2020) promise better performance than the conventional methods in terms of environmental footprint. However, such direct recycling processes are still being tested and need to be further developed before mass scale implementation. Moreover, the shift towards cell chemistries with lower content of critical and valuable resources, such as Cobalt, may pose a threat to the economic incentive of recycling. The processes currently used will thus need to transform in order to recover a broader fraction of materials that can make the activity more economically viable (Zhou et al., 2020). With further improvement, novel techniques, such as high-intensity ultrasonication (Lei et al., 2021) or advanced hydrometallurgy (Mohr et al., 2020a), may also increase the recovery yields and the overall efficiency of recycling. Second life applications also show promising performance, with potentially lower energy requirements than recycling. However, the extent to which energy savings can be achieved must still be validated with real data (Wewer et al., 2021; Sommerville et al., 2021). As the scope of this research lies on the manufacturing stages, the EoL is not further analyzed.

2.5. Remarks of literature review

In general, the profound lack of transparency weakens the robustness and comparability of results with just a limited number of studies fully disclosing primary data. Only if LCA results from different studies using own reliable primary data are compared, the investigated relationships between the LCI and the LCA result can be justified or falsified. The extensive use of secondary data, i.e. databases and other literature sources, hinders this, as the data is merely replicated with potential flaws being propagated. Furthermore, LCA studies based on primary data and using a B–U approach are preferred to reliably identify and analyze the environmental hotspots in LIB production. Only 17% of the studies reviewed (Thomitzek et al., 2019a; Degen and Schütte, 2022; Erakca et al., 2021; Wang et al., 2017; Pettinger and Dong, 2017; Thomitzek et al., 2019b; von Drachenfels et al., 2021; Wessel et al., 2021; Li et al., 2014; Shu et al., 2021; Kim et al., 2016) are based entirely on primary data and modeled with the B–U approach. However, only four of those studies (Degen and Schütte, 2022; Wang et al., 2017; Li et al., 2014; Shu et al., 2021; Kim et al., 2016) are LCAs, making a total of only 8% of the LCA studies examined meeting the stated requirements. Moreover, two of these studies are investigating novel cell chemistries: Li et al. (2014) investigate a LIB with a silicon Nano-wire anode on pilot scale, whereas Wang et al. (2017) investigate a battery with Li-rich cathode from lab to industrial scale. The LCA study of Degen and Schütte (2022) considers only environmental burdens arising from direct energy consumption during cell manufacturing, excluding materials.

Accordingly, there are only two LCA studies (Shu et al., 2021; Kim et al., 2016) using both, primary data and a B–U approach to examine a mature battery technology. Particularly at the laboratory level such a study would be important in order to evaluate scale-up effects and to apply them to prospective LCAs of emerging battery technologies. Hence, the following LCA for LIB cell production at lab-scale aims at closing this existing gap. Own primary data, obtained by in-house measurements, provide the basis for this analysis.

3. LCA of lab-scale LIB cell production

The expressed need for lab-scale LCAs led to the conduction of an own assessment described in the following. The LCA methodology underlying this work is defined by the ISO standards 14040/14044 (ISO 14044:2006, 2006). LCA is a standardized method analyzing environmental aspects as well as impacts of a product, system or service throughout its whole life cycle. Thereby, the LCI of this work underlies major principles of MEFA which investigates energy and material inputs to a system, flows within that system, and outputs of that system (Hendriks et al., 2000), and can be controlled by simple mass balancing (Ayres and Ayres, 2002; Brunner and Rechberger, 2004; Fischer-Kowalski, 1998).

3.1. Goal and scope definition

The major goal of this work is to identify environmental hotspots associated with the production of a lab-scale LIB cell production, based on primary data for each production step, partly gained by in-house measurements employing a bottom-up approach. Because the assessment is centered on a battery already existing in the market, an attributional instead of a consequential LCA is conducted, as the latter tends to focus on prospective market changes (Ekvall et al., 2020). By comparing the environmental impacts with those of industrial LIBs covered in the literature review, the effect of production scales on the LCA results is additionally discussed. The results of this study shall enable the retrospective investigation of scaling effects, which in turn can be applied to emerging batteries. Hence, the results of this work are of high relevance to LCA practitioners in the battery field but also to battery developers alike. The investigated battery is the KIT 20 pouch cell fabricated in the Battery Technology Center (BTC) at the Karlsruhe Institute of Technology (KIT). One single cell weighs 0.54 kg, has a rated capacity of 20 Ah, and a nominal voltage of 3.7 V delivering a gravimetric energy density of 141 Wh/kg. The cell consists of the active materials NMC111 for cathode and graphite for anode, Polyethylene terephthalate based separator, 1 M $LiPF_6$ in EC/DMC (1:1) wt% + 3%

VC electrolyte and dimensions of 179 mm × 236 mm x 7.4 mm (Karlsruhe Institute of Technology, 2020). Additional information on the cell, such as charge and discharge characteristics or cyclization data, can be found in the data sheet provided in the SI. The functional unit is 1 Wh of cell energy capacity. Sensitivity analyses are carried out for different electricity mixes, different loss rates and dry room throughput rates. In addition, different scenarios, consisting of combinations of those three parameters, are performed emulating the effects of upscaling production. Given that most other studies reviewed have assessed the environmental footprint of the batteries on the pack level instead of the cell level, it also becomes necessary to extend the system boundaries of the system herein presented in order to ease comparability with literature. A generic battery pack composed of the KIT 20 cells and additional components such as battery management system (BMS) and housing is additionally modeled, followed by a calculation of its life cycle impacts. Lastly, a comparison of the latter against those in other studies shall ease the interpretation and validation of the results obtained.

3.2. System boundaries

The cradle-to-gate analysis considers the pre-chain of precursor materials (i.e. raw material extraction and processing), as well as the cell manufacturing itself, while excluding use- and End-of-Life- (EoL) phase which, however, has been investigated already in other studies (Mohr et al., 2020c; Peters et al., 2019). The manufacturing process of the KIT 20 cell has been previously described in detail by Erakca et al. (2021) and is summarized in Fig. 7. A more comprehensive view, illustrating the precise material, energy and waste flows can be found in Fig. S1 and Table S2 of the SI.

After mixing the respective slurries for cathode and anode, the Aluminum and Copper current collectors are accordingly coated and dried in a two chamber oven, with temperatures of 80 °C in 120 °C in the first and second chamber respectively, with an average coating speed of 0.36 m/min. The electrodes are then calendered, separated and stacked. The cell stack is dried in a vacuum dryer afterwards, which is located in the dry room to ensure low humidity levels while transporting the vacuum dried sheets into the packing stage. For the specific case, the conditioning system of the dry room remains switched off during vacuum drying and it is switched on as soon as the transportation to the next step begins. The 100 m^2 sized dry room has an ambient temperature of 22 °C and a dew point temperature of −70 °C. In the following step, the cell stack is packed in a pouch bag and sealed, followed by electrolyte filling. The cell is then formatted in an air-conditioned room ensuring there is no significant heat evolution during this process. A degassing stage in the dry room follows next where the gas pocket attached to the cell is pierced and cut off. At the BTC, slitting and roll pressing, which are optional steps in pouch cell production, are excluded. Also, aging and End-of-Line testing are not performed. Thus, the analysis is carried out until the end of degassing step. As mentioned before, the analysis of the battery pack demands for an extension of the system boundaries to account for the pack assembly process and additional pack components, which is described in detail in the corresponding section 4.3.

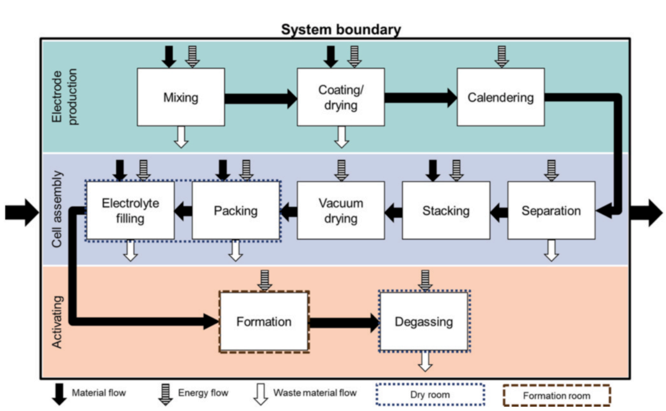

Fig. 7. System boundaries and considered production steps.

3.3. Assumptions and limitations

This study gives continuity to the work by Erakca et al. (2021) where an EFA has been presented and is complemented with further on-site measurements during the fabrication of the KIT 20 cell. Due to its laboratory character, there are differences in the KIT 20 cell production process when compared to large scale LIB manufacturing, mainly related to the production volumes and associated specific material and energy demand. A theoretical production capacity of four cells per day has been estimated based on direct observation of the facilities and equipment as well as on dialog with the personnel in charge. With 280 working days per year, this corresponds to a production volume of 1120 cells or 85 kWh. This annual volume could potentially characterize a small pilot scale plant. However, low process efficiencies, high material loss rates, abundance of manual steps as well as poor process interconnectivity have led to the classification of the production level as lab-scale. Data collection and cell production were staggered rather than chronological. The KIT 20 electrodes are in reality purchased, meaning that the measurements related to mixing, coating, drying and calendering are separately performed at another laboratory. It is assumed, nevertheless, that these processes are directly connected to the investigated production line. Moreover, the energy and material flows for cathode mixing, coating, and drying, as well as the waste cathode slurry were initially measured for the chemistry NMC622. The material data was later on adapted to reflect the proportions of NMC111 cathode material. According to an interview with an expert in the field, it is reasonable to use the same energy data, since different NMC chemistries require very similar amounts of energy during the mixing process. Likewise, similar densities are reported for NMC111 (4.7 g/cm^3) (Cerdas et al., 2018) and NMC622 (4.76 g/cm^3) (Zhu et al., 2019) leading to the assumption that the NMC111 slurry waste is the same as the measured value for NMC622. Since no measurements were performed for anodes, its energy requirement is assumed to be 15% less than that of cathodes (Erakca et al., 2021). The amount of cathode and anode slurry on the electrodes is calculated based on weight differences between samples with coated and uncoated Aluminum foil, which are subsequently scaled-up according to the electrode area. The energy data for the dry room is based on load values for a month (May 2019) in which it was used intensively. The difference of the load values of the entire building for days with switched-on and switched-off dry room are identified, yielding in an operation power of 64.8 kW (Erakca et al., 2021). Cell formation is based on own calculations, where the energy supplied during the three-staged cyclization is added to the cycler's own energy requirement. Energy for preheating or system start-up as well as waste material are included in all necessary steps and distributed among the number of cells produced. Assumptions made for the transportation and infrastructure analysis can be found in Table S3 in the SI. A detailed description of the modeling for the battery pack is provided further in this document.

3.4. Data sources

The baseline model has been built considering input of electricity from the German mix for the year 2019 with 46% fossils as reported by AG Energiebilanzen e.V. (AGEB) (AG Energiebilanzen, 2022). Moreover, a scenario with the average European electricity mix (ENTSO-E as presented in Ecoinvent V3.7.1) and a hypothetical scenario with 100% renewables (consisting of 50% solar and 50% wind energy) are presented. A detailed composition of the inventory data for the electricity mix can be found in Section S3 of the SI. The background data for pre-chain processing, transportation, infrastructure and production waste treatment is extracted from Ecoinvent V3.7.1 (cut-off, unit). In addition, inventory data extracted from Peters and Weil (2018) is used for the modeling of battery cell materials. Specifically, this relates to the inventory data for the production of NMC, current collectors, separators, and cell tabs, which the respective authors modified based on Ellingsen et al. (2014). PVDF and SBR binder are based on Bauer et al. (2015) and Zackrisson et al. (2010) respectively. The estimation of energy demand is based on the analysis for the KIT 20 cell provided by Erakca et al. (2021) and supplemented with own energy data for mixing, separation, and stacking as explained in detail in the previous section. A detailed description of the energy measurement procedure, including details of the measurement device, assumptions and operation conditions can also be found in the Supplemental Information provided by Erakca et al. (2021). The MEFA follows the bottom-up modeling approach, where the demand for each step of cell production is analyzed according to the respective operating conditions. The data is controlled and validated using mass and energy balances to ensure the law of conservation throughout the entire manufacturing process. The complete inventories are provided in Tables S9–S45 in the SI.

3.5. Modeling approach

The LCA is modeled and performed in the software openLCA version 1.10. Default providers are chosen for the processes, with 'unit processes' as preferred process type. Due to its scope and retention of all aspects to be investigated, the International Reference Life Cycle Data System (ILCD) as provided by the European Commission is chosen for the Life Cycle Impact Assessment (LCIA). The exact method is the ILCD 2011 Midpoint + which is provided in the LCIA method package 2.1.1 by the consultancy and software development company Green Delta (GreenDelta GmbH, 2022). Given that the full LCI is provided in the SI, the LCA can be remodeled using a different LCIA method if desired. According to the recommendations of the Product Environmental Footprint Category Rules for rechargeable batteries by the European Commission (European Commission, 2020), the most relevant impact categories for the study of battery systems are acidification (terrestrial and freshwater), climate change, resource use (energy carriers and minerals) and respiratory inorganics. These categories can be found within the ILCD Midpoint methodology labelled as 'acidification', 'climate change', 'mineral, fossil and renewable resource depletion' and 'particulate matter' respectively. Therefore, these categories are explicitly addressed in the analyses of this study. As already mentioned, a bottom-up approach has been chosen, therefore, each cell manufacturing process was modeled separately and interconnected as the manufacturing chain is modeled with a MEFA oriented approach. Thus, the output of a process is an input for the next one. All measured inputs and outputs of the foreground system are calculated for 1 Wh of cell energy storage. Inventory data for precursors from other literature sources are allocated as indicated in the original source. No internal recycling is considered in the modeling (however, secondary materials are implicitly included via 'market processes' within Ecoinvent), thus all production loss and waste are assumed to be incinerated. The production waste is modeled with an output oriented approach: material and energy inputs are as measured and fixed, whereas the output waste is variable and can be modified for different loss rates when necessary. Transportation inputs are included in each step separately, whereas infrastructure and the total energy consumption of the dry room have been considered in a final stage. The latter eases the analysis of the effects of different throughput rates for the processes taking place in the dry room. Given that the system is composed only of single-output processes, no allocation is necessary.

A study of the effects on the environmental footprint produced by using different electricity mixes as well as by changing other production parameters, such as loss rates and throughputs, has been performed by means of a sensitivity analysis in chapter 4.2. The modeling of the battery pack can be seen as an extension of the previously described system to incorporate further components and to account for the effects of additional mass shares on the energy density and the system's impacts. Further details of this process can be found in chapter 4.3.

4. Results and discussion

In the following the LCA results for the KIT 20 battery cell and a theoretical battery pack will be presented. The analysis of results and further discussion herein presented will be focused on the categories 'acidification', 'climate change', 'mineral, fossil and renewable resource depletion' and 'particulate matter' respectively. A complete view on the results for all sixteen categories of the ILCD method can be found in Table S8 of the SI.

4.1. Baseline model

The baseline conditions for cell manufacturing on laboratory level have been presented in previous sections. A lab-scale production line fed with electricity from the German grid, characterized by low throughputs and high specific material and energy demand leads to the results observed in Fig. 8. A breakdown of the contributions from each production stage eases the identification of the most relevant hotspots in each impact category.

It becomes clear that the operation of the dry room, the most energy-intensive process, is the main contributor to the total impacts in three of the four categories. It accounts for about 56%, 79% and 48% of the emissions in 'acidification', 'climate change' and 'particulate matter', respectively. Its contribution is less significant in 'resource depletion', accounting only for about 6% of the total. Significant contributions from anode coating/drying and cathode mixing are also found in every category. The pre-chains of these two processes are in fact the main drivers of 'resource depletion', contributing approximately 42% each to the total impacts. In particular, Copper mining for the anode current collector and Cobalt extraction for the cathode active material have the largest influence. The emissions of Nitrogen oxides and Sulphur dioxide arising from the demand of fossil based German electricity, especially high for the dry room, have the largest influence in 'acidification'. Similarly, Carbon dioxide emissions from the same energy mix are the determining factor for 'climate change'. Small particulates and Sulphur dioxide emitted along the pre-chains of Copper for the anode current collector and of the cathode active material, as well as during the burning of fossil fuels (hard coal and lignite) within the electricity production are the most relevant agents in 'particulate matter'.

In addition, high loss rates during fabrication are reported mainly due to lab character of the investigated manufacturing process. The average loss rate for the slurries, Copper, and Aluminum foil is of about 54% material, which is considered as a main driver of environmental impacts. It is expected that under conditions of large scale production with higher efficiency, material loss and the associated environmental

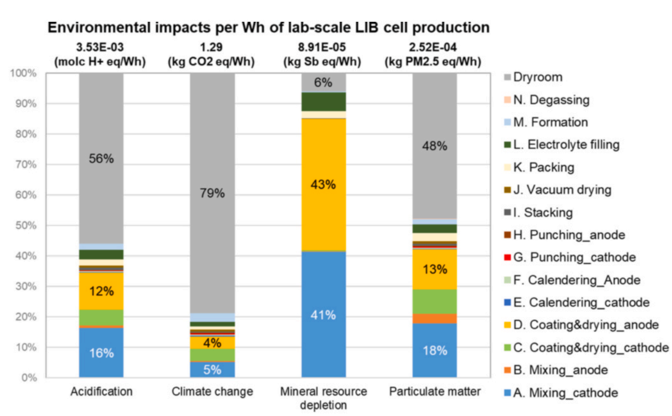

Fig. 8. Environmental impacts per Wh of lab-scale LIB cell production for the selected impact categories.

burdens can be reduced significantly.

Several reasons lead to the substantial electricity demand for the dry room. The first and main factor being the throughput (4 cells/day), which is very low due to the lab-scale production. Additionally, for a throughput of four cells per day, the dry room area (100 m^2) at BTC is over-dimensioned. Moreover, the specific room operates at a dew point temperature of −70 °C, well below the −60 °C to −40 °C used in industry (Thomitzek et al., 2019b). It is recognized that an increase of the throughput could lead to a considerable reduction of the dry room energy consumption and consequently of the environmental impacts. Although the dry room as a single unit has the largest impact on 'climate change', at approximately 87%, the impact is determined by the aggregate energy demand along the entire production line. This is highly influenced by the underlying energy mix of the production line, which in this case relates to the German grid which still contains a high share of fossil fuels.

4.2. Sensitivity analysis

The analysis so far relates to a battery system fabricated using non-optimized manufacturing methods, characteristic of lab-scale production. It is of interest to understand the potential effects that changing certain conditions, i.e. energy mix, material loss rate and throughput, may have on the calculated footprint of the battery cell. Sensitivity to energy mix is of interest in the context of ongoing global efforts to decarbonize the energy sector, while material loss rate and throughput are influenced by production scale and efficiency. This chapter describes a simplified yet practical approach that illustrates the sensitivity to a dynamic environment in which the use of energy and material resources becomes more efficient, as it is expected with the introduction of economies of scale and increased penetration of clean energy sources. In real life, these dynamics are complex and may require an iterative analysis that takes into account the potential introduction of new variables (e.g. expansion of infrastructure, local increase of power demand …) not considered in the baseline study. However, despite the large degree of uncertainty involved, a simplistic view is deemed as sufficient to understand the basic principles and potential of scale-up techniques.

4.2.1. Energy mix

The rapid evolution of electricity markets leads to quick obsolescence of some data sets contained in commercial databases, most of which are used for background system modeling. For such reason, it was necessary to substitute the inventories for German electricity production as found in Ecoinvent 3.7 (for the year 2017) with a more recent dataset (German mix in 2019) to provide a more up-to-date discussion of results. To ensure consistency, the same dataset structure for electricity production considered in Ecoinvent has been maintained, given that this database is still used for most other background processes in our system. This structure establishes three different voltage levels (high, medium and low) at which different types of generation technologies supply electricity to the grid. In particular, it stipulates that the electricity used in industry and modern laboratories is extracted at the medium voltage level, which also neglects the production from photovoltaic (PV) systems as these are considered to supply only on the low voltage level (Ecoinvent. https, 2022). In the real world, however, it is possible that large PV installation will supply electricity in the medium voltage level.

Fig. 9 shows the percentage composition of the German mix in 2019 as considered for the baseline modeling for the supply of electricity. This energy mix contains a share of about 46% of fossil fuel based electricity which, combined with the dismissal of medium level cleaner generation technologies such as PV systems, leads to high specific greenhouse gas emissions and to the previously observed climate change potential.

Assuming that the described battery manufacturing processes could potentially be reproduced and/or scaled-up in any geographical region but also at any point in time, it becomes of interest to determine the sensitivity of a battery cell's footprint to a changing electricity mix. Two additional scenarios have been modeled to assess such sensitivity: the first scenario assumes that cell production is made with the average European electricity mix (ENTSO-E as presented in Ecoinvent 3.7.1 and illustrated in Fig. 9); the second scenario is a hypothetical model using renewably sourced electricity with a default share of 50/50 from solar and wind energy as these are the fastest growing technologies in the market (International Energy Agency. Renewables, 2021, 2021). In real life, however, the decarbonization of the grid will likely be achieved by integrating a broader set of technologies most suitable to the conditions of a specific area (Ram et al., 2019). The results for the four selected impact categories are displayed in Fig. 10.

Considerable deviations from the baseline can be observed in every category when substituting the electricity mix. The 'acidification' potential undergoes an increase of about 53% with respect to the baseline when using the average European mix, whereas the use of renewables leads to a reduction of about half the initial value. The increase in the EU scenario is attributed to greater emissions of Sulphur dioxide, linked to coal power generation mainly from Poland and Spain according to the reported mix from Ecoinvent 3.7. The sensitivity in 'climate change' displays a reduction of about 20% for the EU scenario and drastically drops in the renewable scenario, descending to about 20% of the baseline value. The CO_2 intensiveness in both scenarios is fairly lower than for the German case. Although the absolute intensity of fossil fuels is similar in the German and European grid (~46% and ~43%, respectively), electricity generation from lignite is higher in Germany and therefore more carbon intensive. 'Resource depletion' remains

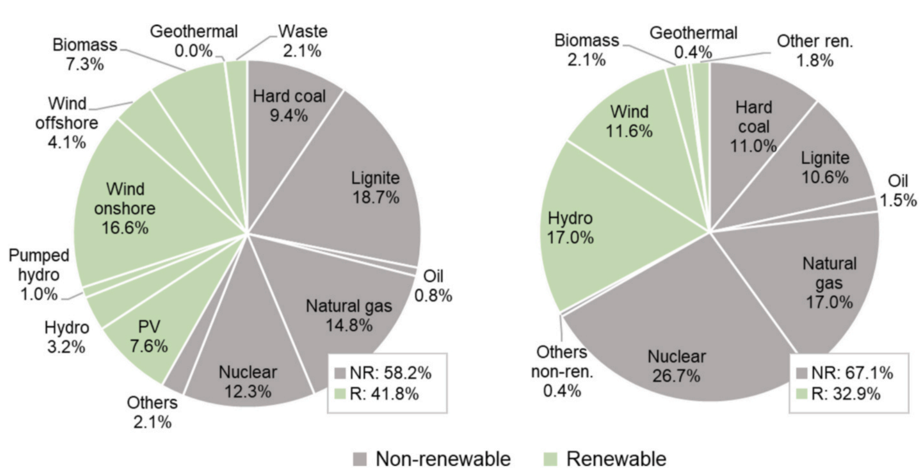

Fig. 9. Composition of the electricity mix for Germany for the year 2019 as reported by AGEB (left) and of the ENTSO-E electricity mix in Ecoinvent 3.7.1 for the year 2017 (right).

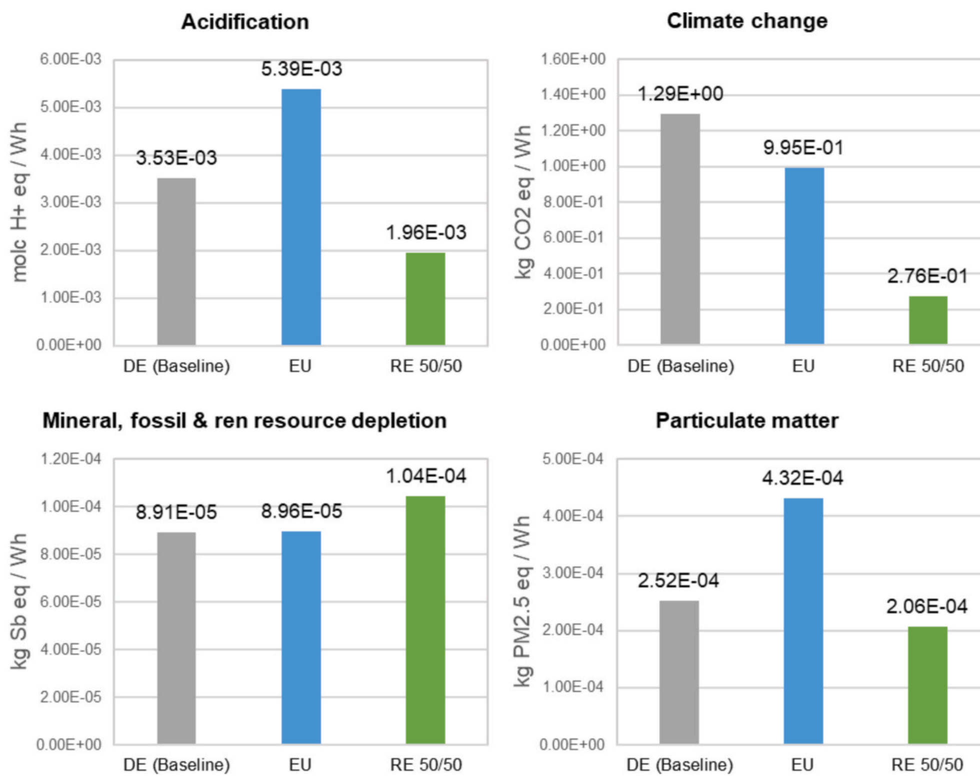

Fig. 10. Sensitivity to electricity mix for the selected impact categories.
DE = German mix 2019 as reported by AGEB, EU = ENTSO-E mix 2017 as provided in Ecoinvent 3.7.1,
RE 50/50 = hypothetical renewable mix with 50% solar and 50% wind energy.

approximately the same with EU electricity but has a 17% increase when renewable energy is used. This increase is attributable to the broader use of silver associated with the manufacture of solar modules, as well as the use of other valuable metals in the required inverters for both PV and wind systems. The International Technology Roadmap for Photovoltaic states, however, that the silver content in the modules has been gradually reduced, and that this trend is expected to continue over the next years (VDMA. International, 2021). Therefore, the influence of PV systems on 'resource depletion' could become less significant. On the other hand, the eventual demand increase of permanent magnets for wind turbines, not yet fully characterized in the database, might raise concerns in this category. In 'particulate matter', an increase of 70% and a decrease of 18% can be observed for the EU and RE 50/50 scenarios respectively. Similar to 'acidification', power generation systems in Serbia, Poland and Spain are associated to large release of particulates and Sulphur dioxide into the atmosphere (Ecoinvent 3.7.1).

4.2.2. Loss rate

The baseline model includes an average loss rate for the slurries, Copper and Aluminum foil of almost 54%. These losses occur mainly during coating, drying and punching. In the coating and drying step, rips in the foil frequently occur due to the laboratory character of the process requiring its disposal and the re-clamping of new electrode foil. In addition, coating parameters need to be adjusted during the beginning of the coating process making the sections of coated foil prior to the desired configuration not suitable for further use. Unlike most processes at industrial scale, punching at the lab-scale is not optimized for maximum resource efficiency. This leads to large sections of the coated film being cut out without further recycling or reuse. A sensitivity analysis is carried out considering different levels of material loss in an attempt to emulate the effects of implementing optimized manufacturing techniques which should, allegedly, lead to improved resource efficiency. Fig. 11 illustrates the sensitivity to different material

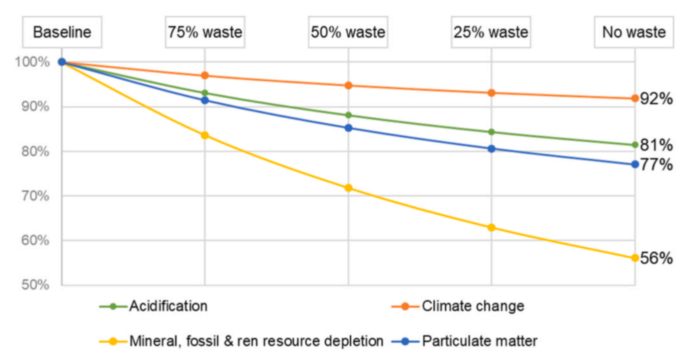

Fig. 11. Percentage variation of environmental burdens under different material loss rates.

loss rates in the four assessed impact categories. These can be read either as absolute loss rates of 40.5%, 27%, 13.5% and 0% (compared to the baseline loss rate of 54%) or as relative 75%, 50%, 25% and 0% with regard to the baseline value.

A moderate sensitivity can be observed in the impact categories 'climate change', 'acidification', and 'particulate matter', with impacts potentially decreasing down to 92%, 81% and 77% respectively with regard to the baseline if no material is wasted. In general, reduced material consumption leads to lower energy demand and process emissions originating in the pre-chain of such materials. A greater potential lies in 'resource depletion', where more significant reductions can be expected. A relative reduction of 25% of the initial loss rate, will already lead to a drop down of the impacts to about 84% of the baseline, reaching a minimum value of about 56% as the theoretical limit in the ideal no-waste scenario. This larger influence can be explained when considering the decreasing demand for Copper and Cobalt, which in fact are the largest contributors due to their consistently high impact characterization factors in this category.

4.2.3. Dry room throughput variation

The research focus of lab-scale operations, resulting in smaller production volumes, ultimately results in diminished interest for material and energy optimization techniques in this stage. Thus, the underlying low utilization rates of equipment prevail, leading to high specific energy consumption during their operation. As a consequence, a product fabricated under such conditions will normally entail an environmental footprint larger than that of the same product manufactured at an industrial level (Ellingsen et al., 2014). Given that the operation of the dry room has been identified as the main contributor in most impact categories, the sensitivity to the throughput rate in this stage is the focus of analysis. Initially estimated for a production volume of four cells per day (baseline), the environmental profile of the KIT 20 cell is recalculated for different throughput values in the dry room, ranging from five to 500 cells per day as seen in Fig. 12.

A decrease of the contributions arising from the operation of the dry room becomes evident in every category, with a steep reduction in the range between five and 50 cells produced per day. This behavior is especially noticeable in 'climate change', where the relative impact reduction in this range is of about 67%. In the categories 'acidification' and 'particulate matter', the percentage reduction of the impacts in the same range is of about 50% and 42% respectively. The slope of this decrease becomes less significant in the range between 50 and 500 cells per day in these three categories since the contributions of the dry room no longer play a relevant role. For the specific case of 'resource depletion', the total impacts remain approximately constant at all throughput rates given that the operation of the dry room entailed low contributions even at low production volumes (about 5% in the baseline analysis).

4.2.4. Optimistic scale-up scenario

It is of interest in this research to understand the dynamics between production scale and environmental footprint for the studied cells and to estimate the degree of influence that the first has on the latter. The lab-scale manufacturing conditions established in the baseline analysis characterize a battery cell whose environmental performance at this level shall not be used as a market benchmark. This means that a comparison with market-established counterparts, most often manufactured in large volumes, will only illustrate the potential lying within upscaling techniques. Shifting cell manufacturing to a more favorable industrial environment would transform its footprint, but the potential magnitude of this effect remains uncertain. To address this uncertainty, a theoretical scenario aiming to reflect ideal larger scale production while also using energy inputs from renewable sources has been modeled. In particular, this scenario is characterized by a throughput of 400 cells per

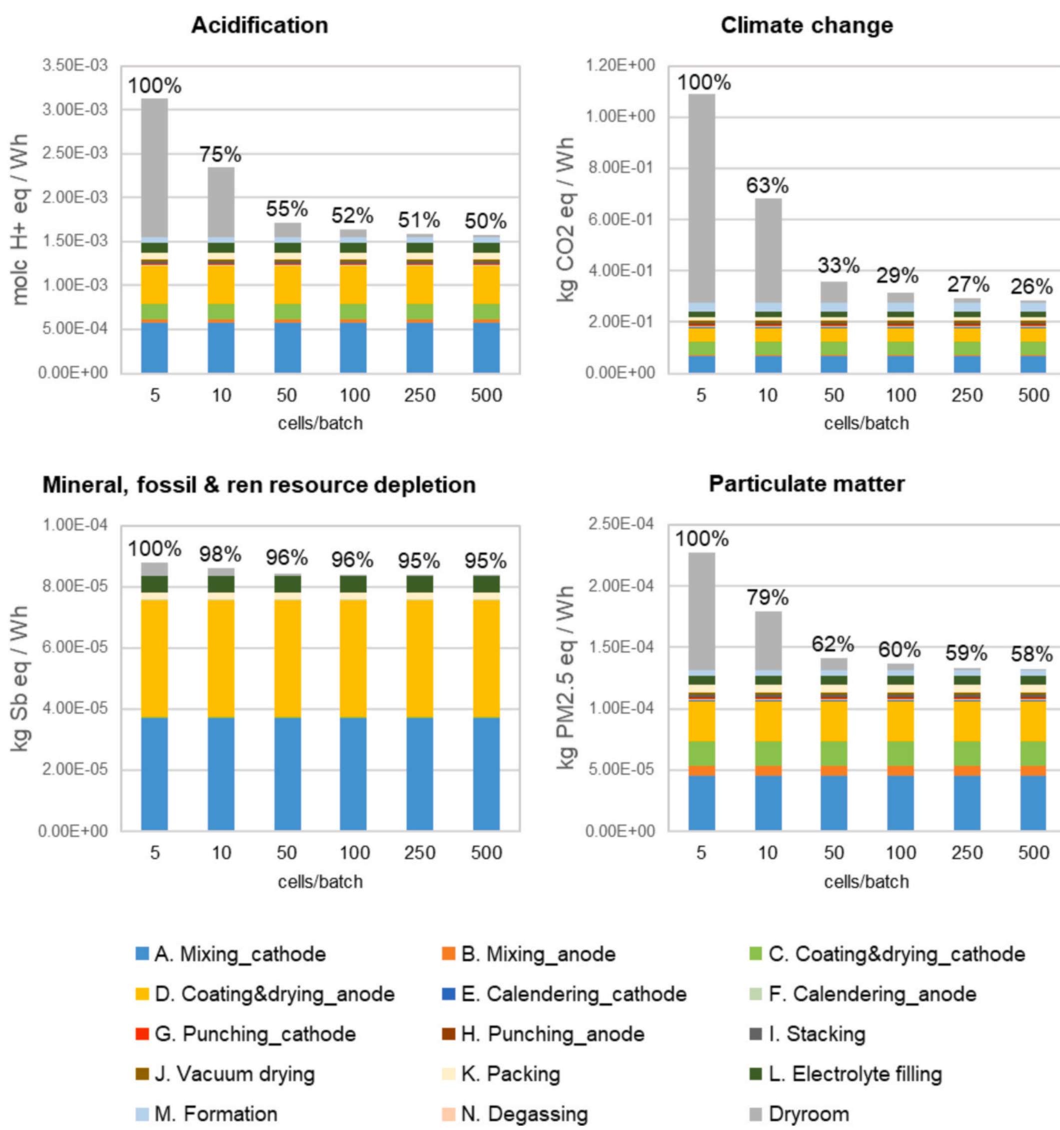

Fig. 12. Sensitivity to dry room throughput.

day in the dry room, 8% loss rate (value from an industrial scale LIB manufacturer (Pettinger and Dong, 2017)) and electricity from solar and wind power systems (50/50 ratio). Fig. 13 displays the percentage variation of the environmental impacts between the baseline and this model scenario. It is worth noting that, while this scenario intends to provide insight of the effects of upscaling, the use of electricity exclusively from renewable sources grants it an optimistic character. The results shall be interpreted on an indicative level, providing only a picture of the potential room for improvement between different production scales in the context of an energy transition towards high penetration of renewables systems. With a minimum potential reduction of about 44% in 'resource depletion' and a maximum drop of about 92% in 'climate change', the magnitude of the upscaling effects becomes clear. The effects of lower specific energy demand per Wh achieved with higher throughput rates in combination with the low pollutant and greenhouse gas emissions of electricity from renewable sources lead to a critical reduction in three out of four categories. The potential decrease in 'resource depletion', albeit significant, remains driven by the influence of lower material loss rate.

4.3. Analysis of battery pack

In previous sections, the environmental performance of a battery pouch cell, namely KIT 20, has been described. While the obtained results allow drawing a set of conclusions on their own, a direct comparison with other results found in literature is not suitable. In particular, the system boundaries in most LCAs from literature describe a battery pack comprising not only the cells but also additional components such as the BMS, external housing and, in some cases, even a cooling system. This entails additional material and energy flows that consequently lead to changes of the environmental burdens. In addition, due to the changing mass composition, the energy density of the system must be recalculated. Ultimately, these effects are reflected in the product's footprint. In order to ease a fairer comparison with literature, it becomes necessary to extend the boundaries for the production of the KIT 20 cell to account for the additional impacts associated to the manufacturing of a full battery pack.

4.3.1. System description

Within the framework of this study, primary data acquisition is possible only for the production of cells. Therefore, secondary sources to complement the modeling of the battery pack are resorted. The unified inventories described by Peters and Weil (2018) have been implemented since these ease comparability with other studies. For a theoretical battery pack with a composition per unit of mass of 76.7%, 4.7% and 18.6% for cells, BMS and housing respectively, the energy density is of about 108.15 Wh/kg.

The extension of system boundaries for the manufacture of the battery pack is illustrated in Fig. 14. A cradle-to-gate analysis is carried out, starting from energy conversion and raw material extraction throughout the production of the whole battery pack, including the previously described KIT 20 cell production. The use- and EoL phase of the pack are not considered.

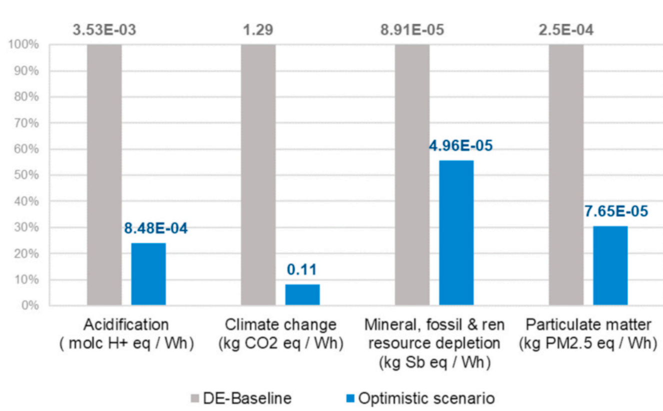

Fig. 13. Comparison of baseline model vs optimistic scenario with electricity from renewables and zero loss rate.

4.3.2. System analysis

Ellingsen et al. (2014) found that the impacts of energy demand for pack assembly are minimal. In addition Dai et al. (2019) assumed the assembly to be a manual process, entailing no significant additional environmental burdens. Consequently, the energy demand of pack assembly in this study is also assumed to be zero. Fig. 15 displays the aggregated environmental impacts of the battery pack for the four different impact categories 'acidification', 'climate change', 'mineral, fossil and renewable resource depletion' and 'particulate matter', distinguishing the contributions from the main components (cells, BMS and housing) as well as other contributor factors (i.e. transport and infrastructure). Thereby, the baseline lab-scale scenario with German electricity mix as well as two scale-up scenarios, representing a pilot scale battery production are analyzed. Both scale-up scenarios are characterized by a dry room throughput of 400 cells per day and a loss rate of 8%, but are different in terms of energy mix, using the German and European energy mix respectively as shown in Fig. 9.

Unsurprisingly, the contributions from the cells dominate the impacts in every category regardless of the scenario assumed. Reasons for this are the intrinsic criticality of the cells accounting also for a large share (77%) of the total weight of the battery pack. In addition, significant contributions from the BMS can be found, particularly in the impact category 'resource depletion'. This is greatly influenced by the consumption of Tantalum for the electronic components within the BMS. Likewise, the energy demand and associated emissions for the prechain of these electronics lead to considerable impacts in the remaining categories. However, considerable reductions, in all categories are obtained by the scale-up scenarios, especially striking for the climate change potential. Compared to the lab-scale baseline scenario, a maximum impact reduction of about 84% and 86% can be observed in the DE and EU scale-up scenarios respectively.

4.3.3. Comparison with literature

In order to gain broader understanding of the environmental performance of the modeled KIT 20 battery pack, a comparison with literature values is drawn in the following. Fig. 16 illustrates the climate change potential for battery pack production, expressed in CO_2-eq. per Wh battery storage capacity, as found in several literature sources. Climate change potential has been chosen as the impact category to be analyzed, since it is the most frequently reported value. A distinction of the production scales (laboratory, pilot and industrial) is made. Whenever identifiable, the annual production volume is indicated in descending order on the vertical axis. The average magnitude of each production scale has been represented with a cross. In addition, the energy modeling approach is considered by representing values stemming from T-D approach with triangles, B–U approach with circles and mixtures or unclear approaches with diamonds. The different cathode chemistries used in the studies are indicated in the legend.

Four different scenarios associated to the KIT 20 battery are considered: Baseline-DE scenario (DE-energy mix, 4 cells/day dry room throughput, 54% loss rate), Baseline-EU scenario (EU-energy mix, 4 cells/day dry room throughput, 54% loss rate), scale-up-DE scenario (DE-energy mix, 400 cells/day dry room throughput, 8% loss rate) and scale-up-EU scenario (EU-energy mix, 400 cells/day dry room throughput, 8% loss rate). Overall, 13 reported values have been identified.

Only two values for lab-scale LIB production have been reported, deriving both from this case study. However, a significant difference of 23% can be observed between the values with German and European energy mix, which is in line with the investigation in chapter 4.2.1 due

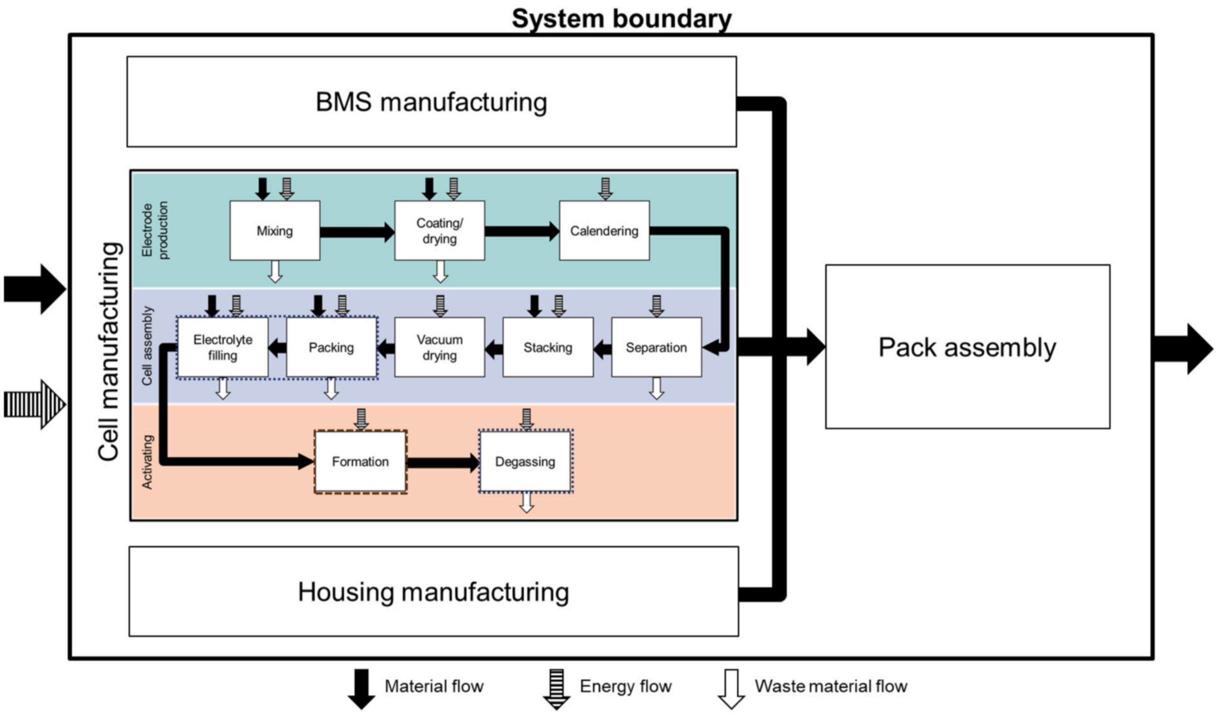

Fig. 14. System boundary for the analysis of the battery pack.

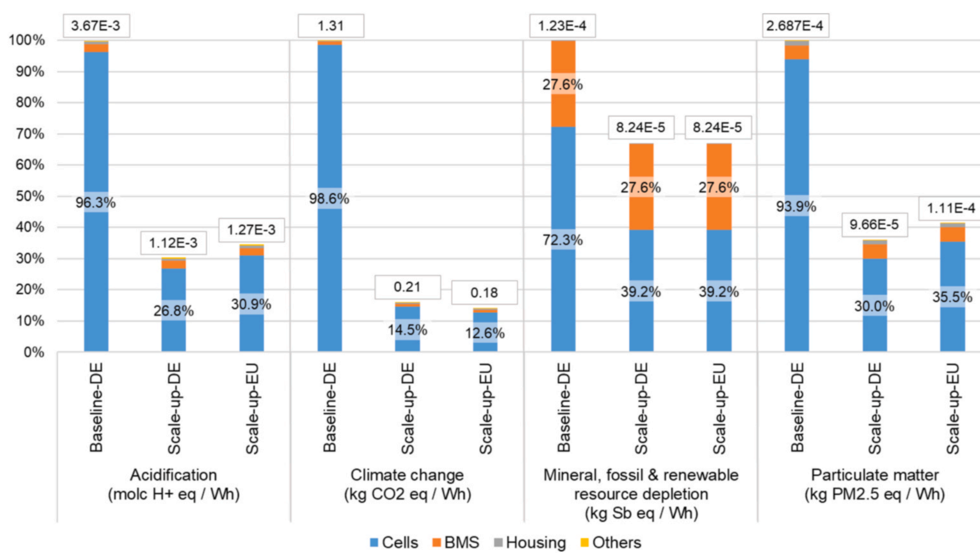

Fig. 15. Environmental profile of the KIT 20 battery pack.

to the lower CO_2 intensiveness of the European energy mix compared to the German one.

At the pilot scale, a total of three values have been determined, of which two are the scaled-up scenarios for the KIT 20 battery of this study and another for a battery cell fabricated using the German electricity mix (von Drachenfels et al., 2021), however, without indicating the production volume. Given that the reported value is on the cell level, it was necessary to aggregate the impacts of the remaining components of the battery pack used in that study on top of the cell value, resulting in a comparable climate change potential as for the lab-scale scenario of this study.

With a set of eight values, the majority of the studies are on an industrial scale (Chordia et al., 2021; Dai et al., 2019; Ellingsen et al., 2014; Philippot et al., 2019; Sun et al., 2020; Shu et al., 2021; Kim et al., 2016; Crenna et al., 2021). Thereby, the production volumes are ranging from 56 MWh up to 34.8 GWh. The differences in the results among the varying industrial scale studies are small and could likely be absorbed within the uncertainty range of each study. In addition, different cell types such as pouch (Ellingsen et al., 2014; Sun et al., 2020; Kim et al., 2016), cylindrical (Chordia et al., 2021; Philippot et al., 2019) and prismatic (Dai et al., 2019; Crenna et al., 2021) cells but also diverse cathode chemistries were used in the battery packs of these studies. Moreover, the potential influence of using different background databases and impact assessment methods on the study results has not been assessed. For a more robust comparison, it would be advisable to remodel the LCIs of the studies using a common background database and to recalculate the LCA using a common impact assessment method. Potential effects of the diverse energy modeling approaches (T-D, B–U,

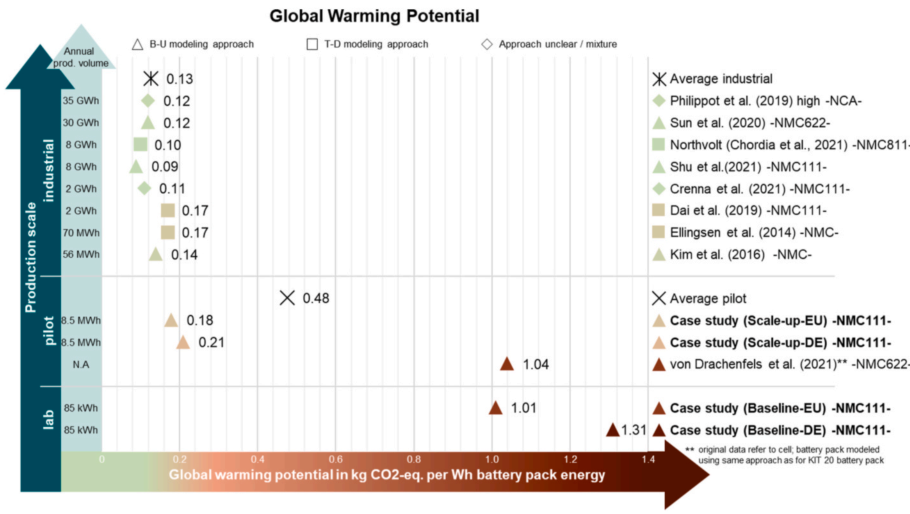

Fig. 16. Global warming potential in CO2-eq. per Wh battery storage capacity for different LCA studies on varying production scales.

mixture/unclear) could correlate with the differences between the study results. At first glance, the values of the industrial scale studies using B–U approach seem to yield slightly smaller results than those using an unclear or T-D approach. However, the closeness and irregular distribution of the results within the industrial scale, as well as the overall small number of studies, does not allow for a clear and reliable conclusion. Besides, this impression changes insofar as the results of all production scales are considered. Although all studies at the lab and pilot scales use the B–U approach to model cell production energy demand, some of the results are an order of magnitude larger than those at industrial scale using the T-D approach.

It has been demonstrated in previous sections that the environmental footprint of battery cells is heavily influenced by the volumes and scale of production. Naturally, this effect also persists at the pack level and is particularly evident at the lower range of the production volume, namely from lab to pilot scale. This becomes clear when comparing the baseline scenario with the scale-up scenarios of this study. Thereby, the climate change potential could be reduced by 83% when increasing the production volume from four to 400 cells per day. As previously described, switching from German to the less CO_2 intensive European energy mix would lead to a comparatively lower reduction of 23%. Simultaneously, it is expected that the benefits obtained by increasing the production scale gradually become less significant and down to negligible as the production volume increases, thus setting a lower limit for the environmental impact of the battery. Therefore, it is not surprising that the highest value of 1.31 kg CO_2-eq. per Wh is found at the lab-scale for the baseline scenario of this study with German electricity mix, whereas the lowest value of 0.09 kg CO_2-eq. per Wh, which is 93% lower than the lab-scale value, belongs to a Gigawatt scale battery production (Shu et al., 2021). The scale-up scenarios of this study, corresponding to higher pilot or even small industrial manufacturing, lead to results very similar in magnitude to other reported values in the industrial scale, underlining the diminishing impact of the production scale on the LCA result after a certain volume. This trend can also be observed in Fig. 16 when looking at the full range of different production scales and volumes and the already mentioned similarity of the industrial scale results. It seems that the production scale and volume up to a certain point has a much higher, if not the highest, impact on the results. Nevertheless, as shown in the literature review, there are numerous studies lacking information on production scale or volume, which would, however, be indispensable for a valid evaluation as well as reliable comparison of LCA results.

4.4. Relevance of production scales in environmental assessments

The influence of the production scale on the environmental performance of a product should be assessed, in particular, when conducting prospective LCAs for developing technologies. Anticipating the environmental impacts of an emerging technology, not only at the laboratory level but at larger scales as well, allows for a pre-evaluation of the compliance with existing environmental policies and legislations, and enables early reorientation and design improvements towards a more sustainable profile of the technology (Cucurachi et al., 2018; Moni et al., 2020; Tsoy et al., 2020). At the same time, the uncertainty surrounding the technical performance and the manufacturing methods of novel technologies, especially at larger production scales as often only lab-scale manufacturing data is available, represents a challenge when performing prospective LCAs (Moni et al., 2020; Tsoy et al., 2020; Simon et al., 2016; Thonemann et al., 2020). The utility of first scale-up attempts is demonstrated in this study by illustrating the magnitude of the gap in the results obtained at different production levels (see Figs. 6 and 16). Understandably, the performance at lab-scale is not representative of the true potential of a certain technology, but marks the top limit from which improvements can be achieved. Accordingly, scaling up allows not only for a 'more probable' picture of environmental performance, but enables also a fairer comparison with well-established and competing technologies, ultimately setting the benchmark of potential environmental claims. Over the past few years, the upscaling of lab-scale inventory data to higher production scales, enabling a prospective analysis of potential environmental burdens, has met keen research interest. In their review article, Tsoy et al. (2020) examine various scale-up techniques commonly used in ex-ante LCAs that could be applied also to novel battery technologies in the development stage. Especially, the commonly used scaling method presented by Piccinno et al. (2016), which is based on process engineering equations, could be applied on chemical constituents of emerging batteries currently existing at lab-scale. Caduff et al. (2011) demonstrate the possibility of using past advances to determine empirical learning effects and scaling curves that could be applied to prospective analyses. This increase in research for scale-up methods of LCI data for emerging technologies (von Drachenfels et al., 2021; Piccinno et al., 2016; Tsoy et al., 2020; Simon et al., 2016; Caduff et al., 2011; Caduff et al., 2014; Shibasaki, 2009; Zhou et al., 2017), results in a broad range of methodologies with different levels of complexity, rather than a standalone 'holy grail' solution (Moni et al., 2020; Simon et al., 2016; Thonemann et al., 2020). The extent to which these methods are suitable for emerging battery technologies and the relevant criteria defining the adequacy of scaling methods must yet be further studied.

The scale-up procedure described in this study, by means of simple extrapolations of material and energy flows, has led to an estimation of the climate change potential within a magnitude close to the average of industrial systems from literature. While this simplistic approach serves as a good proxy to illustrate the potential differences between systems fabricated at different scales, it neglects possible side effects of real-life scale-up. Lab-scale equipment and specific processing techniques may largely differ from those required at pilot or industrial lines, as they may prove unsuitable for large production volumes (e.g., due to material inefficiencies, insufficient velocities, large operation costs, etc.) (Moni et al., 2020). Similarly, thermal processes such as heating and drying often switch from electricity to natural gas as energy carrier, introducing new variables that ultimately get reflected in the environmental performance of the product (Shibasaki et al., 2007). As observed for the production of the KIT 20 cell, there is little interconnection between processes at the lab, leading as consequence to an increased need of multiple intermediate manual steps. Contrary to this, the widespread concept of Lean Manufacturing in industry seeks to increase productivity by optimizing production and response times as well as reducing material losses. Some strategies to achieve this is eliminating manual operations, implementing layouts that allow for a steady flow of material and automating processes whenever possible. In some cases, this will require additional infrastructure and machinery (e.g. conveyor belts), that demand energy and other consumables while reducing the specific needs of the product. Given the large degree of uncertainty at the current state, these effects have not been considered. Likewise, energy recovery approaches potentially applicable in cell formation, or in the form of heat recovery during coating and drying, are not accounted for in this scale-up (Moni et al., 2020; Thonemann et al., 2020). Within the scope of this study, the magnitude of these effects and their influence on the final result remain unclear, demanding for further research in this field. Moreover, the adequacy of scale-up methods could be tested with the provision and comparison of data for mature systems obtained at different manufacturing scales. This would also facilitate the extrapolation of data from mature technologies in the assessment of emerging battery concepts, better achieved with a B–U perspective. Given the current lack of research in such direction, the study at hand shall serve as a first step in filling this gap not only by providing a lab-scale LCA with bottom-up primary data obtained by in-house measurements, but also by investigating possible effects of scale-up with a simple extrapolation approach.

5. Conclusions

The study herein conducted has aimed to identify and fill information gaps in the field of environmental sustainability assessments of LIB cell manufacturing. An extensive literature review of studies on the sustainability assessment of LIBs has been conducted, examining data sources, modeling approaches, as well as production volumes and scales, demonstrating that, despite the valuable progress and growing number of studies in this area, there is still a very limited amount of primary data available describing material and energy flows of battery manufacturing. Moreover, a fundamental lack of transparency has been observed negatively affecting the traceability and comparability of results. Hence, a need for LCAs based on transparent LCIs generated with primary data exists, which shall enable the understanding of the dynamics determining the environmental profile of LIB cell production at different production scales.

Through transparent and comprehensible system modeling using primary data obtained by in-house measurements, this study presents a detailed breakdown of the environmental profile of a lab-scale battery cell production, providing new datasets to the LCA community and facilitating the understanding of the environmental criticalities of this system in four main impact categories, namely 'acidification', 'climate change potential', 'resource depletion' and 'particulate matter'. The hotspots identified in the baseline analysis, namely the cathode electrode paste, the anode current collector (Copper), and the energy requirements for coating and drying, as well as dry room use, are in line with those identified in the literature. The higher order of magnitude of the impacts obtained in this study are related to process inefficiencies which are characteristic of lab-scale manufacturing. Low utilization rates and small production volumes are common at this stage, resulting in higher specific energy requirements and lower material efficiencies compared to values from literature that have been calculated at larger scales. In this specific case, high material loss rates during electrode fabrication and low product throughput in the dry room are among the main impact drivers.

Sensitivity analyses have been conducted to address the uncertainty of the results and to provide insight into the potential impact of scaled-up production. Thereby, sensitivities to different electricity grids, different dry room throughputs, and different loss rates have been examined. A theoretical scenario combining all three variables (50/50 solar and wind energy mix, 400 cells per day throughput, and 8% loss rate) has been analyzed to emulate ideal larger scale production. While the use of the EU electricity mix leads to a reduction in 'climate change', it increases the footprint in the remaining three categories. Using the renewable 50/50 mix results in drastic reductions in almost all categories, with an exception on resource depletion. As expected, increasing the throughput of cells in the dry room, reduces the cell footprint significantly in three of the four impact categories evaluated. In addition, ensuring low material loss rates, particularly for Cobalt and Copper, will grant the largest impact reductions related to resource criticality. Lastly, if scale-up is accompanied by a transition to clean energy sources, as presented in the theoretical optimal scenario, the combined benefits have the potential to drastically reduce the footprint to a small fraction of the initial estimates.

When other components beyond the cells are to be considered, as in the modeling of a full battery pack, a six fold difference in 'climate change' between laboratory and pilot scale battery production has been found. The results for the pilot scale model were obtained by simple extrapolations of mass and energy flows and are also comparable to other values reported in the literature for industrial scale systems. This illustrates the large influence that the production volumes and scales have on the environmental performance of a product and the usefulness of simple scale-up methods in gaining insights in such direction. Further research is indispensable to better understand scale-up techniques and to reduce the uncertainties relating thereto. This is crucial for the conduction of prospective LCAs for emerging battery technologies that often rely on limited data obtained in lab-scale production lines. Further LCA studies of mature technologies at different production levels, using primary and transparent LCI data, might facilitate the development and validation of adequate scale-up methodologies.

CRediT authorship contribution statement

Merve Erakca: Conceptualization, Methodology, Software, Validation, Investigation, Data curation, Writing – original draft, Writing – review & editing, Visualization. **Sebastián Pinto Bautista:** Conceptualization, Methodology, Software, Validation, Data curation, Writing – original draft, Writing – review & editing, Visualization. **Samineh Moghaddas:** Methodology, Software, Investigation, Data curation, Writing – original draft, Visualization. **Manuel Baumann:** Conceptualization, Methodology, Validation, Writing – review & editing, Supervision, Project administration, and, Funding acquisition. **Werner Bauer:** Investigation, Resources. **Lea Leuthner:** Investigation, Resources. **Marcel Weil:** Conceptualization, Validation, Writing – review & editing, Supervision, Project administration, and, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

All data used are included in the supplementary information.

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Appendix A. Supplementary data

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