Towards more flexibility and transparency in life cycle inventories for Lithium-ion batteries

Eleonora Crenna*, Marcel Gauch, Rolf Widmer, Patrick Wäger, Roland Hischier

Technology & Society Laboratory, Empa, Lerchenfeldstrasse 5, 9014 St. Gallen (Switzerland)

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ABSTRACT

Electric vehicles are gaining increasing room in the global market, since they are seen amongst the most promising solutions to cope with the growing concerns related to climate change and environmental pollution. The successful evolution of the transportation sector towards electro-mobility depends on the battery chemistry and technology, and its environmental impacts. However, the poor availability of data at the commercial production scale and the diversity in modelling choices make evaluating the environmental impacts of Lithium-ion batteries (LIB) difficult and uncertain. We aim at contributing to the creation of flexible and transparent life cycle inventories (LCI) of LIB for background databases by means of a consequently modular approach that will be applicable in the future as common framework to model new generations of LIB. In the present paper, we focus on (i) compiling modular LCI datasets of current and near-future market LIB chemistries, namely NMC111, NMC811 and NCA, by using the most recent data from existing sources, and (ii) exemplarily assessing the environmental impacts of the three modelled chemistries. This assessment takes into consideration a wide range of impact categories, with a focus on climate change and the comparison with the available literature in the sector. The whole is complemented with several sensitivity analyses, which show the relevance of transparency when making choices in compiling the LCI.

1. Introduction

Electric vehicles are gaining increasing room in the global market, since they are seen amongst the most promising solutions to cope with the growing concerns related to climate change and environmental pollution. At European level, electro-mobility is considered as a priority to move to a clean and circular economy and achieve the climate neutrality target set through the European Green Deal (European Commission, 2019).

The successful evolution of the transportation sector towards electro-mobility depends on the battery technology (Crabtree, 2019), which is accepted as the key solution for mobility in the near future. Therefore, characterizing the impacts along the supply chain of Lithium-ion batteries (hereafter referred to as LIB) is of upmost relevance in order to capture the environmental impacts of electric vehicles and to ensure their sustainability (Rajaeeifar et al., 2020). Life cycle assessment (LCA) is seen as the methodology of choice in order to provide a comprehensive picture of the environmental sustainability of LIB (Ness et al., 2007). Indeed, LCA is a standardized systems-thinking approach, used to assess the environmental challenges along the life cycle of products (ISO, 2006).

Over the last decade, many LCA studies have been performed to compare the sustainability of mobility options, including electric vehicles (e.g. Del Pero et al., 2018; Yang et al., 2020). Besides the production mix for the electricity consumed when driving with electric vehicles, the results heavily depend on the assumptions behind the life cycle inventory (LCI) of batteries, while the remaining parts (e.g. construction and maintenance of the vehicle itself) show less importance (Notter et al., 2010; Cox et al., 2018). Nonetheless, the evaluation of environmental impacts of LIB is still difficult and uncertain.

A recent literature review about LCA studies of industrial LIB (Peters et al., 2017) retrieved more than hundred publications produced over the past two decades. Amongst these, only a very small number provides original LCI data in terms of a transparent list of materials and energy demand along the life cycle of LIB. Moreover, these few publications show rather controversial results, especially when it comes to quantifying the impacts of LIB production. Indeed, studies differ up to three orders of magnitude in the assessment of the energy demand in the
various production steps. For instance, Ellingsen et al. (2014) report high values with 586 MJ/kWh battery cell, whilst Notter et al. (2010) and Dai et al. (2019) report much lower figures of about 3 to 170 MJ/kWh. This large variability is reflected in the life cycle impact assessment (LCIA) results, e.g. concerning climate change related impacts, with a bandwidth of circa 50–500 kg CO	extsubscript{2} eq per kWh battery capacity (see Ellingsen et al., 2014; 2017).

The reason behind the wide variability of results lies in the assessment of different chemistries and technologies, the use of data from different production scales (e.g. pilot operation vs full production line), the application of different approaches (e.g. top-down vs bottom-up for calculations related to the manufacturing process) and assumptions to model the whole LCI of LIB (Romare and Dahllöf, 2017; Ellingsen et al., 2017; Cerdas et al., 2018; Peters and Weil, 2018; Raugei and Winfield, 2019).

Currently, the database ecoinvent – one of the most utilized background databases for LCA – includes only one LIB type, namely a LIB with lithium-manganese oxide (LMO) cathode. However, this chemistry is increasingly leaving space to LIB with nickel-cobalt-manganese oxide (NMC) and nickel-cobalt-aluminium oxide (NCA) cathodes, which are more suitable for automotive applications given their higher energy capacity and improved durability (Bunsen et al., 2018; Raugei and Winfield, 2019).

Based on these premises, we aim at contributing to the creation of flexible and transparent LCI of LIB for LCA background databases, by means of a consequently modular structure that can also be adopted as a common framework to model the LCI of future generation LIB. Indeed, through such a modular approach, we aim to break down in an easy-to-adapt manner the inventory model into the different materials and processes. This modular approach offers a simplified, flexible and consistent way of modelling a complex system, such as the production of LIB, thus facilitating in the future the modelling of new types of LIB which result from the fast technology developments in the battery field in a consistent and simpler way.

In this paper, the modular approach is exemplarily applied to current and near-future market LIB chemistries, namely NMC111, NMC811 and NCA. We focus on the following specific objectives: (i) to compile LCI datasets in a strictly modular way (using ecoinvent for their exemplary inclusion into a consistent LCA database) by making use of the most recent data from the available literature, and (ii) to assess the environmental impacts of the modelled LIB. These updated LIB datasets, which are meant to be usable in all LCA database environments, build on recent data from existing sources (both industrial measurements and expert estimates), and are intended to achieve the highest degree possible of modularity, allowing for traceability of data sources. Hence, although we compile LCI from existing sources, we propose three LIB chemistries for their direct use in background LCA databases in which they are currently not available, including regrouping of data and adjustments based on the recent technology developments.

The present paper is structured as follows. Section 2.1 provides an overview of the modular approach for the life cycle inventory modelling of LIB, which is applicable to all LIB types under study. In Section 2.2., we provide the details regarding the analysis of the impacts of the modelled LIB at different levels of detail (e.g. battery pack, cell and their components) through an LCA case study, in which we also compare alternative modelling options for the battery components. Section 3 discusses the results of the modular approach and the performed LCA exemplification case study, and compares the environmental sustainability of the LIB under study with the results available in literature. Section 4 presents our final conclusions.

2. Material and methods

2.1. Life cycle inventory data of Lithium-ion batteries

The LCI step within the LCA methodology implies the creation of an inventory of input (e.g. natural resources, energy) and output flows (e.g. emissions to air, water and soil) from and to nature, generated by a product system. The inventory of materials and energy flows is compiled within a cradle-to-gate system boundary. Indeed, the inventory covers the activities from the extraction of raw materials to the end of the LIB manufacturing process, allowing to provide the inventory of a complete battery pack to be used in an electric vehicle. The system includes also emissions to the environment, infrastructure and waste treatment in accordance with the ecoinvent guidelines (Weidema et al., 2013).

We compile the life cycle inventory data of LIB manufacturing processes by applying a modular approach. The modules correspond to elements of the battery production system, which represent the LIB components at different levels, from the precursor materials (finer level) via the cells up to the battery pack (higher level) (see boxes in Fig. 1). Hereby, we followed the idea of the Matryoshka or nesting dolls: at the highest level there is the battery pack which includes the battery modules, which in turn embed the battery cells, and so on to the precursor materials. Modules belonging to the same level can be modelled independently from each other and then be interconnected to generate a new module at higher level. For instance, the cathode, the anode, the electrolyte and the separator represent four different modules within the modular inventory, and they belong to the same level that we call “cell level”. These components are modelled independently one from the other, as none of them is input to another. However, they can be linked together based on specific mass ratio to form the battery cell, which represents another module at a higher level in the inventory. The choice of the modules is linked to the main battery materials and components, as previously done in Notter et al. (2010), with the addition of dedicated modules to energy demand (e.g. assembly energy) and more differentiations in the modules at finer levels. The choice of keeping energy as a separate module is based on the potentially higher detail that the literature can offer, allowing to split the energy demand for each step of the assembly phase.

Such modular approach allows for flexibility in terms of selection of alternative materials (e.g. concerning cathode active materials; use of synthetic or natural graphite), so that different types of cells, battery modules and battery packs can be produced and compared for sustainability assessment within a common and consistent framework. Additionally, it allows for an increased transparency in terms of a better traceability of the data sources at different levels of detail. Indeed, the more modules the system is split into, the more transparent it is, with the possibility to identify where specific assumptions were made and fill the data gaps.

To illustrate this modular approach, we selected different LIB types by assessing the current electric vehicle market in view of the most relevant battery chemistries (Irle, 2019; Michaelis et al., 2016). At present, NMC and NCA are the most widely used LIB cathode chemistries in electric vehicles due to their technological maturity, with NMC mainly used in Renault Zoe and Chevrolet Bolt, and Tesla exclusively using NCA (Schmich et al., 2018). Within the NMC family, NMC111, NMC532 and NMC622 cathodes coupled with a graphite anode constitute the current LIB generation (Steen et al., 2017). A promising future development of the NMC chemistry consists in coupling a NMC811 cathode with a silicon-graphite anode, which would be characterized by lower cobalt and higher nickel content, resulting in an improved energy density (Michaelis et al., 2016; Steen et al., 2017; Bunsen et al., 2018).

Thus, within this study we modelled a NMC111/graphite LIB as representative of the current generation. Moreover, we followed the electric vehicle market since several years. Additionally, following our modular approach, we modelled the inventories of the more advanced LIB chemistries NMC811 and NCA, coupled with silicon coated graphite anode, in order to show how the present modular approach allows for an easy development of further LIB inventories.

To compile the inventory of the selected LIB, we performed an extensive literature review of data from both the scientific field and the industry by means of Google Scholar, Scopus, Web of Science and
Retrieved publications include research articles mainly focusing on LCA case studies of electric vehicles and related literature reviews, technical reports from producers and research institutes, publicly available battery manufacturers’ websites and battery specification brochures. Data were selected based on the following main criteria: completeness of the LIB value chain coverage for the sake of data consistency along the whole life cycle of LIB; temporal representativeness (i.e. preference for the most recent data, mainly covering the past 5 years); preference for primary data from LIB manufacturers. Expert opinion from Empa colleagues, specialists in the battery field, was considered and best estimates were applied to eventually fill the gaps.

We identified the main properties of the three LIB (Table 1) and modelled the related bill of materials mainly using the models BatPac and GREET2 from the Argonne National Laboratory (ANL) (Dai et al., 2017; 2018a; 2019). GREET2 provides recent LCI data of different chemistries collected from large-scale industrial material producers, allowing for the use of primary data from a single source. We inventoried data representing a battery pack made of prismatic cells, to be used in a small/medium electric vehicle (Dai et al., 2018a).

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**Table 1**

Main characteristics of the three Lithium-ion battery (LIB) technologies under study.

<table>
<thead>
<tr>
<th></th>
<th>NMC111/graphite</th>
<th>NMC811/Si-graphite</th>
<th>NCA/Si-graphite</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Battery pack weight (kg)</strong></td>
<td>165</td>
<td>158</td>
<td>143</td>
</tr>
<tr>
<td><strong>Energy capacity at pack level (Wh/kg)</strong></td>
<td>143</td>
<td>149</td>
<td>159</td>
</tr>
<tr>
<td><strong>Number of cells per battery pack</strong></td>
<td>140</td>
<td>140</td>
<td>140</td>
</tr>
<tr>
<td><strong>Type of cells</strong></td>
<td>46-Ah prismatic</td>
<td>46-Ah prismatic</td>
<td>46-Ah prismatic</td>
</tr>
<tr>
<td><strong>Energy capacity cells (Wh/kg)</strong></td>
<td>209</td>
<td>209</td>
<td>224</td>
</tr>
</tbody>
</table>

* Energy density as reported in Dai et al. (2018c), in line with the current LIB on the market (e.g. Schmuck et al., 2018).
the electronic components, as available in Dai et al. (2018a, 2019). Further details for modelling each battery component, their translation into the resulting inventory data, required assumptions for this as well as their link with ecoinvent background data are reported in the supplementary materials.

With respect to the used main data sources (i.e. Dai et al., 2017; 2018a; 2019; Nelson et al., 2011) and the existing background database ecoinvent v.3.6, novelties and ad hoc adjustments have been fixed within our approach as shown in Fig. 1. More detailed information can be found in the supplementary material.

In order to assess the differences in given impacts depending on the inventory modelling choices, we modelled the LCI of the following materials and components according to alternative approaches within the developed modular framework: cobalt sulfate and separator in NMC111 LIB, silicon content in the anode of NMC811 and NCA LIB. Details for each of them are reported in the supplementary materials. Additionally, we modelled the energy demand for the production of NMC811 battery pack, assuming that its future manufacturing process is moved from Asia to Europe. Therefore, we modelled two LCI options, one assuming that the value chain starting from electrode manufacture is entirely relocated in Europe, the other that solely the cell and pack assembly occurs in European countries. Thus, the average energy mix of Europe is used for the production of the main components and for cell and pack assembly.

2.2. Life cycle impact assessment

An illustrative LCA case study was conducted to analyse the impacts of the NMC111 LIB presented in details in Section 2.1. In LCIA, midpoint models quantify environmental impacts by linking the use of natural resources and the generation of emissions to an impact on the environment. Such impact is calculated by means of specific factors called characterization factors. Here, we applied the Environmental Footprint (EF) method v.3.0 developed by the European Commission’s Joint Research Centre (EC-JRC) (Zampori and Pant, 2019), as available in SimaPro v.9.0.0.48, and analysed the impacts at midpoint level for the following 16 impact categories: climate change, ozone depletion, ionising radiation, photochemical ozone formation, particulate matter, human toxicity non-cancer, human toxicity cancer, acidification, eutrophication freshwater, eutrophication marine, eutrophication terrestrial, ecotoxicity freshwater, land use, water use, resource use-fossils, and resource use- minerals and metals. The LCIA results are calculated for battery system mass (kg⁻¹) and energy stored (kWh⁻¹).

In a second step, we compared these results with those of the more advanced LIB presented in Section 2.1 (i.e. NMC811 and NCA) and those in current literature, with a focus on climate change due to scarce quantification of potential impacts in other categories or the use of not directly comparable methods.

3. Results and discussion

3.1. Main considerations on the modular approach

We modelled the LCI of three LIB types by breaking their manufacturing process down to smaller parts representing the main battery components, including at a finer level their underpinning materials and processes. Following the idea of modularity initially proposed in Notter et al. (2010), we gathered data from existing sources and regrouped them in modules (the “boxes” reported in Fig. 1) within a common framework. This simplified and structured approach allows for detailed contribution analyses of impacts at higher level of details (see Section 3.2), a consistent comparison of impact results between various LIB types and gives the opportunities for developing other LIB compositions, as we did for the more advanced LIB types analysed in the present study (see Section 3.3). In fact, the LCI of NMC811 and NCA were developed by means of the same modular approach used for the LCI of NMC111 as presented in Fig. 1. By replacing the existing specific chemistry- (e.g. LIB specific energy storage) or technology-dependant parameters, the LCI of the two more advanced LIB types were modelled quickly and with few small changes, starting from the initial NMC111 modular scheme. The use of such a modular approach facilitates more systematic model development, promoting consistency thanks to the adherence to the same modelling scheme and principles, thus setting a common basis for the modelling of various LIB inventories.

By simplifying the LIB production inventory model into the different materials and processes, we were able to attribute the environmental impacts to the specific features (e.g. cell production, cathode precursors), also improving the transparency on electricity requirements and coverage of processes along the production chain of LIB (see Section 3.4). Hence, with this manuscript we present some kind of a new LIB baseline which is transparent in modelling and reporting, in order for other LCA practitioners to know what the assumptions and uncertainties behind each module are and to give them clear guidelines for the development of future LIB models along the same direction.

Concerning the data, although we held as much as possible to one data source reporting the most up-to-date data (2015–2018) from commercial scale production, some adjustments were needed in order to develop a representative baseline that can be used by practitioners. These adjustments, based on estimates from additional sources and expert judgement, might bring uncertainties in the datasets and related impact assessment results. We accounted for respective uncertainties of data in the pedigree matrix associated to the suitable format for the background database.

3.2. Analysis of the LIB: NMC111/graphite as representative example

We modelled NMC111/graphite LIB as a representative example of the application of our modular approach, and we analysed its environmental impact with the purpose of showing that this modular approach allows for a contribution analysis at different level of details (from low, i.e. battery pack, to high, e.g. electrode active material), in a transparent way and with the possibility of tracing the impacts back to the sources.

According to the system units analysed and in line with the current literature, cell manufacture represents the most important contributor to the impacts associated with the production of the LIB pack (Fig. 2). NMC111 cell production makes up to more than 50% of the total impact of the battery pack for 14 out of 16 categories, reaching 91% in the category ‘particulate matter’. Battery pack housing materials (aluminium box, battery terminals and plastic components) cause relatively low share of impacts throughout all categories, mainly due to their lower amount within the battery pack (i.e. less than one third of the battery pack mass). Despite their lower share in mass, a major role is played by the electronic parts, specifically the BMS which contributes to 39% of impact for the category ‘resource use- minerals and metals’, due to its high metal share.

At cell level, the NMC111 positive electrode and the negative current collector made of primary copper have particularly high environmental burdens. This finding is in good accordance with other studies (e.g. Notter et al., 2010; Ellingsen et al., 2014). The impact associated with the production of cathode materials is relatively high in at least 12 impact categories, contributing up to more than 70% of the total impact of the cells for the two categories ‘particulate matter’ and ‘acidification’. Graphite and the other anode components, electrolyte, separator and the positive current collector made of aluminium play a minor role. Copper current collector shows high impact for ‘human toxicity non cancer’ (59%), followed by ‘eutrophication freshwater’ (50%) caused by the discharge of sulfidic tailings from the mining sector. Also its impact on ‘resource use- minerals and metals’ is relatively high (38%), due to the mining operation of primary copper.

NMC111-oxide alone contributes to more than 85% of cathode material impacts for all impact categories. All the other cathode slurry components, including binder, carbon black, etc., are responsible for a
very small environmental impact. Within the cathode active material, the production of precursor, namely NMC111-hydroxide, and the electricity required in the calcination process make up to more than 80% of the environmental burden for all the impact categories considered. Especially for climate change, electricity represents 36% of the total environmental impact for the cathode active material. Most impacts of the precursor production are the result of the use of cobalt sulfate and nickel sulfate, to a minor extent followed by the use of sodium hydroxide, manganese sulfate and the heat from natural gas required for the co-precipitation process.

3.3. Comparison of NMC111, NMC811 and NCA LIB

Comparing the impacts per battery mass system of the NMC111 with the other two chemistries under study (see supplementary material for further details), the production of an NMC111 battery pack generally shows lower impacts than more advanced technologies. In fact, the production of NMC811 and NCA battery packs causes higher impacts for all impact categories, except for ‘particulate matter’. NMC811 and NCA show slightly higher impacts than NMC111 for climate change (respectively 7% and 10%), while the highest difference is reported for the impact category ‘acidification’ (60% and 63% respectively). The latter is specifically due to the high contribution of nickel sulfate in the production of the cathode active material precursors.

The situation looks more diverse when the impacts are assessed according to the not mass-related system unit. NMC111 still performs generally better than the other LIB, with higher impact than both NMC811 and NCA for four impact categories. This can be due to the fact that the lower impact of NMC111 per mass unit is not compensated by the lower energy density of this specific technology, leading to higher environmental burden for these categories.

In the mass based system unit, NCA is the one performing worse compared to both the other LIB for the overwhelming majority of impact categories, while for the energy density-based system NMC811 shows higher impacts for 12 out of 16 impact categories. This exercise comparing the different system units shows how studies evaluating the environmental performance of LIB can lead to different conclusions, not only depending on the assumptions behind the inventory modelling, but also on the choice of the system unit. It is important that the system unit is aligned with the goal and scope of the study to provide adequate and coherent interpretation of the results.

3.4. Comparison of LIB from this study with the available literature

In order to understand the results of the here modelled LIB chemistries (and with this, of the proposed modular approach for LIB modelling in general) with respect to the most recent and available literature on the topic, the environmental impacts of the NMC111 LIB under study were compared with the results reported in the following studies: Dai et al. (2019), Ellingsen et al. (2014), Cox et al. (2020), Notter et al. (2010), Romare & Dahllof (2017) and its updated version Emilson & Dahllof (2019) (Fig. 3). The studies differ for a number of aspects: the chemistry of the battery, the data sourcing and modelling especially referred to the energy requirements along the production chain, and the adopted LCIA method. Indeed, Dai et al. (2019), Ellingsen et al. (2014) and Cox et al. (2020) – whose inventory is partially built on the LCI model of Ellingsen et al. (2014) – analyse the impacts of an NMC111 LIB, while LMO is considered by Notter et al. (2010) and an unspecified average chemistry is presented in the reports by Romare and Dahllof (2017) and its update by Emilson & Dahllof (2019). Concerning the source of data, especially from electrode manufacture to battery assembly, Dai et al. (2019) and Ellingsen et al. (2014) based their estimations on primary data obtained from visits to battery manufacturers, respectively in China and Norway, although the production scale differs (full production vs pilot operation line, respectively). Both authors, including Cox et al. (2020), adopted a top-down approach, while a bottom-up approach is used by Notter et al. (2010), Emilson & Dahllof (2019) and Romare & Dahllof (2017) made their own assumptions based on the available literature, and included scenarios, specifically in the former study with nearly fossil-free energy use. The inventory of Dai et al. (2019) and Notter et al. (2010) is of higher details as the electricity and heat consumptions are reported as process-specific, whilst Ellingsen et al. (2014) report a final aggregated value for battery cell manufacture in terms of electricity required for the whole value chain.
We compared the results in terms of their climate change related impacts, as this category is the most common within the available literature and Global Warming Potential (GWP, kg CO$_2$ eq.) indicator represents one of the main ‘area of concern’ for society when assessing the impacts of electric mobility. All of the studies make use of GWP. However, the indicator is based on IPCC (2006) factors (e.g. from ReCiPe 2008 method, as in Goedkoop et al., 2009), while in our study the impacts of battery manufacture is calculated by means of more up-to-date IPCC factors (Myhre et al., 2013), in accordance with the EF method (Zampori and Pant, 2019). To allow for a fair comparison, we recalculated the climate change impacts of the LIB of the present study by means of ReCiPe 2008 method (Goedkoop et al., 2009). The climate change impact results based on ReCiPe 2008 are circa 5% lower than the related EF based results. In order to use a metric that is independent of the battery size, the battery storage capacity measured in kWh has been adopted as representative functional unit for comparison.

The large variability of the LCIA results for climate change is associated with the variability in the energy demand for producing the LIB. For instance, Ellingsen et al. (2014) assume high energy requirements in the whole production process (56% higher than the energy requirements assumed in our study, see Table 2), leading to high contribution to climate change burden. Instead, decreasing the energy requirements leads to smaller climate change impacts, as presented in the case of Cox et al. (2020).

A lack of transparency in the way energy consumption is estimated and linked to each step of the battery pack production in literature did not make possible so far to identify the source of impacts in view of e.g. improvements in the product design. Differently from these previous studies, the application of the modular approach allowed to discern the production step for each battery component and identify the associated energy demand per each module presented in Fig. 1. Indeed, we could estimate that the battery pack assembly reported in the present study requires only a small amount of energy compared with other relevant LIB components mentioned in Table 2, although its energy demand can vary depending on the technology applied (e.g. manual or machinery-based assembly). The largest energy requirements in the production of the battery are found in the manufacture of cells, followed by upstream processes such as the production of the NMC-precursors, involving drying processes and NMP solvent recovery. The decline in the upper end of the energy demand range in the available literature is mainly due to more recent data for battery production, particularly more realistic measurements of process energies in drying rooms for industrial scale factories and solvent evaporation estimates, which better match with the actual production.

### 3.5. Sensitivity analyses

Sensitivity analyses are performed here in order to assess the differences in given impacts depending on inventory modelling choices. Indeed, the impacts of the LIB are dependant on the LCI modelling choices, with each of them representing a possible source of uncertainty. Variations in one or more parameters may influence the LCIA results.

#### Table 2

<table>
<thead>
<tr>
<th>Component of NMC111 battery pack</th>
<th>kWh/kg battery pack</th>
<th>Ellingsen et al. (2014)</th>
<th>Cox et al. (2020), low range value for current batteries</th>
<th>Cox et al. (2020), average value for current batteries</th>
<th>Cox et al. (2020), high value for current batteries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pack assembly</td>
<td>3.00E-04</td>
<td>4.00E-04</td>
<td>4.00E-04</td>
<td>4.00E-04</td>
<td>4.00E-04</td>
</tr>
<tr>
<td>Cell production</td>
<td>3.40E-00</td>
<td>1.68E+01</td>
<td>9.00E+00</td>
<td>1.44E+01</td>
<td>1.80E+01</td>
</tr>
<tr>
<td>Cathode slurry production</td>
<td>2.28E+00</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Cathode precursor (oxide)</td>
<td>1.84E+00</td>
<td>–</td>
<td>3.03E-02</td>
<td>3.03E-02</td>
<td>3.03E-02</td>
</tr>
<tr>
<td>production</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cathode precursor (hydroxide)</td>
<td>2.88E+00</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>production</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Anode slurry production</td>
<td>3.85E-01</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Total</td>
<td>1.08E+01</td>
<td>1.68E+01</td>
<td>9.03E+00</td>
<td>1.44E+01</td>
<td>1.80E+01</td>
</tr>
</tbody>
</table>

* Sum of both electricity and heat from natural gas.
Below, a summary of the main differences due to modelling variations is reported for the battery mass system results; more detailed comparisons are found in the supplementary material.

**Cobalt sulfate.** The sensitivity analysis of cobalt sulfate showed changes in the environmental burden for all the 16 impact categories analysed, both at the level of detail of cobalt sulfate itself and at lower level (either cell or pack). Indeed, all the LCI based on the economic allocation of copper-cobalt ore mining and processing represent the options with higher impacts compared to the mass allocation based LCI. This is linked to the higher economic value of cobalt (5 times higher than copper over a 10-year period, Dai et al., 2018b), compared to its lower ore grade (0.47% Co vs 2.44% Cu, Dai et al., 2018b). The LCI derived from the default modelling as described in Hischier et al. (2005) shows the lowest impacts for the majority of impact categories, except for land use and minerals and metals resource use. This option does not rely on performance data of the specific product, but on average data from a big chemical company and accounts simply for the chemical reaction of cobalt metal, thus excluding inputs associated with the processing and refining of the material. Comparing the aggregated datasets – both economic- and mass allocation-based – with non-aggregated datasets, we found that the non-aggregated datasets generally report lower impacts. The differences in the LCIA results are attributable to the geography choice of the electricity mix and water used. For instance, the three non-aggregated datasets were assigned with electricity mix from the Democratic Republic of Congo (DRC), where the ore mining and processing occur, and China, where the cobalt refining step is located. On the other hand, the aggregated dataset has been attributed with the solely electricity mix of China, based on the geography of the final refining step. This leads to a higher climate change burden for the aggregated dataset, as the fossil fuel based electricity mix from China as available in ecoinvent v.3.6 generates higher GWP when compared with the DRC one.

Ecoinvent database last release (v.3.7) added the LCI of cobalt hydroxide production, developed by the Cobalt Institute. Due to the unavailability of this data set in SimaPro, software that we use for the LCA, it was not possible to run the complete LCA with this newly published data. Therefore, we performed a rough estimate of how much the impact of both cobalt sulfate and the battery pack could increase by using LCIA results available in ecoinvent database as a starting point (details in supplementary materials). We considered the climate change related impacts for the IPCC2013 method (based on the factors from Myhre et al., 2013), as the LCIA results for the EF 3.0 method were not available. We estimated that the impact of cobalt sulfate at both cobalt sulfate and battery cell level is double the value we originally calculated by adapting the LCI of cobalt sulfate from Lewren (2019) and Dai et al. (2018b). The main reason of this difference relies in the way the supply chain of cobalt hydroxide is modelled. For instance, the data set in ecoinvent v.3.7 accounts for a wider number of input and output flows, thus leading to a higher impact value.

**Separator.** We compiled the LCI of eight separator types for the NMC811 LIB technology, varying the plastic material used (i.e. single layer with 100% PE, or multi-layer with a combination of 80% PP and 20% PE in mass), the type of process used to manufacture the plastic membrane starting from granulate material (i.e. injection moulding vs plastic extrusion, or directly using ‘plastic packaging film’ as a proxy for the final porous membrane) and eventual silica-based coating. At separator level, the use of different types of plastic materials brings about large changes in the environmental burden of all impact categories (2–4%). On the other hand, the plastic injection moulding process shows higher impact than both plastic extrusion and the production of a plastic packaging film respectively, for at least 14 impact categories. Additionally, the silica-coating is cause of higher impacts, especially for ecotoxicity freshwater, since it implies not only the addition of silica, but also the use of acetone, PVDF, and other chemicals mixed to produce the coating slurry, which are known to be toxic for the environment. At cell and pack level, the aforementioned differences become minimal, i.e. less than 1% for all impact categories if comparing the various options with our final LCI choice.

**Silicon content.** The use of silicon and graphite together in the anode is considered to be one of the preferred strategies for LIB commercialization in the near-future market, due to its contribution in increasing the energy density of LIB (Wu et al., 2019). Indeed, higher silicon content in the anode can increase the energy density of the anode itself, which is designed to be lighter and thinner compared to the current anodes available on the market. The increase in energy density at anode level can lead to an increase in the overall battery cell energy density and, on a per kWh basis, to a consequent lower impact of the battery system. In our sensitivity analysis, we increased the silicon content in the anode of NMC811 and NCA LIB from 2% to 5%. Considering that we kept unchanged the energy density of the LIB under study, this variation in silicon content did not lead to substantial changes in terms of environmental impacts. At anode level, the same variation in silicon content implies relatively higher impacts for 13 impact categories ranging between 1% (e.g. eutrophication terrestrial) and 28% (human toxicity- cancer). This slight increase in impact might be counterbalanced by accounting for the variation in LIB energy density, thus leading to potential lower environmental impacts.

**Production place.** The sensitivity analysis about the relocation of NMC811 battery pack production in Europe shows some remarkable changes. The choice of the local average European energy mix leads to lower impact for the overwhelming majority of impact categories. Particular attention is dedicated to climate change category, as the LCIA results of LIB are highly dependant on the electricity mixes considered (Emilson and Dahllöf, 2019). A decrease of respectively 15% and 3% is shown in the GWP indicator when applying the average European energy mix either along the value chain (electrode production, cell and battery assembly) or in the solely cell and pack assembly step. Asian energy mix is highly fossil fuel-based (71% vs 43% in Europe, IEA 2017), while European energy mix shows more share of low-carbon technologies (i.e. nuclear, solar, wind, hydroelectric power and biofuels, making up to 53% of all energy sources compared to 29% in China, IEA 2017). Based on this, an NMC811 battery pack produced with an average European energy mix (even only the assembly steps) results to perform better than a NMC111 fully produced in Asia (Fig. 4).

4. Conclusions and outlook

We compiled, based on a consequent modular approach, up-to-date inventory data for the current LIB chemistry, namely NMC111, and for two more advanced LIB types, namely NMC811 and NCA, and assessed their environmental impacts. As a result, detailed and structured data ready for their inclusion in the ecoinvent database are presented, and due to their high modularity they could be included in other database as well.

In fact, in the modular approach that we implemented, we broke down the battery production system into smaller parts called modules, each of them representing the elements of the battery production, e.g. materials ("anode active material” in Fig. 1) or energy demand ("active material synthesis energy” in Fig. 1). Therefore, the present approach can be adopted easily to model different types of LIB within a common framework (as shown here for NMC811 and NCA, respectively), including future LIB which are the results of the fast technology developments in the battery field. For instance, the LCI of further LIB chemistries could be simply modelled by updating the respective modules within the overall modular scheme. As possible adaptations, different materials (like lithium iron phosphate (LFP), cobalt-free cathodes, anodes with high silicon-content, solid electrolytes) or optimized processes (like tableless electrodes, direct cell assembly to lightweighted battery packs without modules) could be proposed. The presented modular design, characterized by transparency on the sources and assumptions behind each module, allows for flexibility in the modification of existing modules to adapt the framework to new chemistries or technologies, and
The LCI of the exemplary LIB chemistry investigated with this approach (i.e. NMC111) is built on the most up-to-date data (2015–2018), largely being information from commercial-scale industrial material manufacturers principally located in China, which as a whole country represents one of the major producers of LIB so far. The use of these recent data taken from the industrial scale, part of them complemented by the expert opinion of battery specialists, allows performing a more reliable LCA comparison between this currently broadly used chemistry and advanced products, although limits and uncertainties still exist in the LCI, e.g. given by the non-exclusivity in the modelling options, the use of proxies and the subjective choices.

From these calculations, we observed that the three modelled battery cells, in particular their cathodes, are the most important contributors to the environmental impacts associated with the production of the respective LIB, in line with current scientific and technical literature. Results may vary depending on the system unit chosen, with one technology performing better or worse than other technologies depending on the functional unit. This points out the relevance of being consistent with the selected goal and scope of the study.

In our comparison with the available literature, we found that, despite the differences underpinning the LCI, the impact on climate change of the NMC111 LIB herein presented stands in between process-specific bottom-up approaches (e.g. Notter et al., 2010) and top-down approaches (e.g. Ellingsen et al., 2014). This result is mainly a consequence of the use of more recent and representative measurements collected at industrial scale for the energy consumption along the battery production chain, complemented with the expert opinion of battery specialists who were involved in the establishment of the data. However, estimating energy demands still remains a tough task, especially given the confidentiality kept by large-scale industries on their material recipes and energy consumptions. In this context, a next step, which goes beyond the integration of LCI data in the existing database, involves the development of a more detailed, original and complete process-based LCI, addressing the latest technology advancements, by means of further critical assessment of the processes in the LIB production chain. Recently, announced improvements for battery production and assembly technologies show impressive potential for energy demand reductions. This would lead to significantly lower environmental impacts for the batteries than with today’s technologies.

Overall, the LCI data set presented in this manuscript, with their high degree of modularity and traceability of data sources, show the applicability of the underlying modular approach. This approach makes the development of and the comparison with the LCI of future generations of LIB possible, thus allowing to head for a more structured debate within the LIB field and the LCA community.

5. Supplementary material

Detailed life cycle inventory data for the three LIB chemistries under study, required assumptions, alternative LCI modelling choices and contribution analyses are available in the supplementary material documents. The LCI data sets in .spold format are available upon request to the corresponding author.

CRediT authorship contribution statement

Eleonora Crenna: Conceptualization, Methodology, Formal analysis, Investigation, Visualization, Writing – original draft, Writing – review & editing. Marcel Gauch: Conceptualization, Methodology, Writing – review & editing. Rolf Widmer: Methodology, Writing – review & editing. Patrick Wäger: Writing – review & editing. Roland Hischier: Conceptualization, Methodology, Funding acquisition, Project administration, Writing – original draft, Writing – review & editing.

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.

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Supplementary materials


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