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Sodium-Ion Batteries with $Ti_1Al_1TiC_{1.85}$ MXene as Negative Electrode: Life Cycle Assessment and Life Critical Resource Use Analysis

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Abstract: Electrochemical storage systems are an enabling solution for the electric system ecological transition, allowing a deeper penetration of nonprogrammable renewable energy resources, such as wind and solar energy. Lithium-ion batteries (LIBs) are state of the art energy storage technology. Nevertheless, LIBs show critical problems linked to their production, especially for what concerns energy consumption, greenhouse gas emissions, and rare raw materials use. Finding alternative storage technologies seems crucial for support energy transition, but at the same time, it is important to study their sustainability from the very beginning of their technological development. Using this framework, this paper presents a life cycle based environmental-economic assessment, comparing Na-ion coin cells ($Ti_1Al_1TiC_{1.85}$ MXene as anode material) with LIBs. LCA results show that the assessed Sodium-ion batteries (SIBs) are less environmentally friendly than LIBs, an outcome driven by the SIBs' lower energy density. However, if results are shown by mass, SIBs can represent potential alternatives to LIBs. On the other hand, the analysis shows that even Na-ions already use less critical resources, both in absolute and in relative values, highlighting the need, at least for the European Union, to find valid alternatives to LIBs if the 2050 decarbonization targets are to be met.

Keywords: life cycle assessment; commodity life cycle costing; sodium-ion batteries; lithium-ion batteries; MXenes

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1. Introduction

Electrochemical storage systems are qualifying solutions for the Italian electric system transition, helping the electric network to be more flexible and able to host renewable energy sources [1]. Nevertheless, Lithium-ion batteries (LIBs), the current best storage technology, show critical issues linked to their production with special reference to construction process energy consumption, CO_2 and greenhouse gas emissions, and the use of rare raw materials.

For a sustainable development or ecological transition, it is important to find alternative electrochemical storage technologies [2] to be used in conjunction with Li-Ion ones, especially when energy density needs are less stringent [3].

Considering that these technologies are currently under development, it is meaningful to evaluate their sustainability, both in environmental and economic terms [4].

In this perspective, a life cycle approach represents an appropriate way to assess environmental and economic impacts, using Life Cycle Assessment (LCA) and an economic indicator, the Commodity Life Cycle Costing (C-LCC) which quantifies, in economic terms, natural resources use during a product life cycle, focusing on those characterized by a high degree of supply risk (critical materials) [5].

During a LCA analysis, the potential environmental impacts are evaluated throughout the entire life cycle of a product or service. The upstream (material inputs needed for production) and downstream (like waste management) processes associated with the production, use phase, and disposal are also included.

The International Organization for Standardization provides guidelines and requirements for conducting a Life Cycle Assessment according to ISO 14040 [6] and 14044 [7].

The C-LCC indicator is an economic measure of resource use derived from market prices, which aims at quantifying the extent to which a product or process exploits natural resources during its life cycle. This indicator can be computed considering critical materials only (as defined by the European Commission) to assess a product's resilience towards potential supply shocks due to geopolitical factors.

Nowadays, Sodium-ion batteries (SIBs) are promising battery technology and the most auspicious successors to lithium technology, with good theoretical environmental and electrochemical performance. Nevertheless, the up-to-date anode material, hard carbon, suffers from poor cyclability and rate capability [8].

The huge application of electrochemical energy storage devices entails the development of new chemistries. MXenes are a vast class of 2D-materials of the general formula $M_{n+1}X_nT_x$ (M = transition metal, X = C or N, and T = M-terminating group). Considering the peculiar structure, charge transport, and surface properties, MXenes are ideal and considered promising materials for energy storage applications, such as anodes for sodium-ion batteries [9–11]. The work of Ferrara et al. shows the recent articles that summarize the potential of MXenes in different energy storage applications [11].

The environmental impacts of LIBs were intensively investigated [12], however, there is a lack on life cycle assessment of SIBs. Peters et al. published a complete LCA of SIBs, providing a full SIB model and corresponding inventory data [13]. Authors found that, when a similar lifetime is achieved, SIBs are potentially competitive with LIBs in terms of environmental impacts. Other works were focused on different electrode materials [14], costs, or material demand [15,16]. Nevertheless, all works present hard carbon as an anode material.

The performance of new materials or new electrode configuration is typically evaluated using hand-made coin cells that are easy to make and can give reproducible data. During this research, it was very challenging to find any published LCA analyses of coin cell batteries (for laboratory investigation and/or for commercial use), which is noteworthy, considering how extensive they are and how long they have been used for research investigation. Only Benveniste et al. [17], to our knowledge, performed LCA analyses on Li-S battery coin cells.

This study aims at eliminating these gaps by providing a life cycle assessment and resource (commodities) life cycle costing of SIB coin cells with $Ti_1Al_1TiC_{1.85}$ MXene as anode material, and comparing SIB with LIB, considering new methods to compare a pilot laboratory product (sodium) to an industrial one (lithium).

2. Materials and Methods

2.1. Life Cycle Assessment

2.1.1. Goal and Scope

The aim of this study is to analyze the potential environmental impacts of SIBs with $Ti_1Al_1TiC_{1.85}$ MXene as anode material.

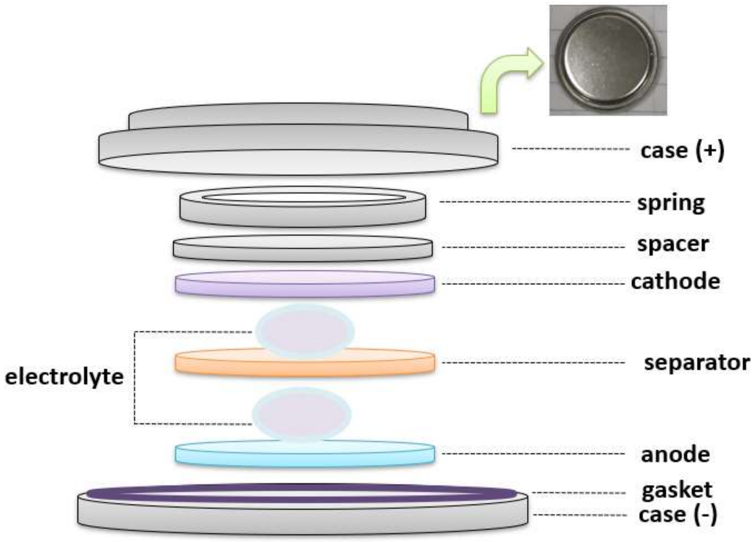
All impacts related to the batteries' production were considered: extraction and processing of raw materials, production of battery components, and their assembly. The end-of-life (EoL) phase is not considered due to lack of data and the early stage of technology development.

The environmental assessment was assessed in SimaPro 8.3 software using Ecoinvent 3.3 ("cut-off" allocation) as a background database and the Environmental Footprint (EF) methodology for impact assessment.

EF methods quantity the environmental performance of products and organizations throughout their life cycle, based on internationally agreed upon, scientifically valid assessment methods [18]. It covers 16 environmental impact categories that are reported in this study, and special attention was given to the climate change and the resource use, minerals and metals, impact categories. Considering energy transition, these are two of the most relevant categories: Climate change, since it constitutes its objective and resource use, mineral and metals, as it is the one that potentially contains the greatest risks [19]. The functional unit is 1 kWh of battery capacity.

2.1.2. Life Cycle Inventory (LCI)

The Life Cycle Assessment study includes extraction and processing of raw materials, production, and assembly of battery components. Battery components are divided into the anode, cathode, separator, and coin or packaging (case, gasket, spring, and spacer) Figure 1.



(**a**)

(**b**)

Figure 1. Na-ion coin battery: (**a**) schematic representation of the Na battery and (**b**) photo of the coin individual parts.

The SIBs in this study represent two stages of technological development: Na_Lab, laboratory scale, and Na_Ind, which represents the hypothetical composition of a SIB based on the chemistry of [20] and considering industrial production and efficiencies deduced from LIB production taken from [21].

To compare results with LIBs, an Industrial coin LIB, Li_Ind, was also considered, starting from data available in [21]. Table 1 summarizes the characteristics of the different batteries.

Table 1. Electrochemical characteristics and performance of the analyzed coin batteries (Na_Lab: Na Laboratory; Na_Ind: Na Industrial; Li_Ind: Li Industrial).

Battery	Cathode	Anode	Cell Voltage	Nominal Capacity	Weight	Battery Energy Density
			V	mAhgMxene^{-1}—Na Ah-Li	g	kWh kg^{-1}
Na_Lab	$Na_{0.44}MnO_2$	Mxene_$Ti_1Al_1TiC_{1.85}$	2.0	110	7.18	1.26×10^{-4}
Na_Ind	$Na_{0.44}MnO_2$	Mxene_$Ti_1Al_1TiC_{1.85}$	2.0	110	6.00	4.29×10^{-4}
Li_Ind	$LiNi_{0.5}Mn_{0.3}C_{0.2}O_2$	Graphite	3.6	20	6.02	3.37×10^{-3}

In the case of the LIB, for anode and cathode weights, a coin cell was reassembled in the laboratory, cutting electrodes extracted from an NMC pouch cell of an automotive battery and considering only one side of the current collector of active materials as in a coin cell (while in pouch cells, the active material is on both sides of the current collector). Amounts of remaining components (electrolyte, separator, etc.) were deduced from [21]. Coin batteries mass composition, by components, is reported in Table 2.

Table 2. Battery coin's mass composition (g), by components.

	Na				Li	
1 Coin	**Laboratory**	**%**	**Industrial**	**%**	**Industrial**	**%**
Cathode	**0.0355**	0.49%	**0.0468**	0.78%	**0.0468**	0.78%
Active material	0.0172	0.24%	0.0351	0.58%	0.0344	0.57%
Binder + carbon black	0.0043	0.06%	0.0011	0.02%	0.0018	0.03%
Al	0.014	0.20%	0.0106	0.18%	0.0106	0.18%
Anode	**0.0191**	0.27%	**0.0227**	0.38%	**0.0414**	0.69%
Active material	0.0041	0.06%	0.0117	0.19%	0.0223	0.37%
Binder + carbon black	0.001	0.01%	0.0004	0.01%	0.0009	0.01%
Al (Na) or Cu (Li)	0.014	0.20%	0.0106	0.18%	0.0182	0.30%
Electrolyte	**1.1845**	16.51%	**0.0217**	0.36%	**0.0217**	0.36%
Separator	**0.0268**	0.37%	**0.0004**	0.01%	**0.0004**	0.01%
Coin (case)	**5.91**	82.36%	**5.91**	98.47%	**5.91**	98.17%
Total weight	**7.1758**	100%	**6.0016**	100%	**6.0204**	100%
Weight excluding case	1.2658	-	0.0916	-	0.1104	-

Mass composition of the Na_Lab battery was determined by primary data, choosing the best performing coin battery described in [20]. The Na_Ind mass composition was determined by combining primary data and assumptions for possible industrial development, considering the current LIBs. In particular, it was established that the maximum amount of cathode material that the coin could contain, hence the corresponding amount of anodes material. The selection and the proportion of nonactive materials (separator, binders . . .) and electrolytes were deduced from [21] in order to simulate industrial production (similar to [13]). Further details of the hypothesis for Na-Ion industrial batter are reported in Table 3 and in Section 3.2.

Table 3. Characteristics of the assessed coin batteries (Na_Lab: Na laboratory scale; Na_Ind: Na Industrial scale: Li-Ind: Li industrial scale).

<table>
<tr><th></th><th></th><th>Na_Lab</th><th>Na_Ind</th><th>Li_Ind</th></tr>
<tr><td rowspan="5">Cathode</td><td rowspan="2">Active material</td><td rowspan="5">Primary data</td><td>Active material weight is the same as in the Li_Ind</td><td>Disk weight: primary data</td></tr>
<tr><td>97% active material</td><td>Active material balance as Li-ion batteries reported by [21]</td></tr>
<tr><td rowspan="2">Binder + carbon black</td><td>3% binder + carbon black</td><td rowspan="2">Binder + carbon black, balance as Li-ion batteries reported by [21]</td></tr>
<tr><td>NMP weight is the same as in the Li_Ind</td></tr>
<tr><td>Al</td><td>Al thickness is the same as in the Li_Ind</td><td>Al thickness calculated assuming the same ratio Al thickness weight/cathode weight as Li-ion batteries reported by [21]</td></tr>
</table>

Table 3. *Cont.*

		Na_Lab	Na_Ind	Li_Ind
Anode	Active material	Primary data	Ratio cathodic active material/anode active material = 3	Disk weight: primary data
			97% active material	Active material balance as Li-ion batteries reported by [21]
			HF weight = stochiometric weight + 10%	
	Binder + carbon black		3% binder + carbon black	Binder + carbon black, balance as Li-ion batteries reported by [21]
			NMP weight is the same as in the Li_Ind	
	Al (Na)		Al thickness is the same as in the Li_Ind	Cu disk thickness from primary data
	Cu (Li)			
Electrolyte		Primary data	The same weight as in the Li_Ind	Weight considering the same ratio electrolyte/cell Weight of the Li-ion batteries reported by [21]
Separator		Primary data	The same weight as in the Li_Ind	Weight considering the same ratio separtor/cell Weight of the Li-ion batteries reported by [21]
			Industrial separator type as the one reported by [13]	
Coin (case)		Primary data		
Energy consumption		Monitoring	As Li-ion cell production reported by [21] + 10% for dry room process	As Li-ion cell production reported by [21]

The coin case represents 82% of the total mass in the case of Na_Lab, and more than 98% for the other batteries. Excluding coin case weight (the same for all battery types), Figure 2 shows the percentage, by mass, of the several components of the batteries considered.

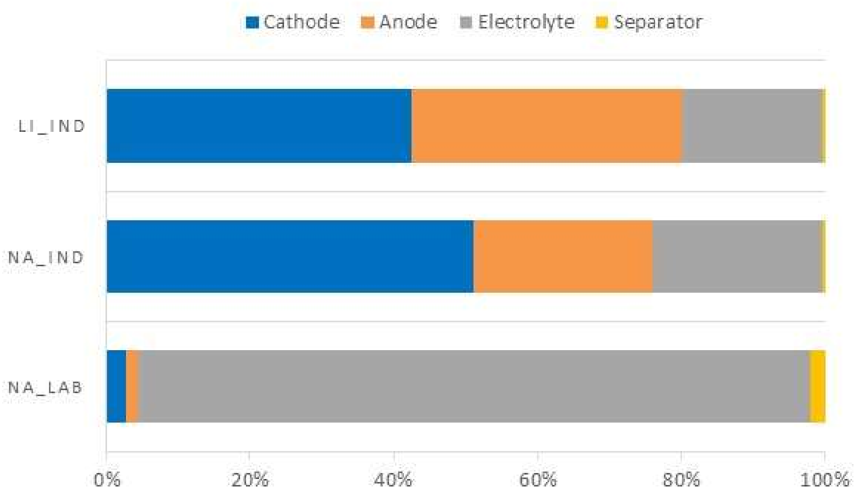


Figure 2. Battery coin's mass balance, by components, excluding coin case weight.

Table 3 provides coin battery characteristics. The full inventory of components and materials can be found in the Supplementary Materials (Supplementary Materials, Section S2)).

2.2. Commodity Life Cycle Cost Indicator (C-LCC)

The environmental performances of SIBs and LIBs, assessed with LCA techniques, have been measured also in terms of resource use through the Commodity Life Cycle Cost indicator (C-LCC) [5]. Such an indicator is based on market prices and quantifies, in monetary units, the extent to which a product exploits natural resources during its life cycle. The indicator is inspired by LCA and life cycle costing (LCC) techniques: costs are treated like characterization factors, while the classification and characterization phases are performed, such as in a conventional Life Cycle Impact Assessment [5].

The C-LCC uses market prices (or their proxies) as a measure of resource scarcity and, for this reason, relies on fewer assumptions with respect to other economic resource scarcity indicators, such as the mineral and fossil depletion indicators developed by ReCiPe [22].

Many studies ([23–25]) argue the need to include "criticality" in LCA studies, given the increasing importance of critical materials for modern and high-tech appliances, as well as technologies related to clean energy production and storage. Critical materials are materials intensively used in several supply chains but are characterized by a high supply risk, which can depend on either physical availability or geo-political factors. Therefore, an alternative version of the C-LCC is also developed, considering only those materials included in the European Commission's list of critical raw materials [26].

The raw materials considered to compute the C-LCC indicator are those included in the Mineral Fossil and Renewable Resource Depletion indicator of the International Reference Life Cycle Data System [27]. Such a list can be expanded, like in this study, to consider materials non included in the Mineral Fossil and Renewable Resource Depletion indicator but nonetheless employed in the life cycle of the batteries considered. Materials considered also include secondary energy sources and energy produced from renewable sources. They do not include water consumption and land-use changes.

Price data come from open-access data sources, such as the International Monetary Fund [28] and Eurostat [29] (the latter for energy prices). In most cases, however, market prices must be proxied with export unit values. International trade data are retrieved from the Comtrade database [30] and, for rare earths, from the Eurostat's Comext database [31] and the United States Trade Commission [32], which both have more detailed data.

Reference prices used in the analysis are average prices calculated over the period of 2011–2020 and expressed in euros (at 2020 prices) (Original price series are expressed in current US dollars; for this reason, they are converted to euros using annual nominal exchange rates and then adjusted for inflation using the Euro Area GDP deflator). A ten-year window is chosen as a compromise. On one hand, it is sufficiently long to limit the influence of short-term fluctuations on the long-term price trends and, on the other end, sufficiently short to reflect expectations of economic agents towards resource availability, at least in the medium-term. Moreover, calculating the average over longer periods might not be the best option to effectively assess the increasing importance that some materials have been experiencing only recently (i.e., cobalt thanks to the breakthrough of lithium-ion batteries). Reference prices are provided in a spreadsheet format in the Supplementary Materials.

Minimum and maximum values in the 1995–2020 period are used in the Monte Carlo uncertainty analysis.

3. Results and Discussion

3.1. Life Cycle Impact Assessment (LCIA) of Na-Ion Battery at Laboratory Scale

The life cycle environmental impacts of the coin battery Na-ion at laboratory scale are shown in Table 4.

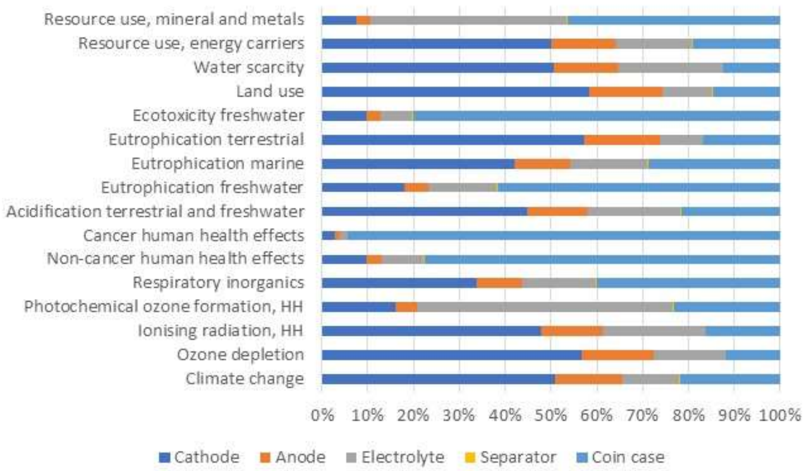
Table 4. Environmental impacts of the Na-ion coin battery at laboratory scale. Data refer to 1 kWh of coin battery capacity.

Impact Categories	Units	Total
Climate change	kg CO_2 eq	5.56×10^4
Ozone depletion	kg CFC11 eq	5.69×10^{-3}
Ionizing radiation, HH	kBq U-235 eq	1.67×10^3
Photochemical ozone formation, HH	kg NMVOC eq	2.25×10^2
Respiratory inorganics	disease inc.	2.56×10^{-3}
Non-cancer human health effects	CTUh	1.07×10^{-2}
Cancer human health effects	CTUh	3.87×10^{-3}
Acidification terrestrial and freshwater	mol H+ eq	3.14×10^2
Eutrophication freshwater	kg P eq	4.53
Eutrophication marine	kg N eq	3.86×10
Eutrophication terrestrial	mol N eq	7.71×10^2
Ecotoxicity freshwater	CTUe	5.37×10^4
Land use	Pt	4.84×10^5
Water scarcity	m3 depriv.	2.17×10^4
Resource use, energy carriers	MJ	6.92×10^5
Resource use, mineral and metals	kg Sb eq	3.05×10^{-1}

In Figure 3, results are presented broken down: (a) the different components; (b) the different components and the energy consumption, and (c) the different components and the energy consumption, excluding the coin case contribution.

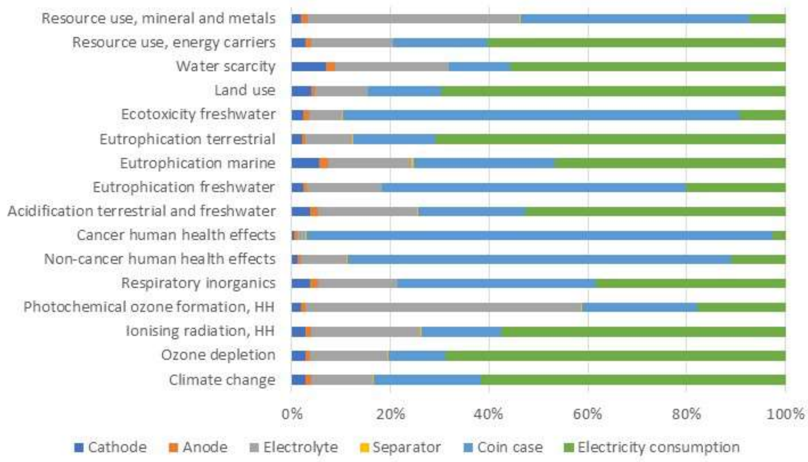
The energy necessary to produce the battery is one of the main contributions to the Climate Change indicator, representing 62% of it. If the coin case is not considered, the contribution rises to 79% (Figure 4).

For the resource use, mineral and metals (RMM) indicator, the electrolyte contributes over 40% (80% if the coin case is not considered in the total).



(**a**)

Figure 3. *Cont.*



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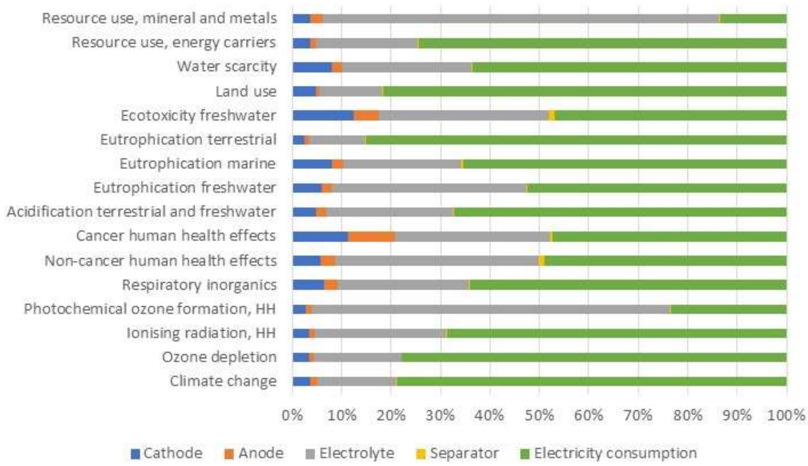


(**c**)

Figure 3. Life cycle impacts on Na-ion coin battery at laboratory scale, broken down: (**a**) the different components; (**b**) the different components and the energy consumption; and (**c**) the different components and the energy consumption, excluding coin case contribution.

If coin case contribution is excluded (which is about 82% by weight of the battery, Table 3), the electrolyte contributes 16% to the GWP indicator, followed by the cathode, anode, and electrolyte. For details, see Figure 4.

Regarding the positive active material production phase, this accounts for about 4% of the Climate change (CC) impact category and if the production of 1 kg of cathode is considered, the energy consumption is the main contribution to the CC impact indicator. Likewise, in the case of the anode, it is the energy consumption the main contribution to the same indicator (Sankey diagrams can be found in the Supplementary Materials (Supplementary Materials, Section S3).

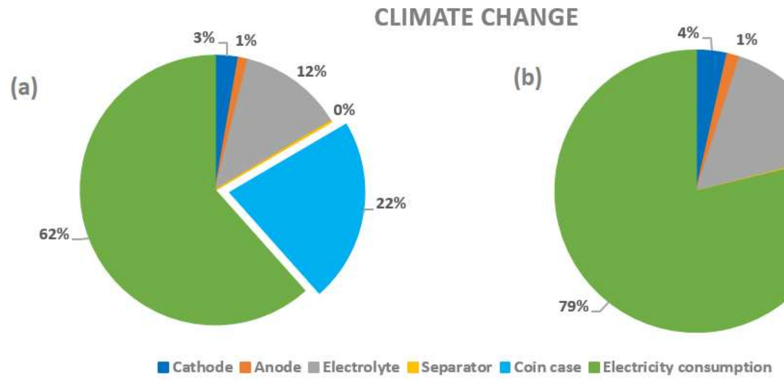


Figure 4. Climate change results in 1 kWh of coin battery capacity, broken down: (**a**) the different components and the energy consumption and (**b**) the different components and the energy consumption, excluding coin case contribution.

Coin case, electrolyte, and energy consumption are the main sources of environmental impacts. These results refer to a laboratory scale and these indications are not directly scalable to a hypothetical industrial scale as materials (for example separator, which affects the amount of electrolyte used) and the processes (which affect energy consumption) could be completely different.

As in the case of Li-ion batteries, the predominant role of the cathode over the anode remains confirmed for the CC and RMM categories, which are the most relevant for decarbonization and circularity.

To our knowledge, the only study available in literature on the potential environmental impacts related to sodium batteries is Peters et al. [13]. According to this study, the electricity consumed during cell production is responsible for 21% of the total CC impacts. It is important to highlight that this study considers the energy requirement identical to that of Li-ion batteries at an industrial level, which is, therefore, a very different reality of the present work.

3.2. Comparison of Na-Ion Coin Battery (Laboratory) with Li-Ion Coin Battery (Industrial)

The LCA methodology application to technologies currently under development (laboratory level, pilot scale or project level), presents two main criticalities: the lack of data (except for the experimental level), which makes these technologies not comparable with existing technologies, and the effective implementation and use of them in future contexts, which are characterized by environmental characteristics and markets different from the situation at the time of the study [33].

To overcome these issues and make LCA an effective decision support tool for environmental policies, it is necessary to adopt an approach that allows both to evaluate the impacts of emerging technologies on an industrial scale, and to consider the future evolution of the system. In this context, there is an innovative application of the methodology defined Ex-ante LCA [34]. The term refers to the "life cycle assessment of a new technology, before it is commercialized, in order to support the decision-making process under development towards the creation of an environmentally competitive technology" [35]. However, although in recent years particular interest has been observed, up to date, there is still no defined and clear procedure or optimal application method.

The methods applied in the Ex-ante LCA evaluation are many and, in this study, the Proxy Technology Transfer—Process (PTTp) is considered among the Technology Development methods [33]. This method involves identifying the most suitable technology on the market to be used as a proxy for the transition from laboratory or pilot scale to industrial scale, enriching the available dataset. For more details on the methods applied in the ex ante LCA assessment, refer to [33].

For the Na-ion battery, considering an industrial production, the Li-ion battery, widely distributed in the market and produced industrially, was taken as a reference (proxy). An industrial version of the Na-ion battery has been assumed: Na_Industrial. Characteristics and hypotheses considered are described in Table 3. The following assumptions were taken into consideration:

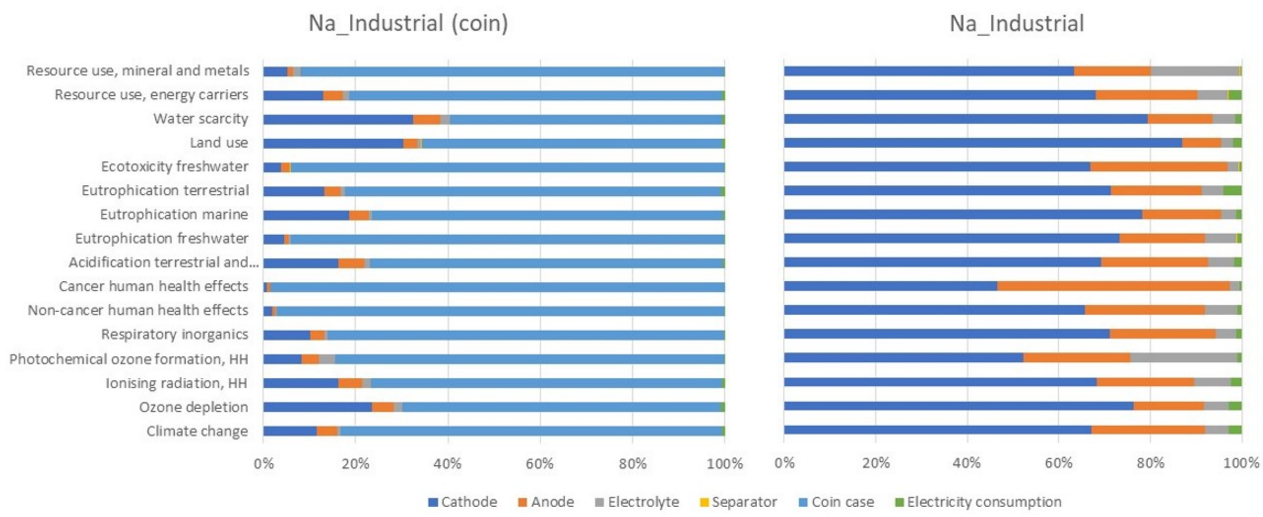
- For anode and cathode: the same ratio active material/binder + carbon black as industrial Li-ion cells (97% active material, 3% binder + carbon black [21]).
- The same amount of electrolyte as in [13].
- The same separator (and separator thickness) as in [13].
- The same energy consumption of the Li-ion NMC cells plus an increase of 10% (both Na-ion electrodes must be produced in the absence of water and oxygen, therefore a dry room is required (maximum 1 ppm water and 2 ppm oxygen) [20].
- Ratio (mass) of cathodic active material/anodic active material = 3 [20].
- Use of substances in the same proportion as Li-ion batteries, or stoichiometric quantity, to simulate industrial use (where the chemicals use is optimized) with an excess of 10%.
- The cathode active material weight is equal to the industrial Li cathode active material weight.

The life cycle environmental impacts of the assessed coin batteries are shown in Table 5. Data refers to 1 kWh capacity.

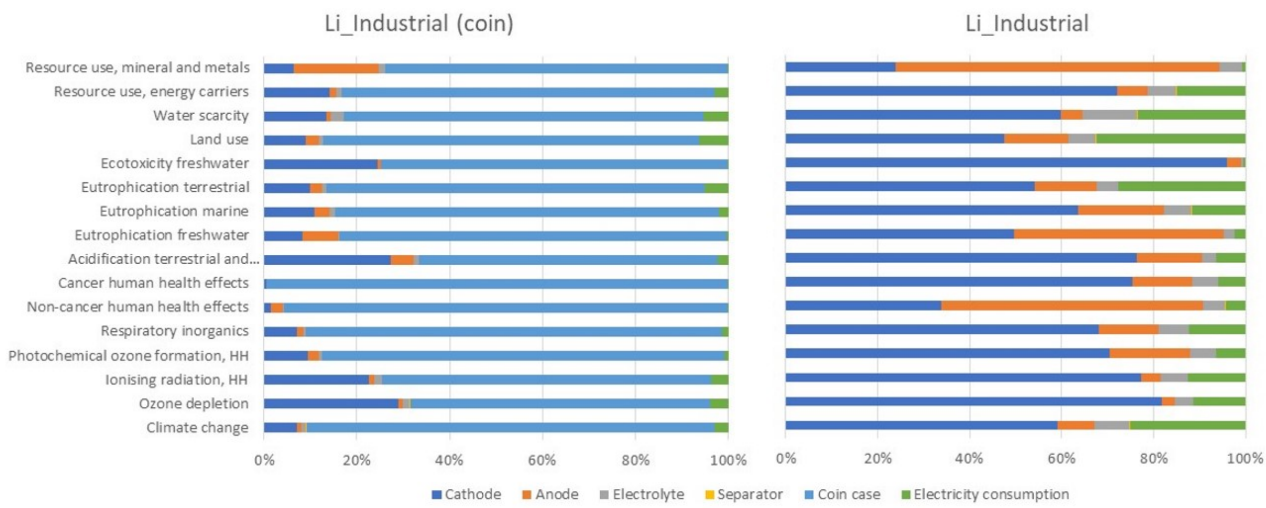
Table 5. Environmental impacts of the assessed coin batteries. Data refers to 1 kWh of coin battery capacity.

Impact Categories	Units	Na_Lab	Na_Ind	Li_Ind
Climate change	kg CO_2 eq	5.56×10^4	5.15×10^3	6.15×10^2
Ozone depletion	kg CFC11 eq	5.69×10^{-3}	3.38×10^{-4}	4.59×10^{-5}
Ionizing radiation, HH	kBq U-235 eq	1.67×10^3	1.25×10^2	1.70×10
Photochemical ozone formation, HH	kg NMVOC eq	2.25×10^2	2.18×10	2.69
Respiratory inorganics	disease inc.	2.56×10^{-3}	4.18×10^{-4}	5.09×10^{-5}
Non-cancer human health effects	CTUh	1.07×10^{-2}	2.99×10^{-3}	3.86×10^{-4}
Cancer human health effects	CTUh	3.87×10^{-3}	1.30×10^{-3}	1.64×10^{-4}
Acidification terrestrial and freshwater	mol H+ eq	3.14×10^2	3.10×10	4.69
Eutrophication freshwater	kg P eq	4.53	1.04	1.49×10^{-1}
Eutrophication marine	kg N eq	3.86×10	5.09	5.94×10^{-1}
Eutrophication terrestrial	mol N eq	7.71×10^2	5.52×10	7.03×10
Ecotoxicity freshwater	CTUe	5.37×10^4	1.60×10^4	2.57×10^3
Land use	Pt	4.84×10^5	3.83×10^4	3.92×10^3
Water scarcity	m3 depriv.	2.17×10^4	1.58×10^3	1.53×10^2
Resource use, energy carriers	MJ	6.92×10^5	5.71×10^4	7.30×10^3
Resource use, mineral and metals	kg Sb eq	3.05×10^{-1}	5.39×10^{-2}	8.54×10^{-3}

In Figure 5, results are shown broken down: (a) the different components and the energy consumption and (b) the different components and the energy consumption, excluding the coin case contribution.



(**a**)



(**b**)

Figure 5. Life cycle impacts result in 1 kWh of battery capacity: (**a**) Na Industrial and (**b**) Li Industrial. On the left side, results are distributed among all the different components, while on the right, the coin case contribution is excluded.

More than 98% of the different batteries' mass represents the coin case. Considering that large-sized batteries will not have a coin structure, the analysis of the environmental results is excludes its contribution. Nevertheless, as the battery size decreases, the environmental importance of the container (coin in this case) increases, and it is inversely proportional to the active component's energy density.

The Li_Ind has the best environmental performance (for all considered impact categories). Considering that the functional unit is 1 kWh of capacity, the worse environmental performances of Na_Ind are due to its lower energy density, eight times lower than Li_Ind (Table 2). It is therefore important for further SIBs development to achieve more competitive energy performances, at least near the LIB's level.

The positive electrode production is the main contribution to the CC impact indicator for both batteries (contributing 67% in the case of Na_Ind and 59% in the case of Li_Ind). During Na cathode production, the most impacting process appears to be the ink production phase, the cathodic active material production, and the use of citric acid (Sankey diagrams can be found in the Supplementary Materials (Supplementary Materials, Section S3). The same result is observed for the Li_Ind; the most impactful process is the production of cathodic active materials.

For the Na_Ind, the negative electrode has a contribution to the CC impact indicator of 25%. Also, in this case, the most impacful process is the ink production phase (Sankey diagrams can be found in the Supplementary Materials (Supplementary Materials, Section S3).

Electrolytes contribute to the Climate change indicator with a percentage below 10% (5% Na Industrial and 8% Li Industrial), while in the case of the separator, the contribution is below 0.2% (0.11% Na Industrial and 0.17% Li Industrial).

For the RMM indicator, the positive electrode production is the main contribution to the impacts. The electrolyte has a contribution of 19% in the case of the Na_Ind. Instead, the anode has a contribution of 17% (Na_Ind), much lower than the 70% obtained for the Li_Ind.

As previously mentioned, SIBs assessed in this study are characterized by a significantly lower energy density than Li-ion ones (Table 2); consequently the functional unit (1 kWh) is correlated to a greater mass of battery and therefore to a higher value of equivalent emissions.

Figure 6 shows the results of the impact assessment for the impact categories of Climate change and Resource use, minerals and metals, expressed in 1 kWh of capacity and 1 kg of battery. These are two of the most relevant categories for the energy transition: the first (Climate change), since it constitutes its objective, and the second (Resource use, minerals and metals), as it is the one that potentially contains the greatest risks [19].

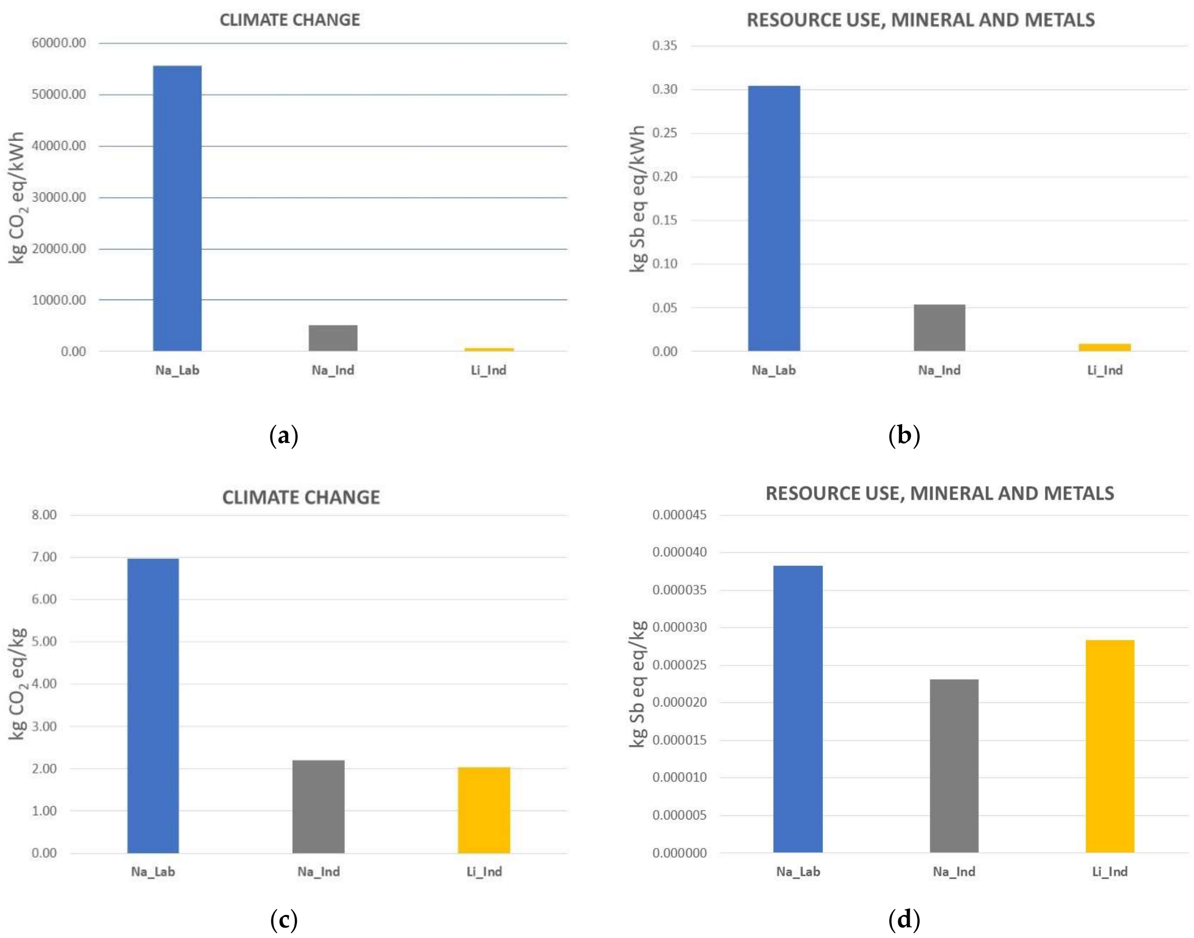


Figure 6. Impact assessment results for the impact categories Climate change and Resource use, minerals and metals, expressed per 1 kWh, (**a**) and (**b**), and per 1 kg of battery, (**c**) and (**d**).

Results for 1 kg of battery show that industrial sodium ion batteries could have CO_2 equivalent emission values very close to that of corresponding LIBs.

For the RMM category, always comparing batteries on a mass basis, the Na_Ind presents an impact reduction of about 20% compared to the Li_Ind. In this case, Na batteries are potential alternatives, as they use neither lithium nor cobalt, both rare materials used in NMC batteries.

3.3. Commodity Life Cycle Cost Indicator

The C-LCC indicator is calculated for both SIBs and LIBs, assuming that both are produced on an industrial scale. In both cases, alongside the baseline indicator, its critical materials counterpart is also computed. Figure 7 shows the baseline results.

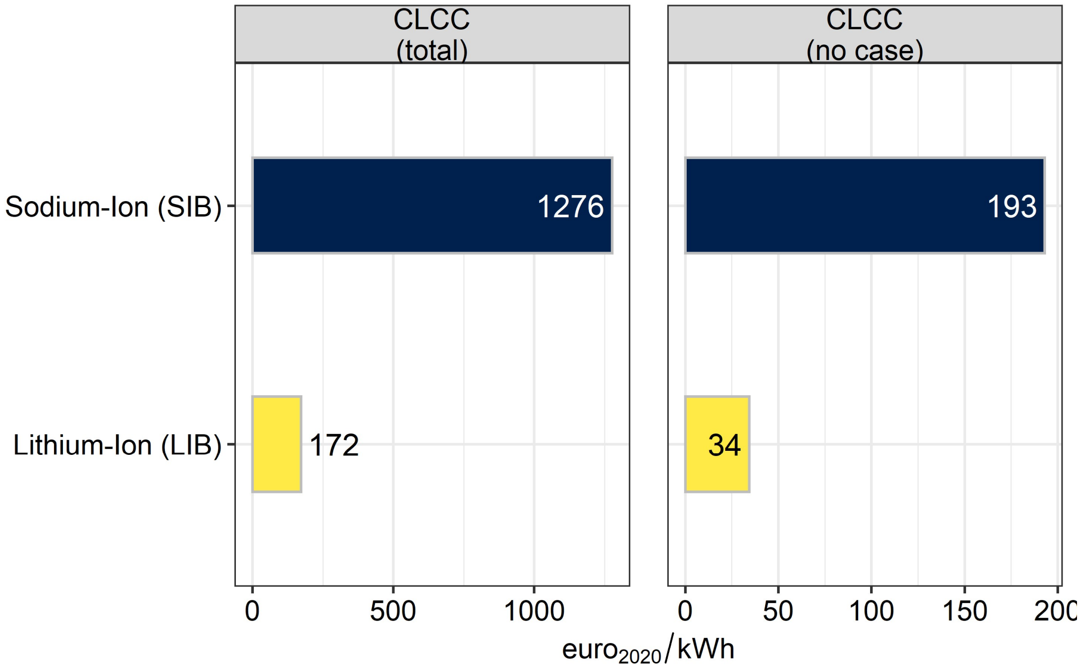


Figure 7. Commodity Life Cycle Cost indicator (C-LCC) calculated for SIBs and LIBs (industrial-scale production).

The SIB is characterized by a value of the C-LCC indicator that is more than seven times bigger than LIBs. This means that, even under the hypothesis that SIBs can be already produced at an industrial scale, its resource consumption is much larger than that of LIBs. Even when the battery case is not considered (which, being made from metal represents a significant share of the total C-LCC value), the picture does not change much, as Figure 8 suggests.

Apart from this case, the cathode is the component that weights the most on the total C-LCC indicator, for both batteries considered. The anode is more than two times more important for SIBs than for LIBs, which, on the contrary, are characterized by a much greater weight of electricity consumption.

The analysis of the C-LCC critical indicator is particularly interesting because the development of SIBs is aimed at finding an alternative to LIBs, which, although highly performing, are batteries that require a relatively high number of critical materials for their production. Figures 9 and 10 show the comparison in both absolute and relative terms.

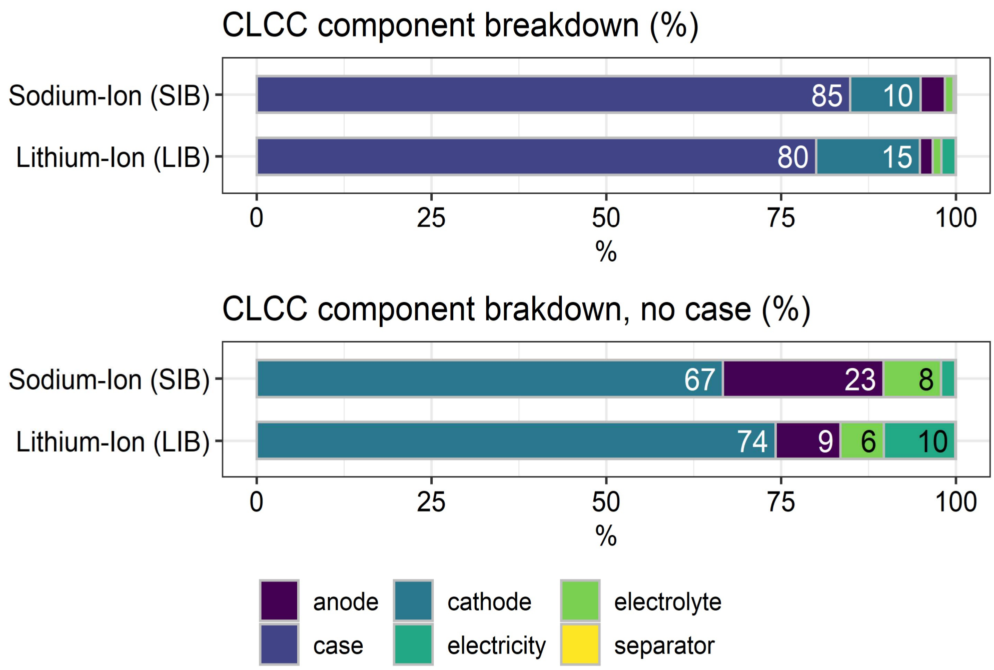


Figure 8. Commodity Life Cycle Cost indicator (C-LCC): component breakdown.

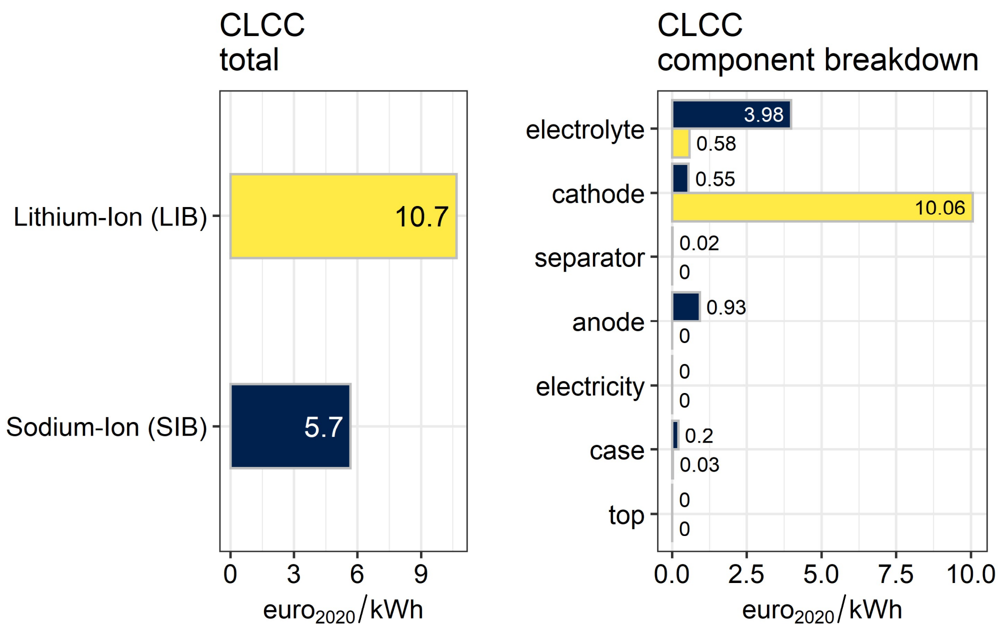


Figure 9. Critical Commodity Life Cycle Cost indicator—absolute values.

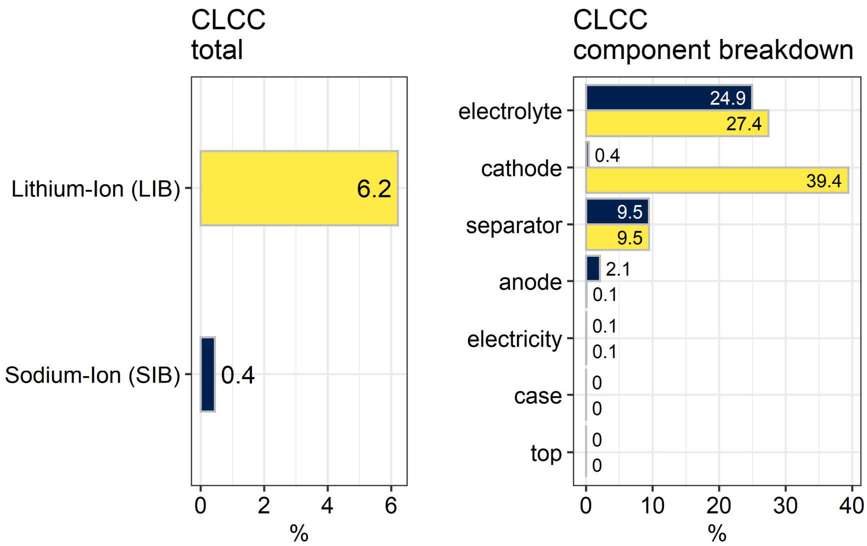


Figure 10. Critical Commodity Life Cycle Cost indicator: relative values (shared with respect to C-LCC total).

LIBs emerge as a battery type for which raw materials have the greatest importance, both in absolute and relative terms. Most of the difference lies on the cathode: the critical C-LCC indicator (calculated for each component) is made up by critical materials for more than 39% in the case of the LIB cathode, which dwarfs the 0.4% of its SIB counterpart.

The C-LCC indicator is based on market prices, which are characterized by high volatility and therefore, uncertainty. For this reason, an uncertainty assessment is performed with the Monte Carlo method. A high number of random prices is generated for each material considered, assuming triangular distributions (Parameters used to describe the triangular distributions are the minimum and maximum prices of each material during the 1995–2020 period and the average 2011–2020 used for the baseline indicator). The C-LCC indicator is therefore calculated for each set of simulated prices and the empirical distribution function is finally used to calculate the probability that, for both LIBs and SIBs, the C-LCC is lower than the baseline value. Figure 11 shows the simulation results.

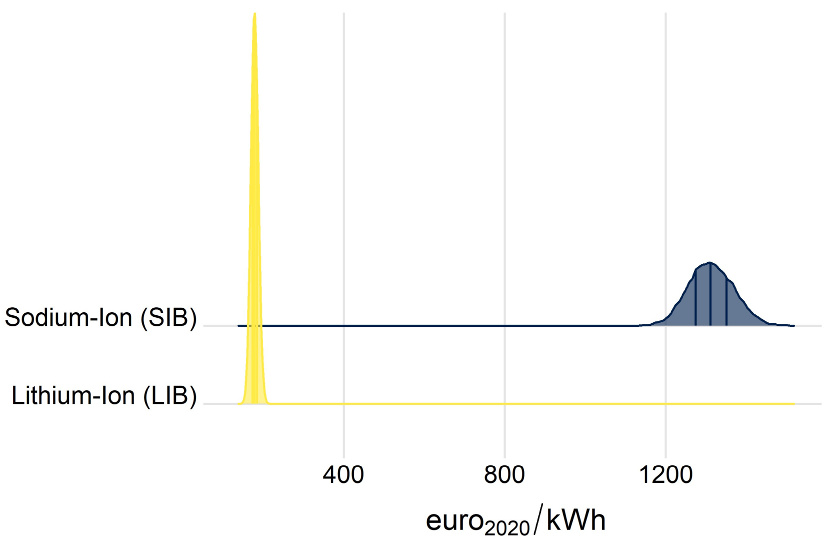


Figure 11. Critical Commodity Life Cycle Cost indicator: Monte Carlo simulation results.

Simulation results, in the case of LIBs, are much more concentrated around the mean and the median with respect to SIBs'. This means that market prices of some materials intensively used in the SIB life cycle are characterized by a higher degree of volatility than those used in an LIB. The probability that the C-LCC indicator calculated for SIBs becomes, due to price volatility, lower than that calculated for LIBs is zero, given the great difference in baseline values. The simulation results also show that the baseline C-LCC values, for both batteries considered, are relatively "optimistic", which means that the probability that, given price volatility, the value of the indicator becomes higher than the baseline is well above 70% in both cases.

4. Conclusions

Electrochemical storage systems could represent one of the efficient solutions towards a sustainable transition for the electricity system. Since these are rapidly expanding technologies, it is essential to evaluate their sustainability in a broad sense, both in environmental and economic terms. Life Cycle Assessment (LCA) and Commodity Life Cycle Costing (C-LCC) represent two suitable tools for evaluating the possible impacts and benefits (environmental and economic) connected to stationary storage systems.

SIBs' LCA was modelled, and an environmental and economic analysis of sodium batteries was developed, comparing these storage systems with the corresponding lithium-ion-based batteries.

LCA results show that the Li-ion-based battery has the best environmental performance, even compared to the hypothesis of an industrial-grade MXenes basedthe sodium ion battery.

The energy density of sodium ion batteries appears to be the limiting factor. In fact, if batteries are compared by mass (1 kg of produced battery), SIB's CO_2 equivalent emission values are very similar to those of the lithium battery, while for the Resource use, mineral and metals impact category, the sodium batteries have a reduction in impacts of about 20% compared to the LIB. In this case, SIBs can represent potential alternatives to LIBs, since they do not require lithium and cobalt for their production, which are rare materials used in these storage systems.

Similarly, the C-LCC results show that SIBs use a much larger amount of natural resources in their life cycle than LIBs do, even assuming that the former are produced on an industrial scale. Materials used in the SIB life cycle are also characterized, on average, by a generally higher volatility, as the Monte Carlo simulations suggest. When the C-LCC indicator is calculated considering critical materials only, however, the picture changes substantially. Even though the baseline LIB C-LCC indicator is more than seven times lower than SIB's, the critical C-LCC of the former is higher than that of the latter in both absolute and relative terms (as a share of the baseline indicator). This means that state-of-the-art LIBs are exposed to a much higher supply risk than their sodium-based counterparts and that the European Union must find reliable and cheap alternatives to LIBs in the decades to come if it is to reach its 2050 decarbonization targets. Although LIB's chemistries with reduced use of critical materials do exist and can be further developed, Lithium itself has been included in the European list of critical materials since 2020. Hence, the use of critical raw materials will remain an issue for LIBs for a long while (at least until a relevant part of raw materials will come from recycling). Nevertheless, apart from critical material use, LIBs will lead environmental performance until SIBs reach their energy density and similar energy efficiency during electrode production. SIBs seem to be a promising alternative characterized by lower potential geopolitical supply risk, but research is needed to reduce dramatically larger natural resource use and higher production cost.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/su14105976/s1. File S1: Na LCA and CLCC [36–40]; File S2: Reference prices.

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