Politecnico di Torino

Master's Thesis

Master of science in Environmental and Land Engineering

Life Cycle Assessment and Development of Si-S battery and comparison with the Li-ion Battery in electric vehicles

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Abstract

This thesis addresses the imperative need to curb global warming by limiting CO_2 emissions, particularly in the transportation sector, to meet the Paris Agreement's goal. Focusing on passenger cars, which contributed significantly to global CO_2 emissions, the study explores the coexistence of conventional and emerging battery technologies within the battery electric vehicle (BEV) industry. While conventional Li-ion batteries are widely used, emerging batteries, such as those incorporating silicon, sulfur, and biomass-derived carbon, show promising properties, although still need to be proven in practice.

In response to the growing emphasis on evaluating environmental impacts throughout a product's lifecycle, this research undertakes a Life Cycle Assessment (LCA) analysis of Silicon-Sulfur (Si-S) and Nickel Manganese Cobalt (NMC) batteries. The primary objective is to comprehensively understand the environmental footprints of these technologies, considering the lifecycle and emphasizing sustainability.

The study delves into the Si-S battery developed in the 2BoSS project at Barcelona's IREC international research institution, comparing it with a conventional NMC lithium-ion battery taken from literature. The Si-S battery, characterized by a Li2S-carbon composite cathode and a silicon nanowire-carbon composite anode, exhibits remarkable potential owing to the abundance of sulfur in the Earth's crust. The thesis aims to pave the way for environmentally friendly and sustainable battery technologies that align with the principles of future sustainable mobility.

The conclusion summarizes the key findings from the LCA analysis, focusing on Si-S and NMC batteries, employing data from the Environmental Footprint database. Results indicate that the Si-S battery, with its innovative materials and circular design, significantly outperforms the NMC battery across various environmental indicators. Energy consumption during production emerges as a crucial factor, prompting the use of renewable energies to mitigate environmental impacts.

While the study adopts a cradle-to-gate approach due to data limitations, ongoing research by various institutions aims to explore practical applications and address uncertainties in the use and end-of-life stages of the Si-S battery. The findings contribute valuable insights into the potential of Si-S batteries and advocate for their adoption in future sustainable mobility, emphasizing environmental and sustainable considerations.

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Introduction

To meet the Paris Agreement's goal of limiting global warming to 1.5°C above pre-industrial levels by 2050, CO_2 emissions must be reduced [1]. COP28 (Conference of the Parties in EU) featured the first comprehensive global assessment under the Paris Agreement, evaluating progress towards the climate goals set by the agreement. The energy sector stands out as an arena where immediate emissions reductions can yield significant impacts. During COP28, the EU and its member countries advocated for global energy objectives, including a shift away from fossil energy. The parties reached an agreement to gradually transition from fossil fuels in the energy sector by 2050 (https://www.consilium.europa.eu/). In recent years, governments have been making significant efforts to reduce CO_2 emissions and fossil fuel consumption in the transport sector by promoting the development of electric vehicles (EVs). Passenger cars using fossil fuels alone contributed to 39% of global CO_2 emissions in 2022 within this sector, according to the IEA's Sustainable Development Scenario [2].

In the current battery electric vehicle (BEV) industry, the coexistence of numerous conventional battery technologies alongside the ongoing research and development of emerging battery technologies is witnessed. Conventional batteries such as lead-acid, alkaline, and lithium-ion are commonly used in our daily lives. However, the presently available commercialized Li-ion batteries (LIBs) are reaching their theoretical energy-density limits, making them incapable of meeting the increasing demands of modern devices. Conversely, new technology batteries, often referred to as next-generation or future batteries, demonstrate superior properties in comparison to their conventional counterparts. It's crucial to note that this potential is mostly based on experiments and theories and hasn't been practically proven yet.[3]

In recent years, there has been a growing emphasis on evaluating the environmental impact of products throughout their entire lifecycle, driven by a heightened awareness of sustainability. This includes a coordinated effort to comprehensively assess the environmental risks and impacts associated with the product's lifecycle.

Achieving net-zero CO_2 emissions within this sector is an obligatory stride towards mitigating the adverse consequences of global warming. Despite the emission-free operational phase of electric vehicles, it is crucial to acknowledge that the production of electric vehicles, particularly concerning the battery, is associated with elevated emissions.

In the IREC international research institution in Barcelona, the 2BoSS project (derived from IREC) aims to advance sustainable battery technology by incorporating silicon, sulfur, and biomass-derived carbon. It will focus on developing innovative, durable batteries with a more circular design, and optimizing the processing of necessary raw materials. The goal is to reduce dependence on critical raw materials (CRM). This battery cell contains a Li_2S-carbon composite as cathode material, a silicon nanowire-carbon composite as anode material, providing specific capacities above 1 Ah g^{-1} and life above 2000 cycles in both cases. In the Earth's crust, sulfur stands out as one of the most abundant elements. When it is paired with lithium (Li), the resulting combination showcases a remarkably high theoretical capacity and energy density, reaching 2600 Wh kg^{-1}. On the other hand, a conventional NCM111-lithium-ion battery taken from the literature stands.

This thesis aims to undertake a comprehensive examination by employing a Life Cycle Assessment analysis for both Silicon-Sulfur (Si-S) and Nickel Manganese Cobalt (NMC) batteries. The primary objective is to gain an in-depth understanding of the environmental impacts associated with these battery technologies. By delving into the life cycle of Si-S and NMC batteries, this analysis will contribute valuable insights into their environmental footprints.

The main goal is to clear the way for advanced solutions that align with the principles of future sustainable mobility. Through this assessment, the research efforts to identify potential areas for improvement and innovation, thus contributing to the development of more environmentally friendly and sustainable battery technologies.

1 Literature Review

In recent years, Life Cycle Assessment (LCA) has found extensive application and adoption across various fields, garnering considerable attention and coverage in the process. Regarding the LCA of lithium-ion batteries in the automotive sectors, seventeen documents were suitable according to Temporelli et al. (2020). The bibliography following 2019 has been analyzed using the Scopus dataset (http://www.scopus.com), yielding an additional nineteen documents that align with the research topic, the papers devoted to the review of previous works are taken for granted. The documents are summarized in *table 1*.

Authors	**Title**	**Year**
Notter, D, A; Gauch, M; Widmer, R; Wager, P; Stamp, A; Zah, R; Althaus, H, J	Contribution of Li-ion batteries to the environmental impact of electric vehicle	2010
Majeau-Bettez, G; Hawkins, T, R; Strømman, A, H	Life Cycle Environmental Assessment of Lithium-Ion and Nickel Metal Hydride Batteries for Plug-In Hybrid and Battery Electric Vehicles	2011
Dunn, J, B; Gaines, L; Barnes, M; Sullivan, J	Material and Energy Flows in the Materials Production, Assembly, and End-of-Life Stages of the Automotive Lithium-Ion Battery Life Cycle	2012
U.S. Environmental Protection Agency	Application of Life-Cycle Assessment to Nanoscale Technology: Lithium-ion Batteries for Electric Vehicles	2013
Ellingsen, L, A, W; Majeau-Bettez, G; Singh, B; Srivastava, A, K; Valøen, L, O; Strømman, A, H	Life Cycle Assessment of a Lithium-Ion Battery Vehicle Pack	2014
Faria, R; Marques, P; Garcia, R; Moura, P; Freire, F; Delgado, J; de Almeida, A, T	Primary and secondary use of electric mobility batteries from a life cycle perspective	2014
Oliveira, L; Messagie, M; Rangaraju, S; Sanfelix, J; Rivas, M, H; Van Mierlo, J	Key issues of lithium-ion batteries from resource depletion to environmental performance indicators	2015
Richa, K; Babbitt, C. W; Nenadic, N, G; Gaustad, G	Environmental trade-offs across cascading lithium-ion battery life cycles	2015
Helmers, E; Weiss, M	Advances and critical aspects in the life cycle assessment of battery electric cars	2017
Romare, M; Dahllöf, L	The Life Cycle Energy Consumption and Greenhouse Gas Emissions from Lithium-Ion Batteries	2017
Cusenza, M, A; Bobba, S; Ardente, F; Cellura, M; Di Persio, F	Energy and environmental assessment of a traction lithium-ion battery pack for plug-in hybrid electric vehicles	2019
Dai, Q; Kelly, J, C; Gaines, L.; Wang, M	Life Cycle Analysis of Lithium-Ion Batteries for Automotive Application	2019
Ioakimidis, C, S; Murillo-Marrodàn, A; Bagheri, A; Thomas, D; Genikomaskis, K	Life Cycle Assessment of a Lithium Iron Phosphate (LFP) Electric Vehicle Battery in Second Life Application Scenarios	2019
Liu, C; Lin, J; Cao, H; Zhang, Y; Sun, Z	Recycling of spent lithium-ion batteries in view of lithium recovery: A critical review	2019
Kallitsis, E; Korre, A; Kelsall, G; Kupfersberger, M; Nie, Z	Environmental life cycle assessment of the production in China of lithium-ion batteries with nickel-cobalt-manganese cathodes utilizing novel electrode chemistries	2020

Sun, X; Luo, X; Zhang, Z; Meng, F; Yang, J	Life cycle assessment of lithium nickel cobalt manganese oxide (NCM) batteries for electric passenger vehicles	2020
The Advanced Rechargeable & Lithium Batteries Association	PEFCR - Product Environmental Footprint Category Rules for High Specific Energy Rechargeable Batteries for Mobile Applications	2020
Wang, F; Deng, Y; Yuan, C	Life cycle assessment of lithium oxygen battery for electric vehicles	2020
Yang, J; Gu, F; Guo, J	Environmental feasibility of secondary use of electric vehicle lithium-ion batteries in communication base stations	2020
Zhu, L; Chen, M	Research on Spent LiFePO4 Electric Vehicle Battery Disposal and Its Life Cycle Inventory Collection in China	2020
Accardo, A; Dotelli, G; Musa, M, L; Spessa, E	Life Cycle Assessment of an NMC Battery for Application to Electric Light-Duty Commercial Vehicles and Comparison with a Sodium-Nickel-Chloride Battery	2021
Iturrondobeitia, M; Akizu-Gardoki, O; Minguez, R; Lizundia, E	Environmental Impact Analysis of Aprotic Li–O2 Batteries Based on Life Cycle Assessment	2021
Koroma, M, S; Costa, D; Cardellini, G; Messagie, M	Life Cycle Assessment of Lithium-ion Battery Pack: Implications of Second life and Changes in Charging Electricity	2021
Rajaeifar, M, A; Marco Raugei, Steubing, B; Hartwell, A; Anderson, P, A; Heidrich, O	Life cycle assessment of lithium-ion battery recycling using pyrometallurgical technologies	2021
Rinne, M; Elomaa, H; Porvali, A; Lundstrom, M	Simulation-based life cycle assessment for hydrometallurgical recycling of mixed LIB and NiMH waste	2021
Benveniste, G; Sanchez, A; Rallo, H; Corchero, C; Amante, B	Comparative life cycle assessment of Li-Sulphur and Li-ion batteries for electric vehicles	2022
Bhosale, A, P; Bodke, K; Babhulkar, A; Amale, S; Mastud, S, A; Chavan, A	Comparative environmental assessment of different battery technologies used for electric vehicles	2022
Chordia, M; Nordelöf, A; Ellingsen, A	Environmental life cycle implications of upscaling lithium-ion battery Production	2022
Quan, J; Zhao, S; Song, D; Wang, T; He, W; Li, G	Comparative life cycle assessment of LFP and NCM batteries including the secondary use and different recycling technologies	2022
Guo, W; Feng, T; Li, W; Hua, L; Meng, Z; Li, K	Comparative life cycle assessment of sodium-ion and lithium iron phosphate batteries in the context of carbon neutrality	2023
Kim, H, C; Lee, S; Wallington, T, J	Cradle-to-Gate and Use-Phase Carbon Footprint of a Commercial Plug-in Hybrid Electric Vehicle Lithium-Ion Battery	2023
Philippot, M, L; Costa, D; Cardellini, G; Sutter, L; Smekens, J; Mierlo, J; Messagie, M	Life cycle assessment of a lithium-ion battery with a silicon anode for electric vehicles	2023

Table 1 Literature regards the LCA of lithium-ion batteries

Notter et al. (2010) performed a "cradle to grave" life cycle analysis comparing the environmental impacts of an electric vehicle with those of an internal combustion engine car. The results revealed that the environmental burdens are dominated by the operation phase in both cases and the major contributions for the electric vehicle are caused by the extraction of critical raw materials used in the battery. This document remains one of the main references for the LCA of lithium-ion batteries cited in several reports.

Majeau-Bettez et al. (2011) presented the life cycle assessment of three lithium-ion battery technologies for plug-in hybrid electric vehicles with a "cradle to gate" approach, also including the use phase.

Dunn et al. (2012) conducted a "cradle to gate" life cycle analysis for a lithium-ion battery with an active cathode material of lithium manganese oxide. Furthermore, an overview of the different possible recycling mechanisms is reported.

U.S. EPA (2013) provided a life cycle assessment using data directly provided by lithium-ion suppliers, manufacturers, and recyclers. The aim was to identify the processes and materials that most contribute to impacts on public health and environment.

Ellingsen et al. (2014) reported a "cradle to gate" analysis for a nickel cobalt manganese traction battery based on primary data with the aim of providing a transparent inventory for this lithium-ion battery technology.

Faria et al. (2014) assessed the life cycle environmental impacts associated with the use of a battery in an electric vehicle and the benefits derived from the use of a battery, no longer suitable for electric mobility, for energy storage in a household.

Oliveira et al. (2015) carried out a "cradle to grave" analysis for lithium manganese oxide (LMO) and lithium iron phosphate (LFP) technologies using secondary data taken from previous paper works.

Richa et al. (2015) performed a study to analyze the environmental trade-offs of cascading reuse of lithium-ion batteries in stationary energy storage at automotive end-of-life with the purpose of extending the life cycle of batteries.

Helmers et al. (2017) presented an overview of the environmental and health-related impacts of the batteries of electric vehicles trying to identify areas of improvements for LCA methodology and battery technology, both.

Romare et al. (2017) reported the findings of the Swedish Energy Agency and the Swedish Transport Administration regarding the energy consumptions and greenhouse gas emissions from lithium-ion batteries. The manufacturing and end of life stages are analyzed based on the literature review highlighting the criticisms related to the recycling of lithium-ion batteries.

Cusenza et al. (2019) conducted a “cradle to grave” life cycle analysis on LMO-NMC traction battery cell considering the application of the battery pack to a plug-in hybrid electric vehicle and modelling the end-of-life stage in accordance with the Waste Batteries Directive (Directive, 2006/66/EC). Furthermore, several assumptions have been made in the study due to lack of primary data so, a sensitivity analysis was conducted.

Dai et al. (2019) performed a “cradle to gate” life cycle analysis for a NCM111 battery pack composed of prismatic cells.

Ioakimidis et al. (2019) provided a life cycle analysis of a LFP battery to examine the environmental impact from the reuse of EV batteries considering four possible scenarios. In all the scenarios, the secondary use of the battery in smart buildings and/or solar panels is contemplated. After the use phase, the battery is directly intended for the second use and subsequent disposed (scenario 1 and 3) or it is firstly disposed and then a new smaller battery is manufactured (scenario 2 and 4).

Liu et al. (2019) analyzed the current situation in the recycling of lithium-ion batteries focusing on the description of the different processes applicable for the extraction of lithium from batteries at the end-of-life stage.

Kallitsis et al. (2020) investigated the environmental burdens associated to the production of a lithium-ion battery with silicon-graphite anode and nickel-cobalt-manganese as cathode active material through a “cradle to gate” analysis.

Sun et al. (2020) evaluated the life cycle environmental impacts of lithium-ion power batteries for passenger electric vehicles to identify key stages that contribute to the overall environmental burden. A “cradle to grave” analysis is performed using primary data even if assumptions were made for the recycling process.

The Advanced Rechargeable & Lithium Batteries Association (2020) provided technical guidance on how to conduct a Product Environmental Footprint (PEF) study. The document contributes to set some rules for developing PEF for high specific energy rechargeable batteries used in the e-mobility.

Wang et al. (2020) performed an analysis regarding lithium oxygen battery use in electric vehicle. A conventional lithium-ion battery (NCM-graphite) is taken as a reference to benchmark the life cycle environmental impact results of the Li-O_2 battery system and a “cradle to gate” analysis is conducted.

Yang et al. (2020) proposed a LCA comparison between repurposed EV lithium-ion batteries and lead-acid batteries used in conventional energy storage systems to identify the environmental impacts. A “cradle to grave” approach is used, and a sensitivity analysis is conducted to assess the reliability of the results.

Zhu et al. (2020) analyzed the dismantling and disposal processes of a spent LFP lithium-ion battery.

Accardo et al. (2021) evaluated a “cradle to grave” life cycle analysis of a NCM111 lithium-ion battery for application to electric light-duty commercial vehicles and compared the results with a sodium-nickel-chloride battery. The results show that the NCM111 battery has the highest impact from production in most of the impact categories, the situation is completely reversed in the use phase.

Iturrondobeitia et al. (2021) compared the life cycle analysis results of aprotic lithium oxygen batteries used in an electric vehicle with the environmental burdens of a reference lithium-ion battery, reference sodium-ion battery and the average value of lithium sulfur batteries considering the same capacity for all the batteries. The aim was to create a road map to enable the practical design of sustainable lithium oxygen batteries within a circular economy prospective.

Koroma et al. (2021) conducted a “cradle to grave” LCA of a lithium-ion battery pack focusing on the global warming potential reduction achievable with the recycling of the battery cells.

Rajaeifar et al. (2021) performed a comparison between two different pyrometallurgical technologies for the recovery of valuable metals from lithium-ion batteries (NCM111). Finding the analogies with results reported in literature was not an easy procedure because of factors that can differ across the studies, such as battery chemistry considered, modelling approach of the recycling process and recycling assumptions.

Rinne et al. (2021) investigated the environmental impact of hydrometallurgical battery recycling process using nickel metal hydride as a reductant for lithium-ion battery waste.

Benveniste et al. (2022) conducted a LCA of a lithium sulfur battery cell to compare it with a conventional lithium-ion battery (NCM) under the same driving distance. The environmental impact assessment results show that the lithium sulfur batteries present a most favorable environmental profile compared to NCM batteries.

Bhosale et al. (2022) compared the environmental impact of lithium-ion battery with lead acid battery with a "cradle to grave" life cycle approach and considering the same automotive application for both batteries.

Chordia et al. (2022) examined the effects of upscaling lithium-ion battery production, from small scale facility to large scale one, remodeling the work done by Ellingsen et al. (2014) for a NCM111 pouch cell into a NCM811 cylindrical cell. The aim was to demonstrate the emissions reduction achievable with the upscaling production.

Quan et al. (2022) quantified the environmental impacts of LFP and NCM batteries using the LCA approach evaluating, also, different recycling methods. The results reveal that NCM battery had better environmental performance than LFP one but shorter service life over the whole life cycle.

Guo et al. (2023) performed a comparison between the environmental impact of a sodium-ion battery with a LFP lithium-ion technology through LCA. The results show that LFP battery has higher environmental performance in the production stage, but NIB seems better in the long-term perspective.

Kim et al. (2023) reported the "cradle to gate" and use phase greenhouse gas emissions for a plug-in hybrid electric vehicle NCM622 battery showing that emissions during the manufacturing and use phase are comparable.

Philippot et al. (2023) evaluated the impact of the entire life cycle of a lithium nickel manganese cobalt oxide battery with a silicon-rich anode comparing it with the state-of-art graphite-based battery using primary data. The results show that considering the same cycle life, silicon-based batteries have lower environmental impacts than graphite-based ones.

In summary, the majority of works regarding the LCA of lithium-ion batteries is related to a "cradle to grave" approach. Some reports consider a "cradle to gate" LCA only and few studies added the use phase. Furthermore, some papers that embrace the end-of-life stage in their analysis, consider only the possible recycling processes for the batteries without including quantitative data. *Table 2* provides a quantitative estimation of the documents including a specific stage of the life cycle assessment in their analysis.

It is important to highlight that most of the research are based on secondary data and previous literature information and, sometimes, data is not reported clearly, especially concerning the end-of-life phase which is often discussed primarily in a theoretical manner. A very small number of documents rely on primary data in their analysis.

LCA phase	Number of documents
Cradle to gate	8
Cradle to gate + use phase	2
Cradle to grave	17
EoL only	3

Table 2 Quantification of the number of documents analyzing a specific LCA stage

The wide range of LCA approaches used to study the environmental performance of Li-ion batteries for electric vehicles, the different functional unit and system boundaries selected, and battery lifetime assumptions make it challenging to compare the various studies.

2 Methodology

There are several methods for analyzing the environmental impacts of materials and the most important ones are Life Cycle Assessment (LCA), Carbon Footprint Assessment, Environmental Impact Assessment (EIA), Material Flow Analysis (MFA), and Ecological Footprint Analysis. Each of them serves specific purposes and provides different levels of detail. One of the most comprehensive methods is Life Cycle Assessment (LCA).

2.1 Life Cycle Assessment (LCA)

LCA is a systematic methodology that evaluates the environmental impact of a product or material throughout its entire life cycle (cradle-to-grave). It considers all stages, from raw material extraction, production, transportation, use, and disposal. LCA quantifies various environmental aspects such as energy consumption, greenhouse gas emissions, water usage, and more. It is also a useful framework to explore environmental tradeoffs between two different products and compare them with each other. The implementation of the LCA is regulated by the International Organization for Standardization (ISO): ISO 14040/14044 Environmental management - Life cycle assessment - Requirements and guidelines. Following the guidelines outlined in ISO 14040, life cycle assessment (LCA) is structured into four distinct stages, each of them playing an important role in the overall assessment of the product's environmental impact or process. These stages include the following main activities: Goal and Scope, Inventory Analysis, Impact Assessment, Interpretation [4].

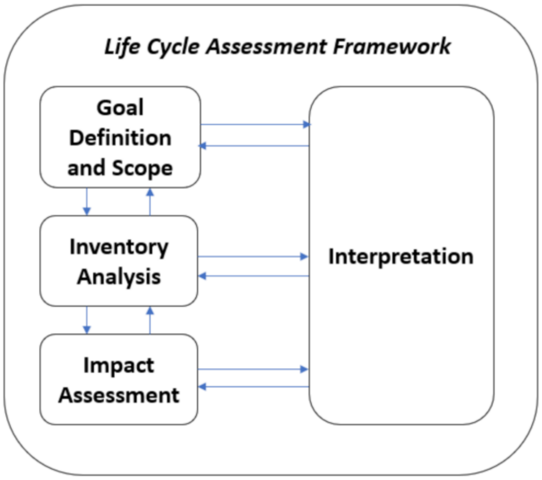

Figure 1 Life Cycle Assessment Framework (ISO 14040, 2006)

The “cradle to gate” approach within the Life Cycle Assessment (LCA) methodology is focused on evaluating the environmental impact of a product or process starting from its initial stages or raw material extraction “cradle” and continuing through to the point of leaving the factory “gate”. In this analysis, LCA considers all the inputs, resources, and environmental burdens involved in manufacturing a product or operating a process until it reaches the factory gate. This includes activities such as raw material extraction, transportation of raw materials to production facilities, component production, product production, and energy consumed during production.

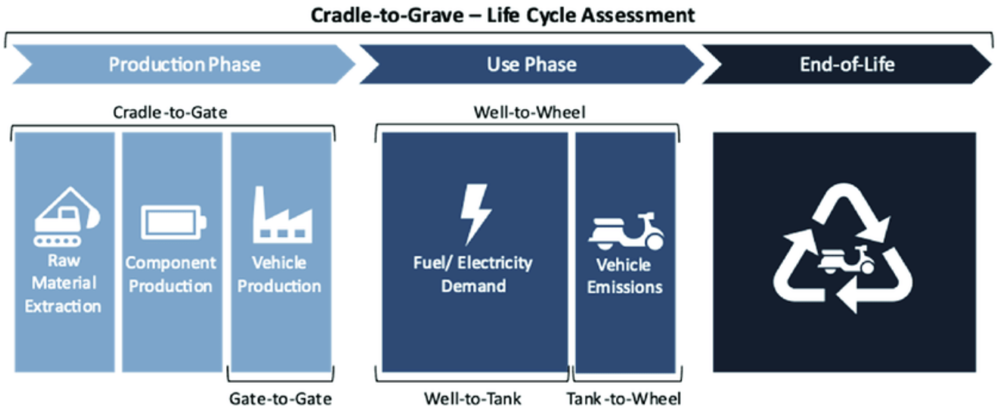

Figure 2 Cradle-to-Grave _ Life Cycle Assessment [5]

2.2 Goal and Scope definitions

In Life Cycle Assessment, the "Goal and Scope" define the purposes and boundaries of the assessment. The goal of the LCA determines the specific reasons and objectives of what you want to achieve with the study, such as assessing the environmental impacts of the product, comparing different processes, or determining opportunities to improve the project under study. The goal guides the overall direction of the LCA. Scope describes boundaries and limitations of the LCA. It determines what will be included and what will be excluded from the study. Functional unit, System boundary, Impact category, or comparison in the case of the comparative study is included in this part.

2.2.1 Functional Unit

In a Life Cycle Assessment (LCA) study, a functional unit is a fundamental and essential concept used to quantify the environmental and resource impacts associated with a product, process, or system. It serves as a reference unit that defines the specific function or purpose of the system being analyzed. The functional unit provides a basis for comparing different alternatives and allows researchers to assess and quantify the environmental and resource-related consequences of producing, using, and disposing of a product or providing a service.

The use of a well-defined functional unit is crucial in LCA because it ensures that the results are meaningful, comparable, and relevant to the intended purpose of the assessment, allowing for informed decision-making and environmental performance evaluation.

2.2.2 System Boundary

The system boundary in an LCA is a defined conceptual boundary that sets the scope of the assessment. It determines which processes, activities, and life cycle stages are included in the analysis and which are excluded.

The system boundary defines the unit processes that should be included within the product system. Preferably, the modeling of the product system should ensure that the inputs and outputs at its boundary consist of elementary flows. It is a critical concept in LCA, as it determines the scope of the study and what is considered in the assessment. The choice of key elements of the system boundary includes temporal scope, spatial scope, inclusion and exclusion criteria, cut-off criteria, and data quality requirement. Among all the elements, the cut-off criteria are important because it establishes thresholds for determining when a process or material's contribution to the overall impact is considered significant enough to be included in the assessment.

When it comes to defining the system boundary, it is important to account for various life cycle stages, unit processes, and flows. These considerations include the procurement of raw materials, inputs, and outputs in the primary manufacturing or processing, the distribution and transportation of products, the production and consumption of fuels, electricity, and heat, as well as the use and maintenance of the products. It also involves addressing the disposal of process wastes and products, the recovery of used products including reuse, recycling, and energy recovery, the production of ancillary materials, the manufacturing, maintenance, and decommissioning of capital equipment, and additional operations such as lighting and heating.

2.3 Life Cycle Inventory (LCI)

Life cycle inventory (LCI) constitutes a methodological phase aimed at compiling a comprehensive record of both input and output flows within a product system. These flows encompass resources like water, energy, and raw materials that are consumed, as well as emissions released into the air, land, and water. This inventory can be constructed through either a review of existing literature or by employing process simulation techniques.

The goal of LCI is to create a comprehensive inventory of all the resources used (such as water, energy, raw materials) and environmental emissions (such as pollutants, greenhouse gases) associated with each stage of the product or process's life cycle. This inventory helps assess the environmental impacts and sustainability of the product or process. It includes collecting data on every process unit within the system boundaries, including consumption, emissions, and product quantity and weight. These data can be primary or secondary. Primary data is the original data collected firsthand from direct sources for a specific research purpose, and the secondary data is the existing data that has been collected by someone else for a different purpose but can be used for research or analysis. The primary data can be collected on-site, while the secondar data can be obtained in literature or databases. In general, it allows for a thorough analysis of the environmental footprint and can inform decisions to reduce the environmental impact and improve the sustainability of products or processes.

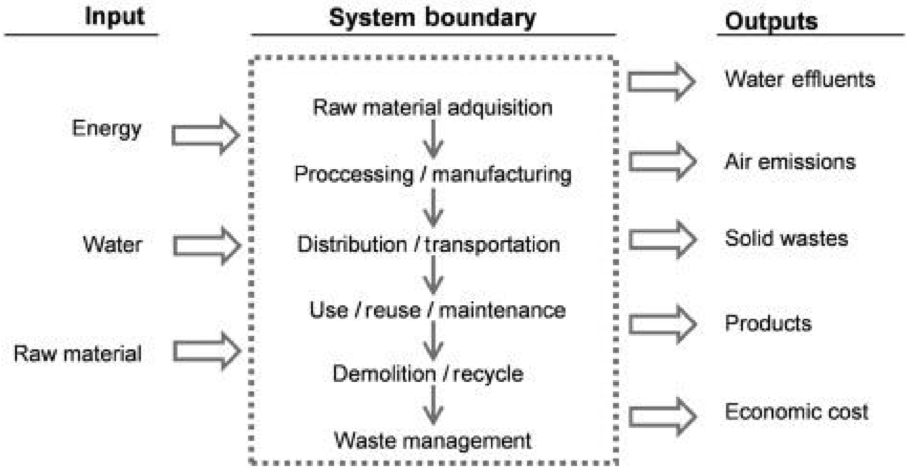

Figure 3 System Boundary [6]

2.4 Life Cycle Impact Assessment (LCIA)

In a Life Cycle Assessment (LCA), the phase known as Life Cycle Impact Assessment (LCIA) enables the evaluation of the potential magnitude of impacts by using data gathered during the Life Cycle Inventory (LCI). This process connects the inventory data with impact categories and metrics, improving the assessment of these impacts. The LCIA phase provides crucial information for interpreting the results of the life cycle analysis. During this stage, impact categories and indicators are used to streamline and represent the outcomes of the Life Cycle Inventory (LCI), with the aim of indicating possible environmental, social, and economic impacts. The aim of this assessment is to:

1. **Identify Impact Categories:** Life Cycle Impact Assessment determines the specific impact categories or indicators that represent various environmental and social aspects related to the life Cycle.
2. **Quantity impact:** LCIA involves the quantification of prospective environmental and social impacts through an examination of inputs and outputs throughout the sections of the life cycle. It assigns numerical values to the recognized impact categories, typically denoted in standardized units, such as kilograms of CO_2 equivalent for assessing global warming potential.
3. **Compare Alternatives:** LCIA enables the comparison of different products, process, or system alternatives by assessing their impact profiles. This information helps stakeholders make informed decisions and select more environmentally and socially sustainable options.

The level of detail, the choice of impact categories to be assessed and the methods used during the LCIA phase depend on the goal and scope of the study.

2.4.1 Impact Category

LCI emissions and resource data are organized and assigned to specific impact categories. Then, they are converted into measurable indicators using factors determined by impact assessment models. These factors help us understand the environmental pressures associated with each unit of emission or resource consumption in different impact categories. This process allows for a comparative analysis of emissions, resource use, and different product options based on these indicators.[7] Indicators should offer insights into the key characteristics influencing the sustainability of both products and processes.[14]

Impact categories considered in the Life Cycle Impact Assessment (LCIA) include climate change, ozone depletion, eutrophication, acidification, human toxicity (cancer and non-cancer related), respiratory inorganics, ionizing radiation, ecotoxicity, photochemical ozone formation, land use, resource depletion, abiotic depletion, particular matter, and water use.

In accordance with the guidelines presented in the European Commission ILCD Handbook, the selection of impact categories in Life Cycle Impact Assessment (LCIA) should be guided by the specific goals and objectives of the study. It should reflect the environmental aspects and concerns that are most relevant to the product, process, or system being analyzed. Impact categories should be chosen to cover a wide range of potential environmental impacts to provide a comprehensive understanding of the environmental performance of the subject under evaluation.[7]

In the different studies, various impact categories are considered based on their objectives. For instance, following Figure 4, the Global Warming Potential has been considered in fourteen different studies, or ten studies examined the Acidification category.

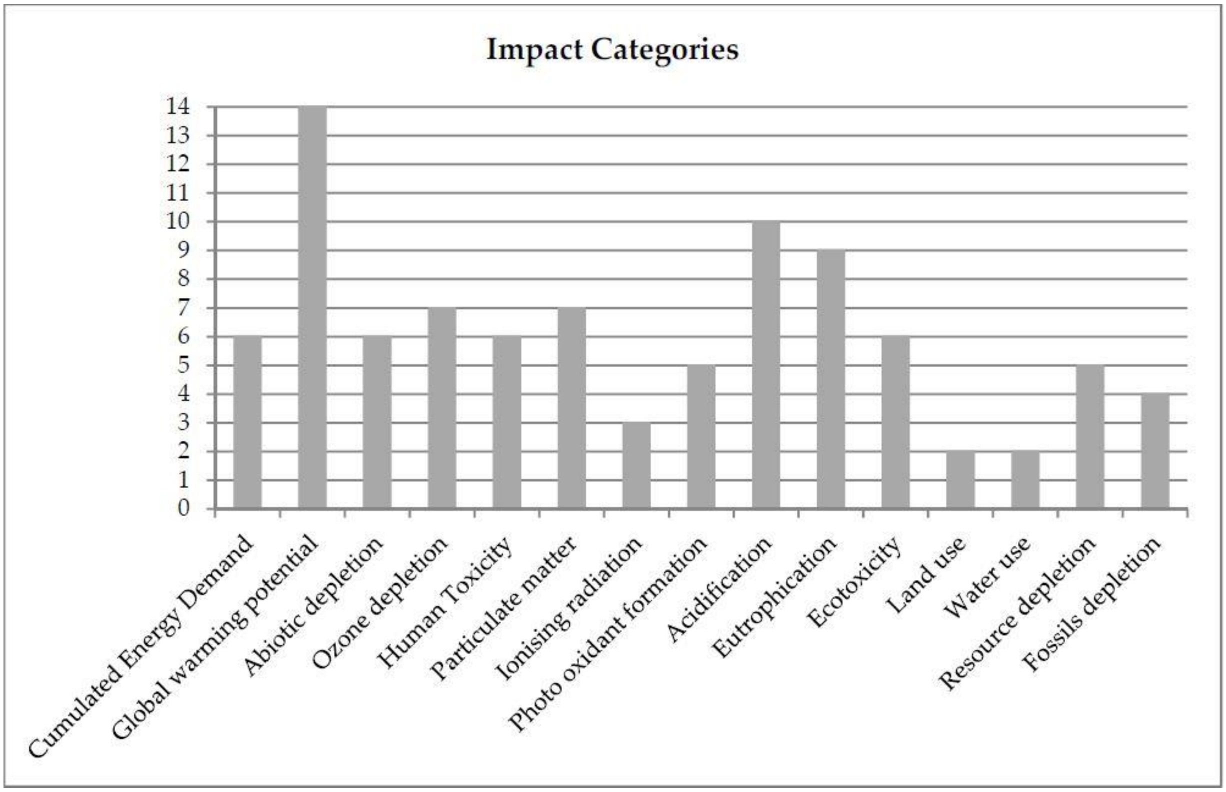

Figure 4 Impact Categories used in the studies [8]

Considering these findings, especially emphasizing impact categories highlighted in nearly 40% of the examined studies and considering their level of significance, it is advisable for an automotive battery Life Cycle Assessment (LCA) to incorporate the following impact categories: global warming potential, acidification, eutrophication, ozone depletion, particulate matter, abiotic depletion, human toxicity, ecotoxicity, and cumulated energy demand.[8]

2.5 Interpretation and Improvements

ISO 14040 defines the Interpretation of the Life Cycle Assessment, a stage in which the results of the assessment are analyzed and evaluated to illustrate meaningful conclusions and provide insights into the environmental effects of a product, process, or system throughout its life cycle. It serves as a vital connection between the data collection and the decision-making process, a comprehensive understanding of the environmental and social aspects related to the life cycle of a subject under assessment. It enables informed and sustainable choices by highlighting areas for improvement and encouraging more environmentally responsible practices. Improvement in LCA refers to the phase where strategies and actions are developed and executed based on LCA findings and recommendations. The goal is to identify opportunities for enhancing sustainability, set specific objectives, develop strategies, implement changes, and monitor progress to minimize environmental and social impacts and promote more responsible practices.[4]

3 LCA of Silicon-Sulfur and NCM battery

All the products that we use in our daily lives are made from raw materials that, depending on the extraction and manufacturing procedures, have an influence on the environment and our health. To evaluate all the products from the environmental point of view, the Life Cycle Assessment (LCA) is applied. Life Cycle Assessment (LCA) is a systematic and comprehensive method used to assess the environmental impacts of a product or process throughout its entire life cycle (ISO 14040). In the context of electric vehicle (EV) batteries, LCA is used for several important reasons: Environmental Impact Assessment, Emissions Reduction, Resource Efficiency, Comparison Analysis, Consumer Information, etc. LCA helps identify the energy consumption, greenhouse gas emissions, particular matter, and other environmental impacts associated with each stage of the battery's life, allowing manufacturers and policymakers to make informed decisions about battery design, production processes, and recycling strategies to minimize the overall environmental footprint of electric vehicles and their associated energy storage systems.

Conducting a life cycle assessment of Si-S and NCM-Graphite batteries allows for a comprehensive evaluation of these battery types in terms of their environmental and sustainability characteristics. Such an analysis holds significant relevance for a wide range of stakeholders, including producers, manufacturers, and consumers, as it assists in making well-informed decisions regarding the application of these batteries in various contexts.

This thesis project was undertaken with the direct involvement of the author at the IREC international research institution, where data collection for the Si-S battery took place. IREC is the Catalonia Institute for Energy Research in Barcelona. Its objective is to promote sustainable development in society by fostering industrial competitiveness, generating scientific knowledge, and generating technology in the realm of energy-related challenges (http://www.irec.cat). All relevant data and assembly parameters were directly acquired from the IREC international research institution (Spain) and in collaboration with the CEA (France). Politecnico di Torino (Italy) involvement not only guaranteed an efficient data flow for LCA and SLCA but also played a crucial role in overseeing task development. In addition, CLEO (Germany) monitored these tasks to facilitate effective communication, dissemination, and exploitation of the results.

On the other hand, the data for the Lithium-ion battery is sourced from the research paper authored by *Accardo, A. et al. (2021).[9]*

Within the next slides, an exhaustive examination of these two batteries will be conducted, aiming to provide a more comprehensive analysis of their characteristics.

3.1 Goal and Scope

This study aims to evaluate the environmental impacts and compare two different batteries using the Life Cycle Assessment (LCA) method.

The first battery under examination is the Lithium-ion battery referred to a study conducted by *Accardo, A et al. (2021)*. This research paper details the application of a conventional and commonly used Lithium Nickel Cobalt Manganese (NCM 111) chemistry featuring ($LiNi_{1/3}Mn_{1/3}Co_{1/3}O2$) as cathode and Graphite as anode. The evaluation conducted in this analysis is based on the data and findings articulated within the referenced research paper and will be examined in the following slides.

The second battery undergoing evaluation is the novel Silicon-Sulfur (Si-S) battery, featuring Silicon as the anode and Lithium Sulfide (Li_2S) as the cathode. This advanced Li-S battery represents the next-generation coin cell prototype, and it was sourced from the IREC international research institution. The development of this battery is attributed to the 2Boss project and Professor Andreu Cabot, leading the "Functional Nanomaterials" research group at IREC, serves as the coordinator for this project. The 2Boss technology aims to significantly decrease the reliance on Critical Raw Material (CRM). It eliminates the use of Cobalt (Co) and graphite, which are present in commercial LIBs, and reduces the demand for Lithium (Li) in Lithium Sulphur Batteries (LSBs) (http://www.2boss.eu).

Since it is a coin cell battery and both pouch and battery pack are still under investigation, an intermediate scale-up analysis was carried out to extend the analysis of the Si-S coin cell to battery packs, based on the NCM battery and other assumptions. This process will be elaborated extensively upon in subsequent steps.

Furthermore, a comparative analysis has been conducted to assess the differences in environmental impacts between the two battery types.

The tool used to evaluate all the phases of the two batteries and provide a comprehensive comparison is the OpenLCA software. OpenLCA enables users to analyze and evaluate the environmental impacts of products, processes, and systems throughout their entire life cycle, from raw material extraction to production, transportation, and end-of-life disposal or recycling. With OpenLCA, users can conduct detailed assessments of resource consumption, energy use, emissions, and various other environmental indicators.

The assessment has included the life cycle phases from “cradle to gate.” A high level of uncertainty associated with the use and recycling phase of the Si-S battery led to this approach.

3.1.1 NCM and Si-S Battery Characterization

3.1.1.1 NCM battery

In the research done by *Accardo, A. et al. (2021)*, the battery electric vehicle under analysis is equipped with an NCM111 cathode with the same molar ratio for the Nickel, Cobalt and Manganese, and a Graphite anode, and includes two battery packs, but for this thesis it is decided to take into account one single battery pack (as a light commercial electric vehicle) with the weight of 226 kg, an energy capacity of 35 kWh, 192 cells, and the weight of 0.856 kg per cell. The key characteristics of this Li-ion battery pack are documented in table 3.

Characteristics	Amount	Unit
Available energy	35	kWh
Cell weight	0.856	kg
Number of cells	192	---
Battery pack weight	226	kg

Table 3 Characteristics of NCM battery pack

General schemes of a lithium-ion battery cell and the components are represented in the figures bellow:

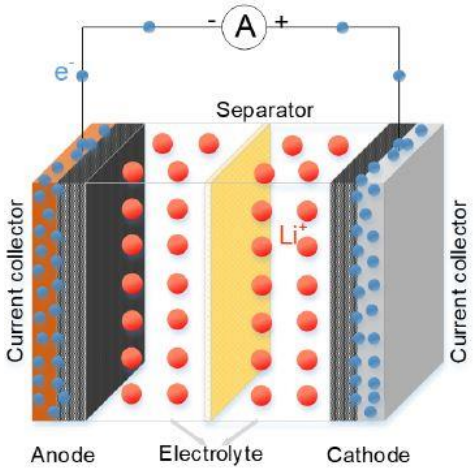

Figure 5 Scheme of a Li-ion cell (Zhu et al., 2020) [48]

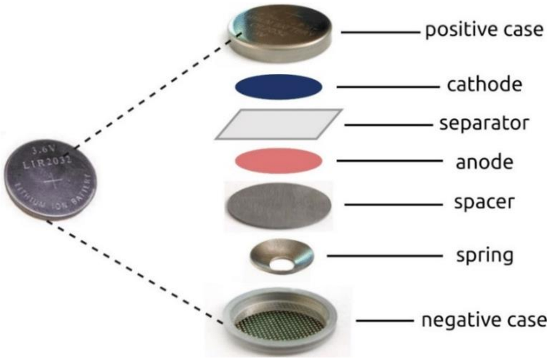

Figure 6 Main components of a coin cell (Zhuo, Ying. 2021) [58]

3.1.1.2 Si-S battery

2BoSS aims to manufacture and validate a novel battery technology using Silicon nanowires for the anode and Lithium Sulfide (Li_2S) for the cathode, both supported by biomass-derived carbons. This technology will also incorporate an active separator (in this study a polypropylene PP fiber will be assumed due to the lack of data for the analysis), an electrolyte composed of lithium hexafluorophosphate (LiPF6) as lithium salt, in a mixture of ethylene carbonate (EC) and diethyl carbonate (DEC) acting as solvents, and a casing. This cell also includes additional components such as a gasket, a spacer, and a spring.

Figure 7 Coin cell test system in IREC

In the smaller scale, a binder Styrene-butadiene-rubber (SBR) holds the active material particles and other components in the electrodes together. For dissolving the active material, a solvent -methyl pyrrolidone (NMP) is used in the cathode of the battery.

Silicon nanowire-carbon composites serves a high specific capacity around 1334 mAh g^{-1} and cycling stability of 2000 cycles. On the other hand, Li_2S-carbon composites loading as cathode material, offering specific capacities around 1200 mAh g^{-1} and useful life above 2000 cycles.

As the characteristics of the Si-S coin cell are important for the scale-up process, they are reported on the table below for the Anode, Cathode, Electrolyte, and Separator. The characteristics of the casing of the coin cell can be neglected since they are not useful for the analysis in this thesis.

ANODE	**mass**	**units**
loading (density of active material in the electrode)	1	mg/cm2
diameter	12	mm
area	1.13	cm2
mass of anode without collector	2.1	mg
mass of active material (Si)	0.94185	mg
capacity	1334	mAh/g
total capacity of anode	1188	mAh
black carbon	0.21	mg
additive	0.072	mg
Biomass-derived carbon	0.94185	mg
COLLECTOR ANODE		
density of the collector	8.9	mg/cm2
diameter	12	mm
area	1.13	cm2
mass of collector	10.2	mg
CATHODE		
loading (density of active material in the electrode)	1	mg/cm2
diameter	12	mm
area	1.13	cm2
mass of cathode without collector	1.13	mg
mass of active material (S)	0.226	mg
capacity	1200	mAh/g
total capacity of cathode	0.54	mAh
black carbon	0.192	mg
solvent	0.256	mg
binder	0.256	mg
Biomass-derived carbon	0.256	mg
COLLECTOR CATHODE		
density of the collector	2.7	mg/cm2
diameter	12	mm
area	1.13	cm2
mass of collector	4.6	mg
ELECTROLYTE		
LiPF6 EC-DEC density	1.25	g/mL
LiPF6 volume (pp separator)	0.04	mL
LiPF6 mass	50	mg
SEPARATOR		
pp density	0.25	g/cm2
diameter	1.6	cm

area	2	cm2
thickness	0.0025	cm
volume	0.00005	cm^3
mass	0.0125	mg

Table 4 Si-S Coin cell characterization, collected from IREC and CEA

3.1.2 Functional Unit

The proper Functional Unit ensures meaningful comparisons by focusing on product's purpose, its function, and specific quantity. In this study, the functional unit was defined as the final product, which is a single battery pack, for both cases. Using one battery pack as the functional unit allows for consistent evaluation of the environmental impacts associated with the production of batteries.

3.1.3 System Boundaries and Assumptions

The system under study ranges from material extraction to component production and passes through the assembly at the plant [Figure 8]. It is essential to note that the Use and the End-of-Life phases of the batteries under consideration have been excluded from the goal of this study. The logic behind this exclusion is the unavailability of the data for the Si-S battery at these phases. In this thesis, it is prioritized to make a reliable comparison between the other phases of the life cycle instead of relying only on data from the literature, as those available are variable and uncertain. Certainly, some assumptions have been incorporated into the analysis of the Si-S battery based on the NCM battery and the literature.

The production stage includes the raw material supply, component production, cell and pack battery assembly, transport, and infrastructure. The bills of the materials and energy required for all the LCA stages of the NMC111 battery were determined based on reference literature.

The specific emissions of each material and energy source were taken from the Environmental Footprint database [nexus.openlca.org], although this database has some data gaps. Hence, in some cases, the closest alternative scenarios have been considered.

The production of both cell and battery components, as well as processes associated with their manufacturing, are addressed in the stages related to the component production and battery manufacturing.

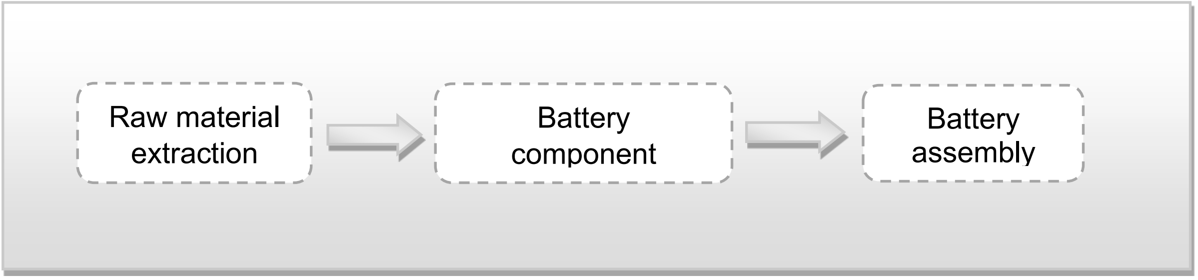

Figure 8 System boundary of the battery life cycle

Addressing the assumptions made in this study concerning the Si-S battery, those associated to transportation and energy inputs are more significant. Given the absence of information from the manufacturer (IREC) and the non-availability of the cell and pack details, the objective was to fill this data gap using the best available alternatives. This involved referencing the paper by *Accardo, A. et al. (2021)* [9], and considering the literature, such as *Notter DA, et al. (2010)* [21].

Moreover, the limitations of the Environmental Footprint necessitated certain assumptions, including the substitution of the active separator with Polypropylene (PP) fiber and the replacement of Silicon nanowire with Silicon Carbide.

3.1.4 Impact Categories

Several impact assessment methodologies can be used to evaluate environmental impacts such as Environmental Footprint, Impact 2002+, CML, ReCiPe. The outcomes of the LCA analysis are categorized into Environmental indicators that combine the environmental impacts link to the material and flows within the input and output of the study system. As mentioned, in this thesis the Environmental Footprint [nexus.openlca.org] was dedicated in OpenLCA software and ten environmental indicators were used. They are listed in the below table.

Indicator	Description	Unit
Global Warming Potential (Climate Change)	Global warming potential (GWP) is defined as the cumulative radiative forcing, both direct and indirect effects, over a specified time horizon resulting from the emission of a unit mass of gas related to some reference gas (CO_2) [1]	kg CO_2 eq
Acidification	Characterized by the increasing hydrogen ion (H+) concentrations in soil or water. It may reach levels of toxic to plants, animals, and microorganisms.[16]	mol H+ eq
Eutrophication	The gradual rise in phosphorus, nitrogen, and other nutrients in an aging aquatic ecosystem, like a lake.[17]	kg N eq
Ozon Depletion	Gradual thinning of Earth's ozone layer in the upper atmosphere caused by the release of chemical compounds.[17]	kg CFC11 eq
Particulate matter	Stands for the mixture of solid particles and liquid droplets found in the air.	disease inc.
Human Toxicity, cancer	Potential harm of a unit of chemical released into the environment.[18]	CTUh
Human Toxicity, non-cancer	Potential adverse effects on human health arising from exposure to toxic substances that do not specifically cause cancer.[24]	CTUh
Ecotoxicity	a measure of the environmental impact due to the release of toxic compounds such as benzene, toluene, xylene, and di-chlorobenzene.[19]	CTUe

Climate change-Land use and land use change	Illustrating the utilization of land, this falls under the subset of climate change considerations.	kg CO_2 eq
Resource use, minerals, and metals	Evaluates the environmental impact associated with the extraction and utilization of minerals and metals throughout the life cycle of a product or process.[25]	MJ

Table 5 Indicators used for the results interpretation

3.2 Battery Life Cycle Inventory

The third phase of the study involves conducting an Inventory analysis, wherein the Si-S battery under investigation is evaluated by analyzing the inputs (materials, energy…) and outputs (products, waste, emission...) along the whole value chain, including component production to the battery assembly, according to ISO 14040. It provides an understanding of the data collection, validation and every action that has been made for the system modeling. As the Functional Unit (FU) of the study is 1 item of the battery pack, the Si-S coin cell should be scaled up into the pouch cell and then battery pack in order to have a better understanding and comparison to the NCM battery. Moreover, coin cells are too small, and it requires a huge amount of them to run a vehicle in a battery pack which is not logical.

It is essential to note that the bills of the materials and energy required for all the LCA stages of the NCM battery were determined based on literature reference *Accardo, A. et al. (2021).* Therefore, the main focus in this part will be on the Si-S battery.

To begin the discussion on the Si-S battery life cycle inventory, it is essential to initially address the up-scaling process before presenting the inventory data.

3.2.1 Manufacturing phase (up-scaling)

Automotive battery packs are typically structured in a pack–module–cell arrangement, where cells are grouped into modules, and these modules are subsequently assembled into packs.[20]

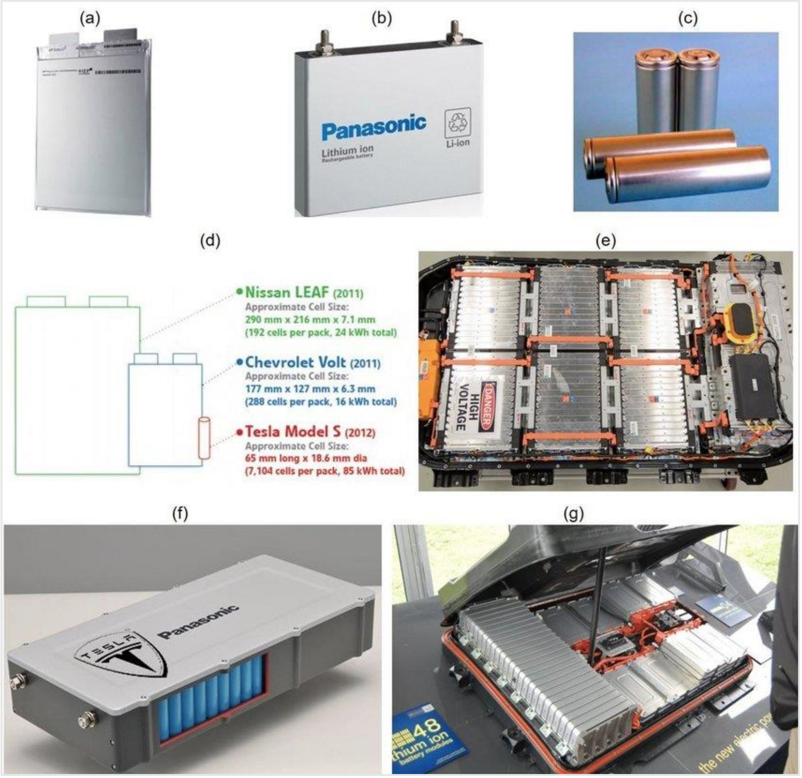

Figure 9 Typical EV battery cells: (a) the pouch cell; (b) the prismatic cell; (c) the cylindrical cell; (d) approximate battery cell size of popular EVs (e) the 60-kWh battery pack fully assembled by LG Chem in Korea, which employs 288 prismatic pouch cells; (f) Tesla's battery module, which consists of hundreds of cylindrical cells; (g) Nissan LEAF battery pack. [57]

In general, Cathode and Anode materials are two important parts of every battery because they are the main source of the enhancement of a battery.

As it was previously mentioned, the Si-S battery coin cell includes a silicon anode, Li_2S cathode, Electrolyte, Separator, casing.

The Up-scaling procedure applied in this study includes two sections:

3.2.1.1 First section

This phase aims to obtain the mass of the Si-S battery cell and pack based on the NCM battery model. According to data provided by *Accardo, A. et al. (2021)* in section 3.1.1.1, the NCM battery exhibits an energy capacity of 35 kWh per single battery pack, including the mass of 226 kg and 192 cells. To begin, obtaining the mass of a single Si-S pouch cell requires knowledge of its capacity, while this value is unknown. Therefore, the capacity of the LIB cell was computed (145.5 Ah) and assumed to be equivalent to that of the Si-S battery cell. Knowing the specific capacity of this battery, which is the specific capacity of the cathode active material (1200 mAh/g), the mass of the Si-S battery cell was determined (0.121 kg). Subsequently, the total mass of cells within the battery pack was calculated (23.28 kg). This enabled the determination of the total mass of the Si-S battery pack (32.01 kg), maintaining the same ratio between cell and pack mass as observed in the LIB. The detailed formulations for each step in this process are outlined below:

- $\boldsymbol{Total\ mass\ of\ LIB\ Cells}$: $cell\ mass * cell\ numbers \rightarrow 0.856 * 192\ =\ 164.352\ kg$

To obtain the capacity of a LIB cell, knowing the specific capacity and the mass, the formula below can be used:

- $\boldsymbol{Capacity\ of\ a\ LIB\ Cell}$: $cell\ specific\ capacity * cell\ mass \rightarrow \left(\frac{170}{1000}\right) * (0.856 * 1000) = 145.52\ Ah$

To calculate the mass of the Si-S pouch cell given its specific capacity and the LIB cell capacity, the following formula can be applied:

- $\boldsymbol{Mass\ of\ Si-S\ Pouch\ Cell}$: $\frac{LIB\ cell\ capacity}{Si{-}S\ specific\ capacity} \rightarrow \frac{145.52}{1200} = 0.121\ kg$

Considering the number of cells in a Si-S battery pack equals to the one in the LIB pack, it is possible to obtain the total mass of cells in a Si-S pack:

- $\boldsymbol{Total\ mass\ of\ cells\ in\ a\ Si-S\ pack}$: $mass\ of\ Si-S\ cell * cell\ numbers \rightarrow 0.121 * 192 = 23.28\ kg$

Subsequently, based on the assumption applied in this thesis, which involves proportioning the mass of the LIB pack to the mass of the pouch cells, it is feasible to determine the mass of the Si-S battery pack. This is expressed by the proportion:

- $\boldsymbol{Total\ mass\ of\ Si-S\ \ battery\ pack}$: $\frac{mass\ of\ LIB\ battery\ pack}{mass\ of\ LIB\ cells} = \frac{mass\ of\ Si{-}S\ battery\ pack}{mass\ of\ Si{-}S\ cells} \rightarrow \frac{226}{164.35} = \frac{x}{23.28} \rightarrow x = 32.01\ kg$

Here, “x” represents the mass of the Si-S battery pack, and the proportion is set up to relate the known mass values of the LIB pack (226 kg) and the corresponding pouch cells (164.35 kg) to the unknown mass of the Si-S battery pack and its pouch cells, x, and 23.28 kg, respectively. Consequently, it is possible to calculate the proportion of separator and each non-cell component in the Si-S battery pack referring to the LIB battery pack (table 8).

3.2.1.2 Second section

The second part of the production and scale-up process includes the value and proportion of each component (precursor) including Anode, Cathode, Cell, and battery Pack which requires some calculations.

The production of the anode and cathode involves precursors detailed in table section 3.1.1.2 based on the Si-S coin cell. It is essential to determine the value of each component. Thus, the anode and cathode in the Si-S coin cell were proportionately sized up to a unit mass of 1 kg. Given that the mass of each component is 100%, applying proportionality allows us to approximate the scale-up for obtaining 1 kg anode and cathode than can be used in the OpenLCA as an inventory data. The following table outlines this procedure:

(It is worth noting that this procedure is not the main inventory of the materials. The inventory data are in the following sections).

- ***Anode:*** *Sum (silicon, biomass-derived carbon, black carbon, additive, collector) = 0.0123gr*

$$\frac{anode\ mass}{100\%} = \frac{active\ material\ mass\ (Si)}{silicon\%} \rightarrow \frac{0.0123}{100\%} = \frac{0.941}{silicon\%} \rightarrow Silicon\% = 7.61\%$$

$$\Rightarrow \boldsymbol{Silicon\ mass\ in\ 1\ kg\ anode = 0.076\ kg}$$

Subsequently, with the same procedure, it is possible to calculate the value of the other components:

Component	value	Unit
Silicon	0.076	kg
Biomass-derived carbon	0.076	kg
Black carbon	0.017	kg
Additive	0.006	kg
Collector	0.825	kg

Table 6 Anode components in 1kg of Anode

- ***Cathode:*** *Sum (sulfur, biomass-derived carbon, black carbon, solvent, binder, collector) = 0.0057gr*

$$\frac{cathode\ mass}{100\%} = \frac{active\ material\ mass\ (S)}{sulfur\%} \rightarrow \frac{0.0057}{100\%} = \frac{0.226}{sulfur\%} \rightarrow Sulfur\% = 3.927\%$$

$$\Rightarrow \boldsymbol{Sulfur\ mass\ in\ 1\ kg\ cathode = 0.039\ kg}$$

Subsequently, with the same procedure, it is possible to calculate the value of the other components:

Component	value	Unit
Sulfur	0.039	kg
Biomass-derived carbon	0.039	kg
Black carbon	0.033	kg
Solvent	0.044	kg
Binder	0.044	kg
Collector	0.799	kg

Table 7 Cathode components in 1kg of cathode

- ***Electrolyte:*** The electrolyte mass within the coin cell is large due to an excess amount employed in the laboratory analysis. It is imperative to recognize that replicating the same proportion for upscaling to the pouch cell is not advisable, as it may affect reliability.

- ***Casing****:* For the up-scaling calculations, the parts related to the Si-S coin cell casing (gasket, spacer, spring) were removed in order to have the actual mass of the cell components. However, the non-cell materials are taken into account for the battery pack.

- ***Battery pack:*** The percentage of each component and precursor involved in the production of the cell and battery pack was taken from the LIB battery at *Accardo, A. et al. (2021)* and it is indicated in the table below for the 32.01 kg of the Si-S pack:

Component	Percentage (%)
Battery cell	72.72
Polyethylene terephthalate compound (PET)	0.5
Steel hot rolled coil	0.7
Aluminum foil	18.4
Copper sheet	0.3
BMS	5.5
Battery pack	**100**

Table 8 Si-S battery pack - 32.01 kg

It is important to mention that the upscaling method employed here is an approximation. The utilization of this approach was prompted by the absence of comprehensive and reliable data regarding the entire Si-S battery pack and pouch cell in IREC.

3.2.2 Inventory data for the NCM battery

This segment incorporates the input and output information linked to each component of the NCM battery, as referenced from *Accardo, A. et al. (2021)* [9]. In the modeling of the main cell materials of this battery, proxies have been used to ensure that the primary materials were used for the production phase. For other materials, default Ecoinvent database have been used.[9]

In this case, the cathode modelling is the main part of the analysis, as it constitutes the main material of the cell. As mentioned before, the cathode is equipped with an NCM with the same molar ratio for the Nickel, Cobalt, and Manganese. The life cycle inventory of the production of 1kg of this material is reported as below table:

Input Flow	Value	Unit
Cobalt Sulfate	0.536	kg
Nickel Sulfate	0.535	kg
Lithium Carbonate	0.383	kg
Manganese Sulfate	0.522	kg
Sodium Hydroxide	0.844	kg
Ammonium Hydroxide	0.117	kg
Natural gas	42.6	MJ
Electricity	25.2	MJ
De-ionized water	7.6	kg
Output Flow		
Lithium Nickel Cobalt Manganese Hydroxide	1.0	kg

Table 9 Life Cycle Inventory, 1kg - NCM Cathode

As reported in the *Accardo, A. et al. (2021)*, the production per kg of Cell is indicated below:

Input Flow	Value	Unit
Aluminum	0.095	kg
Graphite	0.221	kg
Polyvinylchloride (PVC)	0.034	kg
Heat	23.6	MJ
Electricity	1.4	kWh
Ethylene carbonate (EC)	0.069	kg
Polypropylene (PP)	0.016	kg
Lithium hexafluorophosphate (LiPF6)	0.025	kg
Polyethylene terephthalate (PET)	0.003	kg
Copper	0.184	kg
Dimethyl carbonate (DC)	0.069	kg
Carbon Black	0.027	kg
N-methyl-2-pyrrolidone (NMP)	0.003	kg
NCM Cathode	0.396	kg
Output Flow		
NCM Battery Cell	1.0	kg
NMP Emission to air	0.003	kg

Table 10 Life Cycle Inventory, 1kg - Cell production

Inputs for the Non-cell materials production and the Energy required for the final assembly of the battery are noted as following tables:

Input Flow	Value	Unit
Copper	0.003	kg
Aluminum	0.184	kg
Steel	0.007	kg
Polyethylene terephthalate (PET)	0.005	kg
Electronics	0.004	p

Table 11 Life Cycle Inventory, non-cell materials per 1 kg battery pack

Input Flow	Value	Unit
Electricity	6.5	kWh
Heat, natural gas	7.8	MJ

Table 12 Life Cycle Inventory, energy required for the final assembly of 1 kg battery pack

Input Flow	Value	Unit
Aluminum foil	41.58	kg
BMS	12.43	kg
Copper sheet	0.678	kg
LIB Battery Cell	164.35	kg
Electricity	1469	kWh
Polyethylene terephthalate (PET)	1.13	kg
Steel hot rolled coil	1.58	kg
Thermal energy	1762.8	MJ
Output Flow		
NCM Battery Pack	1	item

Table 13 Life Cycle Inventory, 1 item - LIB Pack

3.2.3 Inventory data for the Si-S battery

This section includes the inputs and outputs associated with each component of the battery, sourced from the Environmental Footprint database. Some data were not presented in this database;

therefore, it was decided to extract them from the reference paper or from the literature. Energy input is based on the energy production in EU, and the data related to transportation was excluded from this thesis due to the insufficient information from the source but in some cases, transportation is considered similar to the reference paper or literature (e.g. electrolyte). Moreover, the separator is considered as a membrane made from PP in all the cases.

Consequently, following the scale-up process in the section 3.2.1, and incorporating certain assumptions based on the reference LIB battery, the inventory data is presented as follow:

Input Flow	**Value**	**Unit**
Biomass-derived carbon	0.076	kg
Carbon black, general purposes	0.016	kg
Copper sheet	0.824	kg
De-ionized water	0.001	kg
Electricity	0.345	MJ
silicon carbide	0.076	kg
Styrene-butadiene-rubber (SBR)	0.005	kg
Output Flow		
Silicon Anode	1.0	kg

Table 14 Life Cycle Inventory, 1kg - Silicon Anode

Input Flow	**Value**	**Unit**
Aluminum foil	0.799	kg
Biomass-derived carbon	0.039	kg
Carbon black, general purposes	0.033	kg
De-ionized water	0.001	kg
Electricity	0.345	MJ
Methylpyrolidone	0.044	kg
Styrene-butadiene-rubber (SBR)	0.044	kg
Sulphur	0.039	kg
Output Flow		
Sulphur Cathode	1.0	kg

Table 15 Life Cycle Inventory, 1kg - Sulphur Cathode

The following table considers the Biomass-derived carbon investigated in the IREC by 2Boss project as support for the active electrode materials (Li_2S and Si). This added carbon not only enhances the performance as an electrode in the battery and other electrochemical technologies, but also plays a significant role in cost reduction organic waste (http://www.2boss.eu).

Input Flow	Value	Unit
Carbon fiber	0.0001	kg
Carbon, organic, in soil or biomass stock	0.0035	kg
Copper sulfate_at olant_EU-28+3_s	5.0E-5	kg
De-ionized water	2.0	kg
Ethanol	0.0157	MJ
Potassium chloride (agrarian, 60%K20)	0.001	kg
Sodium sulphite	0.0045	kg
Output Flow		
Biomass-derived carbon	1.0	kg

Table 16 Life Cycle Inventory, 1kg - Biomass-derived carbon

Electrolyte production involves various materials, including phosphorous pentachloride (PCI5), lithium fluoride (LiF), and hexafluorophosphate (LiPF6), each with its dedicated production process. The production processes for these materials are reported in tables, leading to the synthesis of the final product, the electrolyte.[21]

Input Flow	Value	Unit
Chlorine dioxide	0.363	kg
Phosphoryl chloride	0.703	kg
Electricity	0.002	kWh
Thermal energy (MJ)	0.086	MJ
Transport	0.458	tkm
Transporting capacity	0.107	tkm
Output Flow		
Phosphorous pentachloride (PCI5)	1.0	kg
Chlorine	0.022	kg
Phosphorus trichloride	0.043	kg
Waste heat	0.007	MJ

Table 17 Life Cycle Inventory, 1kg - Phosphorous pentachloride (PCI5)

Input Flow	Value	Unit
Ammonia, as 100% NH3	0.032	kg
De-ionized water	2.21	kg
Hydrogen fluoride	0.806	kg
Lithium carbonate	1.49	kg
Thermal energy (MJ)	1.21	MJ
Transport	1.4	tkm
Transporting capacity	0.233	tkm
Output Flow		
Lithium fluoride (LiF)	1.0	kg
Lithium carbonate	0.067	kg
Carbon dioxide (biogenic)	0.881	kg
Waste heat (in)	0.003	m3
Hydrogen fluoride	0.036	kg

Table 18 Life Cycle Inventory, 1kg - Lithium fluoride (LiF)

Input Flow	Value	Unit
Calcium hydroxide	7.44	kg
Electricity	0.541	MJ
Hydrogen fluoride	4.04	kg
Lithium fluoride (LiF)	0.197	kg
Nitrogen liquid	0.001	kg
Phosphorous pentachloride (PCI5)	1.98	kg
Transport	8.19	tkm
Transporting capacity	1.37	tkm
Output Flow		
LiPF6 Production	1.0	kg
Phosphorous trichloride	0.263	kg
Waste heat	1.95	MJ
Waste water (in)	0.003	m3

Table 19 Life Cycle Inventory, 1kg - LiPF6

Input Flow	Value	Unit
Dimethyle carbonate	0.49	kg
Ethylene carbonate	0.49	kg
Polyethylene terephthalate compound (PET)	0.004	kg
Production of LiPF6	0.02	kg
Transport	600.0	kgkm
Output Flow		
Electrolyte	1.0	kg
Phosphorous trichloride	0.263	kg
Waste heat	1.95	MJ
Waste water (in)	0.003	m3

Table 20 Life Cycle Inventory, 1kg - Electrolyte

The inventory for 1 kg of the Si-S battery cell is reported below, obtained from the methods explained in the previous sections:

- It should be noted that the Electricity and Thermal Energy inputs are considered the same as the LIB inventory data, aiming to have the most reliable inventory data for the Si-S battery.

Input Flow	Value	Unit
Anode	0.221	kg
Cathode	0.396	kg
Electricity	1.4	kWh
De-ionized water	6.65	kg
Electrolyte	0.163	kg
Polyethylene terephthalate compound (PET)	0.007	kg
Polypropylene (PP) fiber	0.016	kg
Thermal energy (MJ)	23.6	MJ
Transport	0.167	tkm
Transporting capacity	0.027	tkm
Output Flow		
Si-S Battery Cell	1.0	kg
1-methyl-2-pyrrolidone	0.003	kg
Waste heat	0.38	MJ

Table 21 Life Cycle Inventory, 1kg - Si-S Battery Cell

The Battery Management System (BMS) manages the operation of battery cells, ensuring they function within safe parameters. This system includes electronic boards, fasteners, and both high- and low-voltage components.[22] The inventory of the Battery Management System is indicated below:

Input Flow	**Value**	**Unit**
Cable 3-core mains power 10A/13A 16AWG mPPE (60 g/m) D6.3	7.106	m
Printed wiring board (SMDs glued)	0.3	m2
Transport	563.74	kgkm
Transporting capacity	93.957	kgkm
Output Flow		
BMS	1.0	kg

Table 22 23 Life Cycle Inventory, 1kg – BMS

Eventually, the inventory for 1 item of the Si-S Battery Pack including cell, non-cell, and BMS is reported in the following table:

Input Flow	**Value**	**Unit**
Aluminum foil	5.891	kg
BMS	1.76	kg
Copper sheet	0.096	kg
Electricity	208.1	kWh
Polyethylene terephthalate compound (PET)	0.16	kg
Si-S Battery Cell	23.28	kg
Steel hot rolled coil	0.224	kg
Thermal energy (MJ)	249.7	MJ
Output Flow		
Si-S Battery Pack	1	item

Table 23 Life Cycle Inventory, 1 item - Si-S Battery Pack

3.3 Life Cycle Impact Assessment Results

Undertaking a Life Cycle Impact Assessment (LCIA) is a crucial stage in evaluating the environmental performance of a product. All of the LCIA analysis in this thesis are based on the 10 indicators mentioned in section 3.1.4, with particular attention to Climate Change as the most comprehensive indicator.

➢ LCIA of Electrodes

The figure below illustrates the LCIA results derived from a cradle-to-gate analysis of four Electrodes (Graphite, NCM, Silicon, Sulfur) extracted from OpenLCA. They are categorized within the anodes and cathodes for 1kg of Li-ion and Si-S battery cell production. This characterization allows us to know the extent of the impact of each electrode across different indicators, knowing their values and units of measurement.

Indicator	Graphite	NCM	Silicon	Sulfur	Unit
Acidification	1.178e-3	2.661e-1	6.667e-4	1.230e-3	mol H+ eq
Climate change	2.623e-1	8.004e+0	2.120e-1	4.680e-1	kg CO_2 eq
Climate change-Land use and land use change	6.616e-5	2.019e-3	1.291e-4	1.856e-4	kg CO_2 eq
Ecotoxicity, freshwater	1.070e-1	1.311e+1	1.124e-1	1.507e-1	CTUe
Eutrophication marine	1.649e-4	9.989e-3	1.166e-4	3.532e-4	kg N eq
Human toxicity, cancer	3.979e-9	4.006e-7	1.158e-9	5.657e-9	CTUh
Human toxicity, non-cancer	3.831e-8	1.334e-6	8.522e-8	4.832e-8	CTUh
Ozone depletion	1.151e-7	7.900e-7	8.602e-11	2.321e-9	kg CFC11 eq
Particulate Matter	3.888e-8	1.195e-6	6.422e-9	2.064e-8	disease inc.
Resource use, minerals, and metals	4.464e-7	2.033e-4	7.134e-8	6.066e-7	kg Sb eq

Table 24 LCIA results for 1kg of each Electrodes production

The chart below compares the different electrodes to have better understanding of the impact categories related to each of them. Each color represents a specific electrode. NCM as the most effective component has an impact of 8 kg CO_2 eq. on climate change.

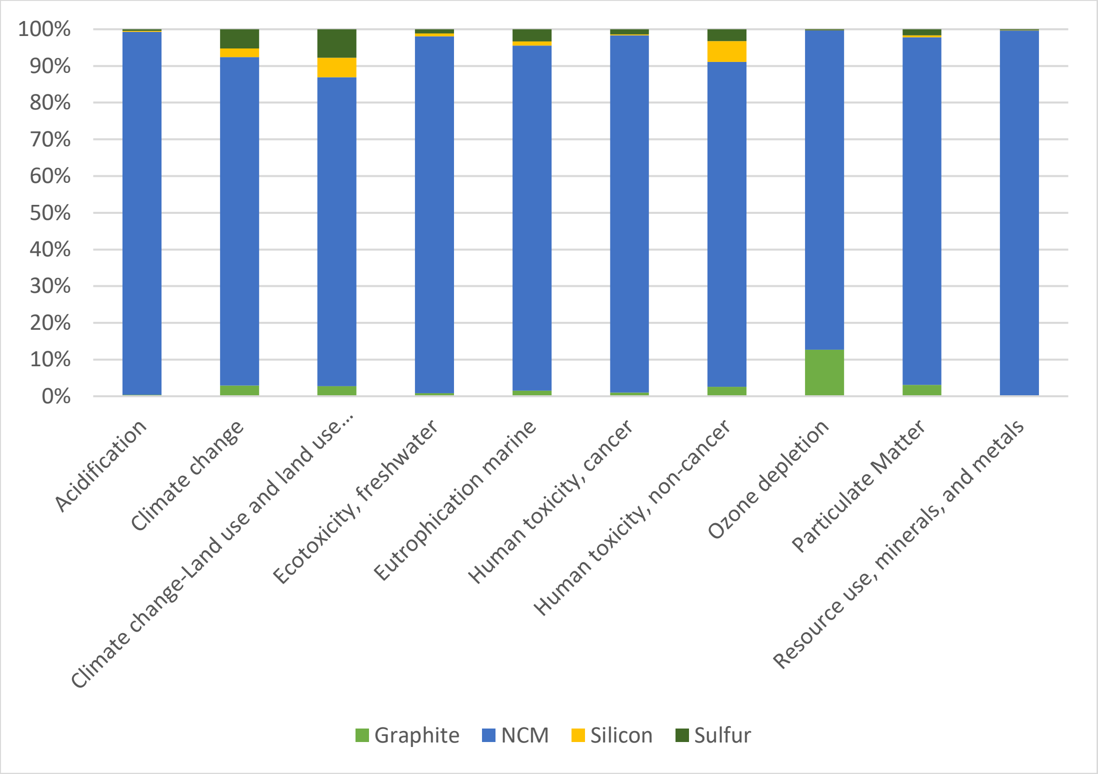

Figure 10 LCIA chart for 1kg of each Electrode production

These results help us understand the environmental impacts of the Electrodes that involve active materials in cell production. As mentioned, the NCM Cathode production stands out as having the highest impact on the environment across all indicators (8.004 kg CO_2 eq. for the climate change category). This notable difference is attributed to the specific preparation processes associated with NCM.

The environmental effects of producing other materials differ based on various indicators. For instance, Graphite production has a relatively high effect in the category of Ozon Depletion (1.15e-7 kg CFC11 eq.) as compared to the Silicon and Sulfur production (better indication in the table above). The next section is dedicated to a detailed analysis of the environmental impacts of 1kg of NCM production.

➢ LCIA of NCM111 cathode production

In order to have a deep understanding of the environmental impacts regarding 1kg NCM111 production, an explicit investigation was conducted for this process. The results of this analyze extracted from the OpenLCA, is reported as follows:

Indicator	Cobalt	Electricity	Lithium Hydroxide	Manganese sulphate	Nickel sulphate	Sodium hydroxide	Thermal Energy	NCM	Unit
Acidification	0.323	0.008	0.014	0.015	0.707	0.003	0.002	1.076	mol H+ eq
Climate change	19.32	2.96	2.19	0.45	2.52	0.65	2.99	31.81	kg CO_2 eq
Climate change-Land use and land use change	0.002	0.002	0.0009	0.0002	0.0006	0.0005	0.0001	0.007	kg CO_2 eq
Ecotoxicity, freshwater	26.62	0.119	2.324	0.393	23.24	0.23	0.025	53	CTUe
Eutrophication marine	0.024	0.001	0.005	0.0005	0.0058	0.0005	0.0007	0.04	kg N eq
Human toxicity, cancer	1.3E-06	2.3E-09	9.7E-08	1.6E-08	1.0E-07	9.5E-09	4.9E-10	1.6E-06	CTUh
Human toxicity, non-cancer	3.5E-06	6.2E-08	6.1E-07	5.7E-08	8.1E-07	2.4E-07	3.5E-09	5.3E-06	CTUh
Ozone depletion	2.4E-06	1.1E-09	1.6E-08	3.5E-10	9.8E-09	5.5E-07	2.7E-11	3.0E-06	kg CFC11 eq
Particulate Matter	3.3E-06	9.0E-08	2.7E-07	1.1E-07	8.8E-07	4.2E-08	1.7E-08	4.8E-06	disease inc.
Resource use, minerals, and metals	0.0005	9.1E-07	1.5E-05	6.7E-06	0.0002	4.6E-06	1.2E-07	0.0008	kg Sb eq

Table 25 LCIA results for 1kg of NCM111 cathode production

The chart below represents the process contribution results for the production of 1 kg of NCM. The indicator considered in this case is Climate Change as the most comprehensive environmental impact indicator. Obviously, the most influential component in the NCM production is Cobalt production. This material carries substantial ecological impacts equal to 19.32 kg CO_2 eq, including deforestation, soil erosion, and water pollution during its extraction. In the case of the battery production, refinement and processing of cobalt can contribute to air and water pollution and releasing harmful byproducts into the environment.[23] Thermal energy from natural gas and Electricity grid mix with the same ratio have the next high impacts on the environment, equal to 3 kg CO_2 eq. The other materials contribute less but still not negligible such as Nickel sulphate and Lithium hydroxide production.

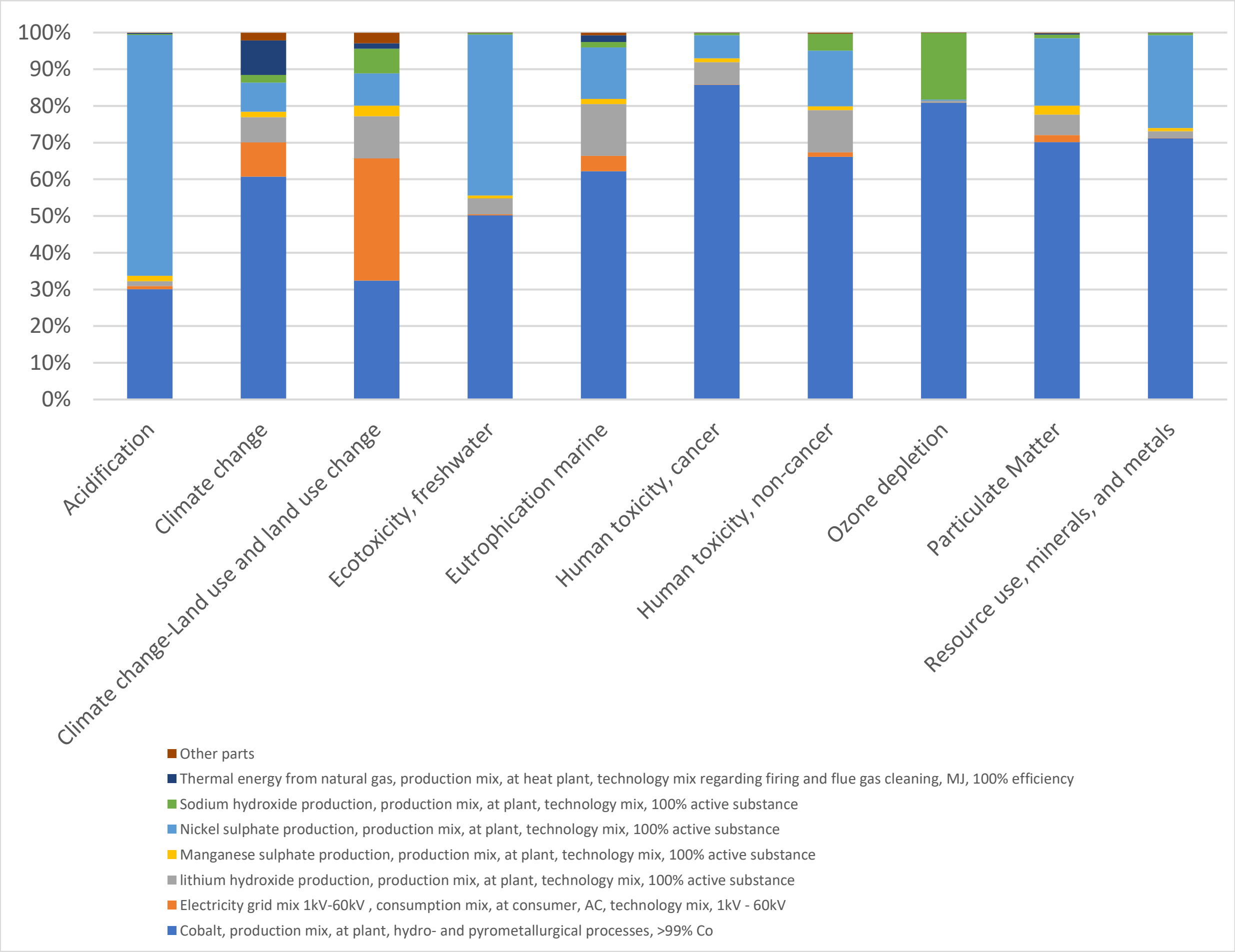

Figure 11 LCIA chart for 1kg of NCM cathode production

➢ LCIA of NCM battery Pack – 1 item

Following the LCIA analysis, in this part the analysis of each battery pack (per 1 item of pack) is represented to have an overview of the most impactful components contributed to the production of the battery packs. Initially, the LCIA of the NCM battery and then for the Si-S battery is reported. The parameters for assessment analysis are Battery Cells, Battery Management System (BMS), Thermal Energy, Electricity, AND Non-cell materials such as Aluminum, Copper, Steel, and PET, although the Non-cell materials have low impacts compared to the other parts. In the Climate Change indicator, the NCM cell production and the Electricity used in this process have the most impact with the values of 1.79e+3 and 6.23e+2 kg CO$_2$ eq, respectively.

Indicator	NCM Cell	BMS	Electricity	Thermal Energy	Aluminum	Copper	Steel	PET	NCM Pack	Unit
Acidification	4.4e+1	2.3e-1	1.8e+0	9.4e-2	1.9e-2	7.1e-4	1.2e-2	9.9e-4	4.7E+01	mol H+ eq
Climate change	1.7e+3	2.5e+1	6.2e+2	1.2e+2	2.4e+1	3.3e-1	4.1e+0	8.2e-1	2.6E+03	kg CO$_2$ eq
Climate change- Land use and land use change	4.6e-1	4.9e-2	5.5e-1	4.6e-3	1.1e-2	2.2e-4	6.9e-4	3.2e-4	1.08	kg CO$_2$ eq
Ecotoxicity, freshwater	2.2e+3	2.4e+1	2.5e+1	1.0e+0	3.9e+0	3.7e-1	5.2e-1	2.1e-2	2.2E+03	CTUe
Eutrophication marine	1.8e+0	2.6e-2	3.5e-1	3.0e-2	1.8e-2	1.9e-4	2.0e-3	2.2e-4	2.2E+00	kg N eq
Human toxicity, cancer	6.7e-5	1.6e-7	5.0e-7	2.0e-8	6.8e-8	2.7e-9	1.7e-8	5.7e-10	6.8E-05	CTUh
Human toxicity, non-cancer	2.3e-4	1.1e-5	1.3e-5	1.4e-7	2.6e-6	3.0e-7	8.8e-7	3.4e-9	2.6E-04	CTUh
Ozone depletion	1.4e-4	2.3e-9	2.3e-7	1.1e-9	2.3e-7	3.9e-11	-2.4e-11	6.2e-12	1.5E-04	kg CFC11 eq
Particulate Matter	2.1e-4	3.2e-6	1.9e-5	7.1e-7	1.7e-8	5.6e-9	3.6e-7	7.6e-9	2.3E-04	disease inc.
Resource use, minerals and metals	3.4e-2	6.7e-3	1.9e-4	5.0e-6	4.9e-6	4.6e-8	1.1e-4	9.9e-8	4.1E-02	kg Sb eq

Table 26 LCIA results for 1 item NCM battery Pack production

In the chart, the significant contribution of NCM Cell is highlighted (70%) as the reason previously explained in the preceding page related to the NCM production. Only in the category of Climate Change-Land use and land use change, the contribution of electricity is more than the Cell.

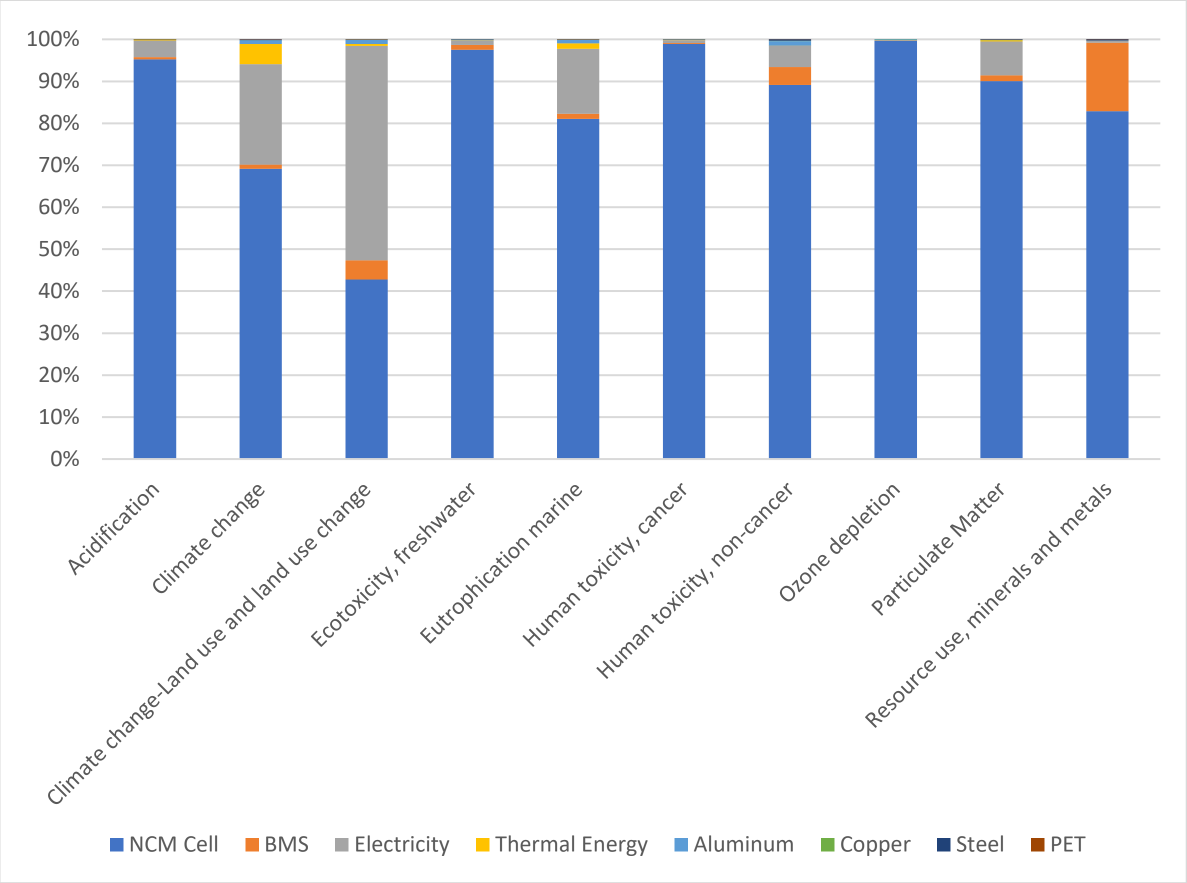

Figure 12 LCIA chart for 1 item NCM battery Pack production

➢ LCIA of Si-S battery Pack – 1 item

Si-S Battery Pack is the next battery to be analyzed for its production phase, from the environmental impacts point of view. The numerical data are presented in the following table:

Indicator	Si-S Cell	BMS	Electricity	Thermal Energy	Aluminum	Copper	Steel	PET	Si-S Pack	Unit
Acidification	1.6e-1	3.3e-2	2.6e-1	1.3e-2	2.8e-3	1.01e-4	1.7e-3	1.4e-4	4.8e-1	mol H+ eq
Climate change	7.8e+1	3.5e+0	8.8e+1	1.7e+1	3.4e+0	4.7e-2	5.8e-1	1.1e-1	1.9e+2	kg CO_2 eq
Climate change-Land use and land use change	2.4e-2	6.9e-3	7.8e-2	6.5e-4	1.5e-3	3.1e-5	9.8e-5	4.5e-5	1.1e-1	kg CO_2 eq
Ecotoxicity, freshwater	1.1e+1	3.4e+0	3.5e+0	1.4e-1	5.5e-1	5.2e-2	7.4e-2	3.0e-3	1.8e+1	CTUe
Eutrophication marine	3.6e-2	3.7e-3	5.0e-2	4.2e-3	2.6e-3	2.7e-5	2.9e-4	3.2e-5	9.7e-2	kg N eq
Human toxicity, cancer	3.3e-7	2.3e-8	7.0e-8	2.8e-9	9.6e-9	3.9e-10	2.5e-9	8.1e-11	4.4e-7	CTUh
Human toxicity, non-cancer	4.1e-6	1.5e-6	1.8e-6	2.0e-8	3.7e-7	4.2e-8	1.2e-7	4.8e-10	8.2e-6	CTUh
Ozone depletion	1.6e-7	3.3e-10	3.3e-8	1.6e-10	3.3e-8	5.5e-12	-3.4e-12	8.8e-13	2.3e-7	kg CFC11 eq
Particulate Matter	1.9e-6	4.5e-7	2.6e-6	1.0e-7	2.4e-9	8.0e-10	5.1e-8	1.0e-9	5.2e-6	disease inc.
Resource use, minerals and metals	9.6e-5	9.5e-4	2.7e-5	7.0e-7	6.9e-7	6.5e-9	1.6e-5	1.4e-8	1.0e-3	kg Sb eq

Table 27 LCIA results per 1 item Si-S battery Pack production

The impacts of the different Si-S battery components are more homogeneous than the NCM battery. In the climate change indicator, 46% and 41% of the contributors to the impact results are related to the Electricity and Si-S Cell, respectively. Across all other indicators, these two components consistently hold higher contributions relative to others, with the exception of the impact attributed to the Battery Management System (BMS) in the Resource use, minerals and metals indicator. The production of the BMS component results in a substantial value of 9.53e-4 kg Sb eq., constituting 87% of the impact for this particular indicator. Furthermore, the Non-cell materials in this battery have a higher effect, specially Aluminum in the Ozon depletion indicator.

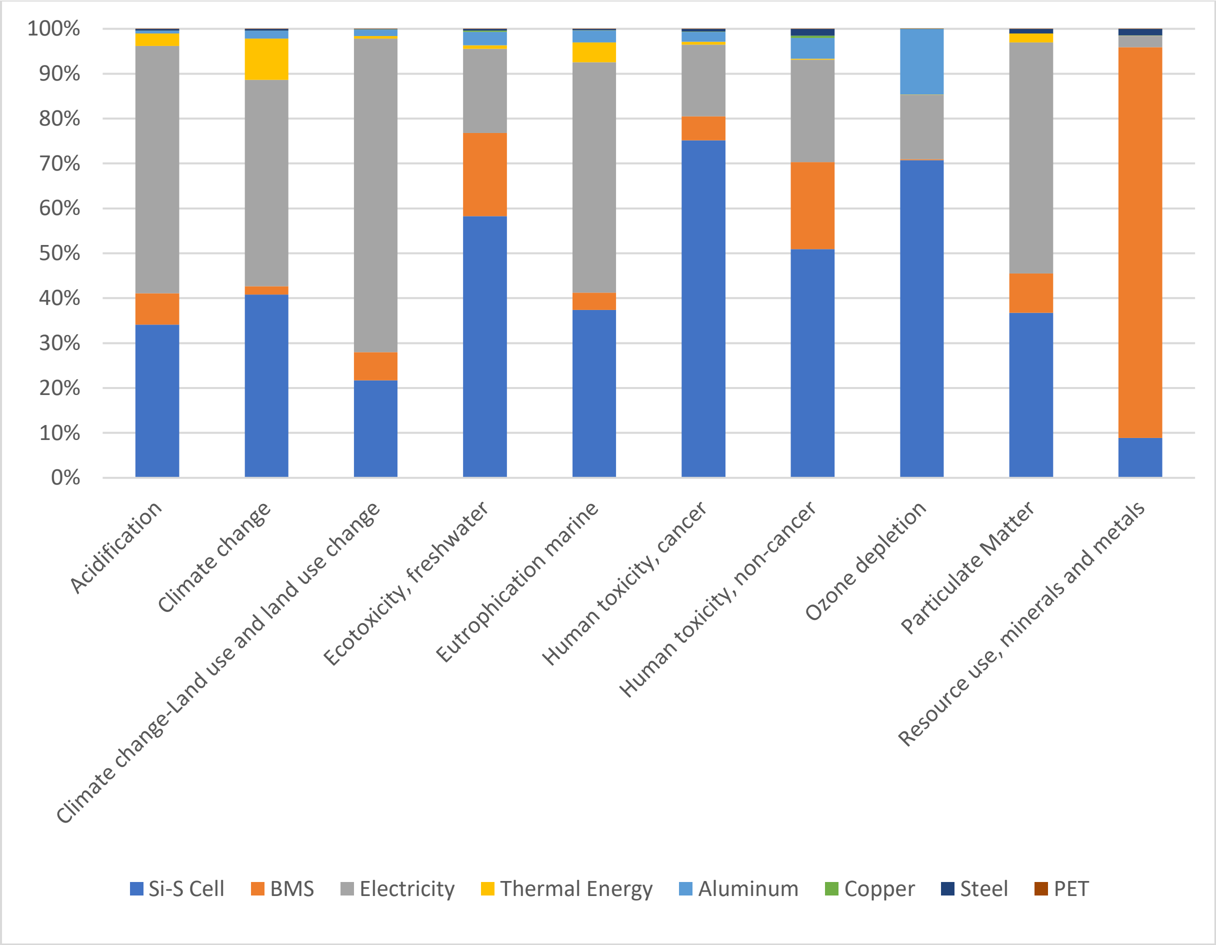

Figure 13 LCIA chart per 1 item Si-S battery Pack production

4 Comparison Between Si-S and Li-ion Battery Pack

This section includes a thorough LCIA comparison between the production of a Si-S battery, initially obtained as a coin cell from IREC and later scaled up to form a battery pack in this study, and a NCM battery pack sourced from *Accardo, A. et al. (2021)*. This process considers all the elements and precursors involved, ranging from the manufacturing of individual cells to the overall production of 1 item battery including both cell and non-cell components. The assessment also takes into account the energy consumption associated with the entire battery production process, such as thermal energy and electricity. This examination aims to provide an understanding of the environmental impacts associated with both battery technologies throughout their life cycle.

Indicator	NCM Battery Pack	Si-S Battery Pack	Unit
Acidification	4.702e+1	4.815e-1	mol H+ eq
Climate change	2.601e+3	1.919e+2	kg CO_2 eq
Climate change-Land use and land use change	1.080e+0	1.118e-1	kg CO_2 eq
Ecotoxicity, freshwater	2.263e+3	1.891e+1	CTUe
Eutrophication marine	2.281e+0	9.766e-2	kg N eq
Human toxicity, cancer	6.852e-5	4.441e-7	CTUh
Human toxicity, non-cancer	2.616e-4	8.210e-6	CTUh
Ozone depletion	1.500e-4	2.310e-7	Kg CFC11 eq
Particulate Matter	2.354e-4	5.234e-6	disease inc.
Resource use, minerals, and metals	4.110e-2	1.095e-3	kg Sb eq

Table 28 LCIA results for Si-S and NCM battery Pack Comparison

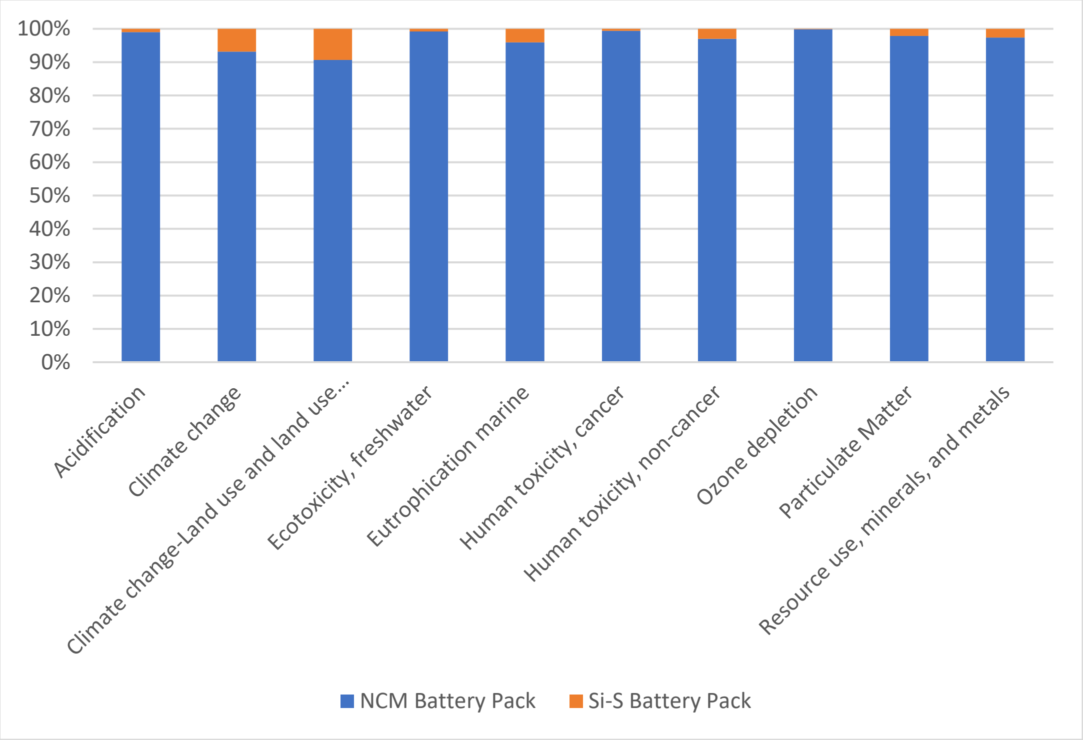

Figure 14 LCIA chart for Si-S and NCM Battery Packs

In all the indicators, a high contribution is observed for the NCM battery when compared to the novel Si-S battery. Considering the numerical table presented earlier, the Si-S battery represents a remarkable reduction in the climate change indicator, indicating a value nearly 13 times lower than that of the NCM battery and it is measured at 192 kg CO_2 equivalent, whereas the NCM battery records 2600 kg CO_2 eq. This severe contrast highlights the environmental advantages associated with the Si-S battery, particularly in mitigating climate change impacts. Moreover, here again the negative impacts of the NCM production due to the presence of the critical raw materials (CRM) is considerable. On the other hand, the extraction, purification, and production processes associated with Silicon and Sulfur has made these materials low impacting.

It is worth mentioning, the Si-S battery is currently in the experimental stage and confined to laboratory-scale testing. Numerous constraints exist regarding its practical application. A more detailed examination of these limitations will be provided in the interpretation section.

5 Interpretation and Potential Improvement

5.1 Interpretation

In the comparison between the Li-ion (NCM111) and Si-S batteries, some key points related to their respective characteristics were determined. Across all of the LCA indicators, the Si-S battery exhibits significantly better response than its counterpart. As noted earlier, the Climate Change impact is much lower for the Si-S battery, recording at 192 kg CO_2 eq., compared to 2600 kg CO_2 eq. for the NCM battery. This improvement can be attributed to various factors related to production and the inherent characteristics of the batteries.

As outlined in Section 3.2.1 (Production phase and scale-up), the mass of the Si-S battery was determined to be 32.01 kg with the obtained capacity of 145.5 Ah. In contrast, the NCM battery had a mass of 226 kg with the same capacity, reflecting the different specific capacities of 1334 mAh g^{-1} and 170 mAh g^{-1} for Si-S and Li-ion batteries, respectively, mentioned at the section 3.1.1. Hence, a lighter battery was achieved with reduced material, while maintaining the same capacity as the LIB.

The other aspect is the LIB reliance on the CRMs, including e.g., natural graphite, lithium, and cobalt. As an alternative to cobalt-based cathode materials, sulfur-based cathode is incorporated. In recent years, IREC and other entities have dedicated substantial efforts to create novel sulfur cathodes, aiming to mitigate the "shuttle effect" and consequently reduce capacity loss over cycling. Sulfur, an abundant and cost-effective element, reacts with lithium through a conversion mechanism, generating soluble products during battery operation that must be managed at the cathode.

On the other hand, silicon can be used instead of graphite anode existed in LIBs, as its capacity is much higher than that of graphite. In this study, Silicon was considered a viable alternative to commercial Lithium in Li-S batteries due to its high specific capacity upon lithiation [26]. These allowed for the creation of a lighter battery resulting in higher efficiency, reduced material requirements in the manufacturing phase, lower cost, absence of CRMs, and consequently, diminished environmental impacts for the Si-S battery.

Recent cost analysis studies in the M. Wentker et al. *A*, demonstrates that alternating the CRM based on NCM811 cathode with sulfur and carbon could potentially reduce the cost up to 24%-30% (71-65 €/kWh) [27]. Given that 2BoSS utilizes critical raw material-free substances such as carbon and sulfur, it has the potential to make substantial cost impacts at the EU level. 2BoSS will also reduce the dependance on the graphite (mainly from China 69% [28]) by using the carbon derived from Biomass. However, reported findings are still limited to demonstrations on the laboratory scale.

Although the Si-S battery has remarkable advantages, it also comes with various drawbacks making its production and especially its utilization complicated for manufacturers and users on the bigger scales, including challenges related to cycling stability due to the volume expansion and poor conductivity during charge-discharge cycles associated with both silicon and sulfur. Despite the 2BoSS project has achieved valuable enhancements and provided solutions such as using nitrogen-doped carbon porous as collectors or using biomass-derived carbon as support for the active electrode materials, considerable research and development efforts are still required to address existing challenges. Overcoming these challenges is essential to enable the widespread application of this battery technology on larger scales, shifting from the laboratory scale to a practical real-world application scale in the future.

5.2 Potential Improvement

As noted in the previous sections, the main improvements considering less environmental impact can be associated with the material chosen in the batteries due to the specific characterization of each material, including e.g., applying Lithium Sulfide (Li2S) as cathode and Silicon nanowire as anode material, or using biomass-derived carbon that all have a potential enhancement on the environmental impacts and cost.

Another crucial improvement for the battery involves optimizing energy consumption during the production phase, regarding sustainability and environmentally friendly purposes. Electricity and Thermal Energy are two main contributors to environmental impacts in the Life Cycle Impact Assessment (LCIA) expressed in section 3.3. Their influence on all indicators is significant, presenting a promising source for potential improvement. In the context of the Si-S battery's impact on the Climate Change category, it is noteworthy that the Electricity Grid mix of the EU and Thermal Energy from Natural gas of the EU collectively account for 46% and 9%, respectively, of the environmental impacts associated with this battery pack production. These two sources directly come from natural gas for the production of thermal energy, and in the case of electricity grid mix, it comes from various sources generating electricity within EU. Nevertheless, this impact can be mitigated by transitioning the energy source used in production directly to renewable energies. Among the various energy sources available in the Environmental Footprint database for electricity, such as biomass, geothermal, hydropower, nuclear, etc., the electricity from Wind Power-technology mix of offshore and onshore in the EU, has been chosen to replace the electricity grid mix. On the other hand, the thermal energy from natural gas has been substituted with the thermal energy sourced from Biogas in the EU. The selection of these two renewable energy sources is based on their availability in the EU, efficiency, as well as their accessibility in the database.

However, the chart below illustrates the environmental impact comparison of the Si-S battery pack production using two discussed renewable energy sources alongside the two conventional energy sources already in use. This result demonstrates the significant influence of the renewable energy sources of Biogas, and Wind Power usage during the production of the Si-S battery. Notably, the environmental impact of the battery with this property is 51% less compared to production with the previous energy sources, equals 94 kg CO_2 eq. This substitution of the energies marks a substantial improvement of the production of the Si-S battery, pursuing the sustainable development goals in the mobility sector.

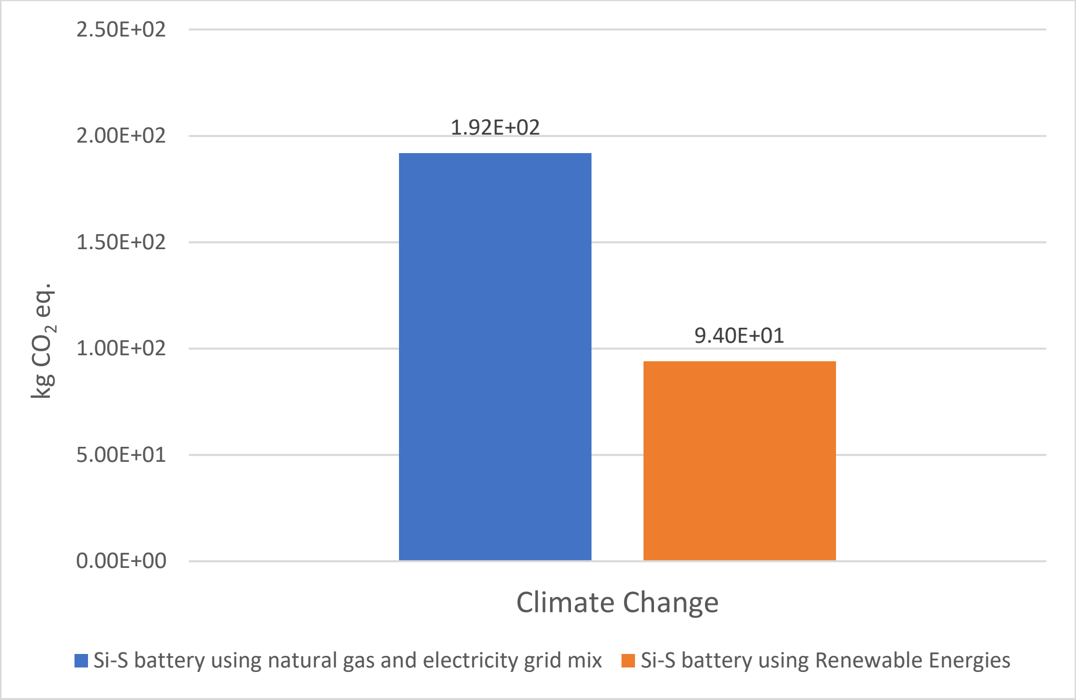

Figure 15 Si-S battery pack production - Renewable & Natural Energy comparison

Furthermore, in the NCM battery, the primary contribution of the electricity and thermal energy was 24% and 5%, respectively. Substituting the basic energies for the production of this battery to the renewable energies discussed above resulted in an enhancement of 23% in Climate Change effects, presented in the graph below. These results show the importance of manufacturing phase of the batteries concerning the renewable energy sources.

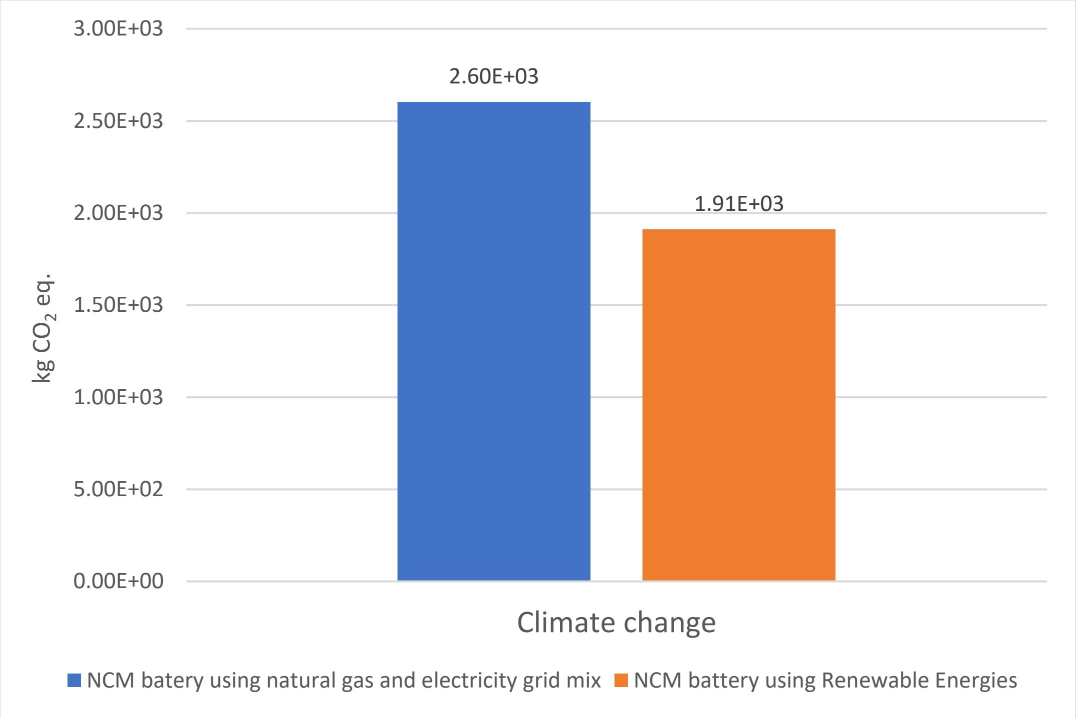

Figure 16 NCM battery pack production - Renewable & Natural Energy comparison

6 Conclusion

This thesis concludes with a summary of the main accomplishments and findings from the analysis conducted. The analysis in this study centered on the LCA of the Si-S battery and NCM-Graphite Lithium-ion battery and comparing them, by using Environmental Footprint database. The goal was to gain insights into the overall characteristics of both batteries and assess potential environmental impacts across various indicators, with a specific emphasis on climate change.

The Si-S battery, produced at IREC on a coin cell scale, was extrapolated to a battery pack size based on available data for the NCM battery pack from the literature, in order to have a better understanding of the analysis and comparison. The LCA results revealed that the Si-S battery pack exhibited significantly lower environmental impact across all indicators compared to the NCM battery pack, since this battery technology eliminates the use of the CRMs such as cobalt, incorporating innovative materials such as Li-S and Si, and using Biomass-derived carbon.

The LCIA results demonstrated that the energy consumption during battery production significantly contributed to environmental impacts, particularly in the Climate Change, Climate Change-Land use and land use change, and Acidification indicators. To mitigate these impacts, renewable energies from EU production were employed, resulting in a substantial reduction in the environmental footprint of both batteries.

The study adopted a cradle-to-gate approach due to a lack of data for the novel Si-S battery and high uncertainties in the use and end of life (EoL) stage. Ongoing research by Politecnico di Torino, IREC, and other partners aims to explore the manufacturing of pouches and battery packs for practical applications of the Si-S battery. The author of this thesis anticipates that this analysis will contribute to future Si-S battery production, with a principal focus on environmental and sustainable considerations.

7 References

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