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Life cycle assessment of sodium-ion batteries

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Sodium-ion batteries are emerging as a potential alternative to lithium-ion batteries. This study presents a prospective life cycle assessment for the production of a sodium-ion battery with a layered transition metal oxide as positive and hard carbon as negative electrode material on battery component level. The complete and transparent inventory data are disclosed, which can easily be used as basis for future environmental assessments. Na-ion batteries are found to be promising under environmental aspects, showing, per kWh of storage capacity, environmental impacts at the lower end of the range published for current Li-ion batteries. Still significant improvement potential is given, especially by reducing the environmental impacts associated with the hard carbon production for the anode and by reducing the nickel content in the cathode active material. For the hard carbons, the use of organic waste can be considered promising in this regard. Nevertheless, when looking at the energy storage capacity over lifetime, achieving a high cycle life and good charge-discharge efficiency are fundamental. This represents the main challenge especially when competing with LFP-LTO type Li-ion batteries, which already show extraordinarily long lifetimes.

Furthermore, it offers a basis for forthcoming comparisons with other post-LIB energy storage technologies like lithium-air, lithium-sulphur batteries, or even fuel cells. 14-17

Methodology

Life Cycle Assessment (LCA) LCA is a standardized methodology for quantifying the environmental impacts of goods, products, or activities. It takes into account the whole life cycle, from resource extraction over production, use phase until the end-of-life handling, and recycling / disposition of as waste. 18,19 This paper quantifies the environmental impacts associated with the production of an SIB consisting of layered oxide and hard carbon electrode materials by means of LCA in order to compare it with existing LIBs. Since the focus is on the battery production, a cradle-to-gate perspective is used, providing results independent from the later application. The functional unit (FU), i.e., the provided service that is used as basis for quantification / comparison, is 1 kWh of storage capacity. In order to be able to assess also the influence of battery cycle life and internal efficiencies, where significant differences exist between battery technologies, 20 a secondary FU is used, i.e., 1 kWh of lifetime energy storage capacity. The cut-off system model is used according to ecoinvent 3.2.21 Thus, the impacts associated with waste treatment or recycling processes are allocated fully to the primary process, leaving waste products available free of burden. This is consistent with previous ecoinvent versions and thus allows for comparing results with existing LCA studies that are based on ecoinvent 2.2.22 Whenever multi-output processes are modelled, their environmental impacts are allocated to the different products according to physical relationships (mass).

Introduction

Na-ion batteries are emerging as a potential alternative to existing lithium based battery technologies. In theory, the maximum achievable specific energy densities of sodium-ion batteries (SIB) are, due to the higher mass and larger ionic radius of Na+ compared to Li+, expected to be slightly lower than those of Li-ion batteries (LIB). Nevertheless, reported energy densities are already higher than those of existing lithium iron phosphate-lithium titanate (LFP-LTO) type LIBs and are expected to exceed also those of lithium iron phosphate-graphite (LFP-C) LIBs. 1-3 Furthermore, SIBs make use of abundant and cheap materials (like sodium instead of lithium, aluminium instead of copper) and are expected to be associated with lower environmental impacts. 4-7 This makes SIBs especially interesting for stationary energy storage systems where weight and volume are less crucial. 8,9 On the other hand, the technology is still in an early phase and no quantification of the potential environmental impacts of the production of such batteries exists. The present paper closes this gap by providing an exhaustive life cycle assessment (LCA) of a representative SIB and the comparison of its environmental performance with existing works on LIBs. 10-13 This provides support for battery developers about environmental hotspots and improvement potentials of future SIBs.

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Battery modelling. The Na-ion battery subject to assessment is based on a layered oxide cathode in combination with a hard carbon anode, the most extensively studied and currently most promising material combination for such batteries.\textsuperscript{23} As composite cathode, a layered oxide in combination with an organic binder (polyvinylene fluoride; PVDF) is used.\textsuperscript{27} The composite anode is based on a hard carbon active material produced from a carbohydrate precursor (sugar), and a water-based binder, styrene-butadiene rubber (SBR) in combination with sodium carboxymethylcellulose (CMC).\textsuperscript{28,29} For both electrodes, aluminium is used as current collector foil for both electrodes since it does not alloy with sodium at low potentials. Sodium hexafluorophosphate (NaPF$_6$) salt in organic solvent is used as electrolyte, while the separator is a conventional polyethylene/polypropylene porous sheet identical to those used in Li-ion batteries.\textsuperscript{30,31} Layout and mass balance of a battery cell are based on existing patents and technical datasheets\textsuperscript{27,30,32} (details are given in the Electronic Supplementary Information (ESI)). Numerous promising material combinations for the production of layered oxide cathodes exist,\textsuperscript{3,9,33} which is why the performance values stated for a generic layered oxide battery are used for the assessment. The SIB, which is exemplarily investigated in this work, shows a cell specific energy density of 128 Wh·kg$^{-1}$, comparable or even slightly above that of existing LFP cells.\textsuperscript{30} Information about achievable lifetime of SIBs is scarce due to the low technical maturity of the technology. Datasheets for pre-commercial layered oxide type batteries state at least 300 charge-discharge cycles with 80% of initial capacity retention, while 2,000 cycles have been proven feasible by research institutions.\textsuperscript{30,34} However, due to the similar cell setup and working principle, SIBs are in principle expected to show comparable lifetime of LiBs once produced with state-of-the-art, industrial equipment. The battery cells are assembled in 18650 type cells casings, which are then packed together with the battery management system (BMS) in a steel casing to form a battery pack comparable to LiB packs. Although the materials used for the SIB might show different properties than those of LiBs, the battery cell and pack production process is assumed to be identical, with final cell assembly and electrolyte filling taking place under dry room conditions. Housing and BMS make up 20% of the total mass of the SIB pack,\textsuperscript{11,12,35} giving a specific energy density of 102 Wh·kg$^{-1}$ for the final battery pack.

The manufacturing of the hard carbon anode from a carbohydrate precursor and the manufacturing of the layered oxide cathode are modelled in detail based on data disclosed in technical datasheets and patents.\textsuperscript{30,32} Cell casing, separator, battery pack housing and the BMS are assumed not to differ significantly from those of existing LiBs, thus inventory data from existing studies on the latter are used. This brings the additional advantage of better comparability with LiBs, since differences that stem from different modelling approaches of these common components are minimised. Figure 1 depicts the production process for a complete Na-ion battery, from the material precursors until the final battery pack as modelled as basis for the environmental assessment. The detailed life cycle inventory data (LCI) for each step of the manufacturing process and the corresponding assumptions can be found in the ESI. Since no large-scale SIB industry is yet established, the production is assumed to be situated in Europe, using the corresponding electricity mixes.

Figure 2 shows the composition of the modelled SIB (battery cell). It is comparable to that of LiBs,\textsuperscript{30} with the anode active material making up a slightly higher share of the battery weight, what is compensated for by the use of lighter aluminium instead of copper for the current collector. The cell casing makes up a relatively high share, what is attributable to the use of 18650 cell packaging; a pouch cell might reduce package weight substantially. The tabulated mass balance of a single 18650 battery cell and further details on the modelling approach can be found in the ESI.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Flow diagram of the production process for the assessed Na-ion battery.}
\end{figure}
Results and sensitivity analysis

Characterization results

The environmental impacts calculated for the production of the described SIB are given in Figure 3 and discussed in the following.

GWP: The anode, and here especially the production of the hard carbon active material, turns out to be an important driver for the global warming potential, being the battery component with the highest contribution to the total GWP (24%). Especially the production of the sugar from sugar beet, which is used as precursor for the hard carbon preparation, is associated with significant GHG emissions (17% of the total GWP). The nitrogen required for maintaining inert atmosphere in the hard carbon production process also contributes a small, but notable share to the impacts (3% of the total). Apart from the hard carbon active material, the aluminium collector foil also shows relevant contributions (almost 6% of the total) from the anode. The cathode production is responsible for 20% of the total GWP, of that 9% only due to the PVDf binder, whose production is highly GHG intensive, and 3% due to the aluminium for the collector foil. Another 8% stem from the production of the layered oxide (active cathode material), and within this the nickel carbonate required as precursor (4%). The electricity consumed during cell and battery pack manufacturing, assumed to be identical to that of existing LIBs, is also responsible for a major share (21%) of the total GWP impacts.

FDP: The profile obtained for fossil depletion potential is similar to that for GWP. Main contributor is the production of the sugar required as hard carbon precursor (16%) and thus the anode (29%). Production of the aluminium used for the anode and cathode collector foil is also important (7%) while the cathode production is less relevant (12%, including collector foil). Here, the nickel carbonate required for the active material is the most important driver. Other key drivers for impacts in this category are the energy demand during cell and pack manufacturing (heat: 15%, electricity: 22%), but also the BMS with 8% and the electrolyte with 6%.

HTP: The human toxicity potential of the battery cells is comparably low: main driver are the electronic components in the BMS, not the battery chemistry itself. BMS and wiring together make up 56% of the total impacts in this category, although the BMS is modelled based on the study by Notter et al. 11, which is already the BMS with the lowest impacts among the LCA studies on LIBs used for comparison. The remaining share comes to about equal amounts from cathode (16%; of that 10% from the nickel carbonate precursor) and anode production (7%; of that 5% from the hard carbon production, with the main driver again being the sugar precursor). The electricity required during battery pack and cell manufacturing contributes another 11%.

MEP: For the marine eutrophication potential, the sugar as hard carbon precursor is the major single contributor (63%). Therefore, 67% of the total impacts stem from the anode, and only 8% from the cathode, again with the nickel carbonate as the main driver for impacts (4%). Other important contributors are the electricity for battery pack and cell manufacturing (8%) and the production of the BMS (7%).

FEP: For freshwater eutrophication, a similar picture as for HTP is obtained, with the electronic components of the BMS being the main driver for impacts in this category (45%). Here, especially the production of the gold required for integrated circuits is relevant (18% of the total). Anode and cathode production contribute about equal shares (12% each), with the main contributors being again the hard carbon precursor (10%) and the nickel carbonate production (9%). Electricity generation for manufacturing makes up another 22%.
**Comparison with Li-ion technology**

In order to obtain a better understanding of the potentials of the assessed SIB, the above results are compared with those of existing studies on the environmental impacts of state-of-the-art LIBs. Several studies exist on LIBs, but these use different life cycle impact assessment (LCIA) methodologies, different LCI databases and very different assumptions regarding the energy intensity of battery cell manufacturing.\(^2\)\(^,\)\(^3\)\(^,\)\(^7\)\(^,\)\(^1\)\(^7\) Therefore, the inventory data of the principal LCA studies on LIBs are recompiled and the manufacturing energy demand and electricity mix used in the different studies is homogenized, using the same average value in all cases (more details in the ESI). This increases the comparability of the studies, putting them on a common base regarding these parameters and, above all, using the same LCIA methodology. Nevertheless, the different studies model also other key components like the BMS or the binder used for the cathode and anode production in very different ways, why the direct comparability of the results is very limited. For example, Bauer\(^10\) uses simple proxies for many battery components (tetrafluoroethylene instead of PVD, benzene instead of carbon black, generic organic chemicals for the electrolyte solvents, etc.), what increases uncertainties and might affect the impacts significantly. Still, a value range is obtained in this way for the potential impacts of LIB production that allows for benchmarking. Figure 4 shows the comparison of the relative impacts obtained for the SIB with those of common LIBs on energy density basis (1 kWh of storage capacity).

On energy capacity basis (1 kWh of storage capacity), the assessed SIB shows promising results, taking into account that the battery chemistry is on a significantly lower technical development level than commercially available LIBs. Impacts obtained for GWP and FDP are at the lower end of the range set up by existing LIBs, while for FEP and HTP the SIB outscores all LIBs. The positive results obtained under toxicity and freshwater eutrophication aspects are mainly due to the use of aluminium instead of copper as current collector in the anode, being copper a very critical substance under these aspects. Only for MEP, the SIB shows the highest impacts among all compared battery types. This is attributable to the use of sugar as anode material precursor and might easily be improved by selecting a different type of precursor, as assessed later in the sensitivity analysis.

**Influence of cycle life**

Battery lifetime is a key factor for environmental impacts of batteries.\(^2\)\(^,\)\(^3\) Since SIBs are still in a very early development phase, it is difficult to predict the stability achievable on medium or even long term. Nevertheless, 2,000 cycles have already been reported for a 18650 type prototype cell and thus seem to be feasible even on short term.\(^3\) The influence of different cycle lives on the overall impact associated with the battery production over its lifetime is assessed in comparison with LIBs, where more reliable information is available in this regard.\(^3\)\(^9\) The cycle lives at 80% depth of discharge (DoD) for the Li-ion batteries are average values from technical specifications, and, if not available, from existing LCA studies: LFP-C: 2,960 cycles; LFP-LTO: 13,850 cycles; LMO-C: 1,070 cycles; NCA-C: 2,200 cycles and NCM-C: 1,650 cycles.\(^2\)\(^0\) The environmental impacts associated with the storage of 1 kWh of electricity over lifetime are shown in Figure 5 (without considering the electricity generation, since the objective is battery comparison). The importance of cycle life is clearly visible, e.g. for the LMO-C type LIB: While achieving very good results per kWh of storage capacity (Figure 4), its low cycle life converts it into the worst scoring LIB type when considering the lifetime storage capacity. Compared to the LIBs, the SIB scores slightly worse in the majority of the assessed categories when assuming a lifetime of only 1,000 cycles, while with
2,000 cycles it already gets into the range of existing LIBs. With 3,000 cycles it clearly outperforms the assessed LIBs in all assessed categories, except the LFP-LTO, which shows extraordinarily high lifetimes. Still, per kWh of storage capacity the impacts of the SIB are lower than those of the LFP-LTO (Figure 5), and with a similar lifetime the SIB would offer better results also compared to this LIB type. In consequence, achieving high cycle life represents one of the main challenges for SIBs in order to excel existing LIB technologies under environmental aspects.

Influence of charge / discharge efficiency

The internal efficiency of batteries varies and has a relevant influence on their life cycle environmental impacts. When also considering the internal efficiency of the batteries, the use phase has to be included. This can be done in a simplified way by only accounting the additional energy required per amount of energy stored due to internal losses. A life expectancy (i.e., capacity retention higher than 80%) of 2,000 charge / discharge cycles at 80% DoD, and an internal efficiency of 90% is assumed for this purpose. Figure 6 shows the influence of varying cell energy efficiency on the overall impact over lifetime (i.e., the share of environmental impacts over lifetime only due to charge-discharge losses), using the European electricity mix. The electricity consumed over battery lifetime due to cell energy efficiency is responsible for around 38% of the impacts caused for GWP, FDP and FEP. For HTP, it makes up roughly 23%, and for MEP and TAP around 19% of the lifetime environmental impacts. Thus, especially for the categories GWP, FDP and FEP a higher sensitivity on the cell energy efficiency is given. The efficiency increase of 2%, for example from 90% to 92%, leads to a reduction of the overall impacts in these categories by about 7%. Naturally, this effect depends also on the used electricity mix and the lifetime of the battery and is more pronounced for long cycle lives. The results demonstrate the importance of the energy efficiency of batteries, which should be more explicitly considered as an important research target for battery development.

Influence of anode hard carbon precursor

Since hard carbon (HC) production, especially that of the sugar precursor, shows high environmental impacts in the majority of the assessed categories, different possible HC precursors are screened: starch, cellulose, organic waste and petroleum coke instead of sugar. Starch and cellulose are alternative carbohydrate precursors, organic waste is used as a generic representative for organic residues like nutshells or fruit peels / wastes and petroleum coke as a fossil precursor. The characterisation results relative to the base case (HC from sugar) are given in Figure 7. More details about the modelling and the corresponding LCI can be found in the ESI. The use of starch or cellulose instead of sugar as HC precursor slightly increases environmental impacts in the majority of the assessed categories, except MEP, where cellulose gives significantly better results. On the other hand, processing organic waste materials shows noteworthy improvement potential, reducing the overall impacts caused by battery production in all categories (for example, by 16% for GWP, 15% for FDP and up to 62% for MEP). High reduction of impacts is achieved especially for MEP, the only category where the SIB showed significantly worse results than the LIBs, basically due to the impacts associated with the sugar beet cultivation. Thus, the use of residues or by-products like banana peels, shaddock peels or apple wastes could be a promising option for reducing the impacts associated with the HC anode and with that the whole battery. Finally, the use of a fossil precursor, petroleum coke, also shows very favourable results, basically because of the much lower amounts of raw material required (a demand of 1.14 kg of coke is estimated per kg of HC compared to 20 kg of carbohydrate; more details see ESI). Nevertheless, while this analysis can show up the tendencies, its limitations have to be taken into account: (i) the HC production process (and the yields), but also the upstream processes could vary significantly depending on the type of residue used; (ii) the precursor might have significant influence on the final electrochemical properties of the HC, and (iii) for
by-products like petroleum coke or residues, the methodology used for allocating the environmental burdens of the main process and the upstream processes can affect the results considerably. Especially for the petroleum coke, the latter can be expected to increase in future, e.g. for growing shares of unconventional oils from tar sands. Thus, a separate exhaustive study of the environmental impacts of HC production would be highly recommendable.

Future improvement potentials

SIBs show some important environmental advantages compared to existing LIB technologies. The possibility to use aluminium both for the anode and the cathode avoids the need for copper, with the latter being one of the main drivers for the impacts caused by the production of LIBs. On the other hand, hard carbon is needed as anode material, whose production from sugar is associated with relatively high impacts, partially neutralizing the benefit of the avoided copper. Thus, a hard carbon with low impacts should be favoured, for example from organic waste materials. The production of the cathode material is also relevant for the overall environmental performance. Especially the need for nickel shows high associated impacts in several impact categories, which stem from nickel mining and nickel sulphate production as precursor for nickel carbonate. Reducing or eliminating the nickel content in the cathode active material should therefore be another objective for reducing impacts. Nevertheless, changing the cathode material composition requires a more in-detail study, since it would change the electrochemical performance of the battery as well.

Energy (electricity and heat) demand for SIB manufacturing, assumed to be identical as for LIBs, is a third important driver for environmental impacts. Improving the energy efficiency of the manufacturing process, strongly driven by the dry room needed for cell assembly,7 could decrease the environmental impacts for both SIBs and LIBs.

Another critical factor, especially under GWP aspects, is the binder used for electrode production. PVdF is used as binder for the cathode, which is also the dominating one in LIBs.35,42 Its production is associated with very high emissions of GHG gases and thus an important contributor to the GWP. In consequence, the use of alternative, water based binders also for the cathode could further reduce GHG emissions,15 both for SIBs and LIBs (more details in the ESI).

Finally, the minimization of the required amount of electronic components (cables, BMS) could improve the environmental performance of SIBs, being these also important contributors to the overall impacts. Again, this applies in the same way to LIBs.

Conclusion

On energy capacity basis (1 kWh of storage capacity), and with an assumed cycle life of 2,000 cycles, the assessed SIB shows promising results already at the lower end of those of existing LIBs. It can be assumed that optimization potential is still given and thus a better performance can be achieved, especially by carefully selecting the cathode composition taking into account environmental aspects and by reducing the impacts associated with the hard carbon. Nevertheless, the cycle life is key for a good performance in this regard, why increasing cycle life is one of the first parameters that should be focused on when aiming at providing alternatives to Li-Ion batteries under environmental aspects. With lifetimes of around 3,000 cycles, the assessed SIB would already outperform existing LIBs under environmental aspects, and, if cycle lives close to those of LFP-LTO type LIBs could be achieved, even these. In the same way, the internal charge/discharge efficiency plays a key role, and achieving an efficiency only slightly above that of current LIBs can provide substantial advantages over lifetime.

When taking into account the low technical maturity of SIBs, the improvements that can be made in comparison to existing LIBs are promising. Still, they are not fundamental, why also economic advantages are required for their future success. The cost of LIBs is partially driven by the high cost of raw materials, which could probably limit their application in large-scale in energy storage. The use of more abundant raw materials in SIBs will bring advantages in this regard. A full economic assessment will be required to comprehensively demonstrate the possible advantages of Na-ion batteries under this perspective.

Furthermore, the used impact assessment methodology fails to quantify the (metal) resource depletion in a satisfactory way, considered to be one of the strengths of SIBs. A dedicated study of these aspects would provide further insights into the future potentials of SIBs.

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Abbreviations

Battery chemistries
C Carbon (graphite for battery electrodes / anodes)
HC Hard Carbon
LFP Lithium Iron Phosphate
LMO Lithium Manganese Oxide
NCA Lithium Nickel Cobalt Aluminium Oxide
NCM Lithium Cobalt Manganese Oxide
NMMT Sodium Nickel Manganese Magnesium Titanium Oxide
LTO Lithium Titanate

Environmental impact categories
CED Cumulative Energy Demand
CED_n Renewable Energy Demand
FDP Fossil Depletion Potential
FEP Freshwater Eutrophication Potential
FETP Freshwater Eco-Toxicity Potential
GWP Global Warming Potential
HTP Human Toxicity Potential
MDP Metal Depletion Potential
MEP Marine Eutrophication Potential
METP Marine Eco-Toxicity Potential
ODP Ozone Depletion Potential
PMF Particulate Matter Formation
POF Photochemical Ozone Formation
TAP Terrestrial Acidification Potential
TETP Terrestrial Eco-Toxicity Potential

Others
CMC Carboxymethylcellulose
DWC Dimethyl Carbonate
DoD Depth of Discharge
EC Ethylene Carbonate
GHG Greenhouse Gas
HC Hard Carbon
LCA Life Cycle Assessment
LCI Life Cycle Inventory
LIB Lithium-Ion Battery
NMP N-Methyl-2-Pyrrolidone
PVDF Polyvinylidenefluoride
SBR Styrene- Butadiene Rubber
SIB Sodium-Ion Battery
TOC Toxic Organic Compounds

References
ToC entry

Life cycle assessment for the production of a sodium-ion battery with a layered transition metal oxide and hard carbon.

Broader context

Sodium-ion batteries (SIBs) are emerging as potential alternative/complementary to lithium-ion batteries (LIBs). However, no quantification of the potential environmental impacts for the production of SIBs exists. This work closes this gap presenting a prospective life cycle assessment for the production of a sodium-ion battery with a layered transition metal oxide as positive and hard carbon as negative electrode material on battery component level. SIBs are found to be promising under environmental aspects, showing, per kWh of storage capacity, environmental impacts at the lower end of the range published for current LIBs. Still significant improvement potential is given, especially by reducing the environmental impacts associated with the hard carbon production and by reducing the nickel content in the cathode. For hard carbons, the use of organic waste can be considered promising in this regard. Regarding the energy storage capacity over lifetime, achieving a high cycle life is one of the most important parameter when aiming at providing alternatives to LIBs under environmental aspects. In the same way, the internal charge/discharge efficiency plays a key role, and achieving an efficiency only slightly above that of current LIBs can provide substantial advantages over lifetime.