POLYTECHNIC UNIVERSITY OF TURIN

Master’s degree course in Environmental and Land Engineering

Master Thesis

A Life Cycle Assessment of Lithium-Sulfur battery Cathodes

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SUMMERY

Since lithium-sulfur (Li-S) batteries have a far higher energy density than other batteries, they have a huge potential to replace current energy storage chemistries. Closing the current data gap is the necessary step for the estimation of the potential environmental implications related to Li-S cathodes to support the development of greener Li-S batteries. This study performs a comparative life cycle assessment (LCA) using cradle-to-gate boundaries of five Li-S battery cathodes with high sulfur loadings (1.5-15 mg.cm^2). The environmental impact can be decreased by a factor of up to 5 depending on the battery selected. When ordinary lithium-ion batteries and Li-S batteries are evaluated using secondary data from the Ecoinvent 3.6 database, the latter has a lower environmental effect per kWh of storage capacity.

It was also fined that the electrolyte plays a significant part in the environmental impacts connected with performance of Li-S batteries. Sensitivity analyses reveals that reducing the amount of utilized electrolytes can minimize the specific consequences by up to 70%. Overall, this thesis highlights how Li-S technology can be used to develop more ecologically friendly batteries that can replace current energy storage technologies.

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I am thrilled about my future journey in this field and the events that will happen forward, I will continue so energetic and enthusiastic to my next academic and career life.

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Chapter 1: Introduction and Methodology

1.1 Introduction

The development of renewable sources and more environmentally friendly energy storage technologies is required due to the very large increase in energy demand and decrease the high dependency of non-renewable energy. The transition from fossil fuel consumption to cleaner, zero-emission renewable energy in the transportation and industrial sectors depends largely on rechargeable batteries. In order to create a zero-carbon economy that is environmentally sustainable, there is an increasing tendency of putting strict environmental rules into place. For instance, the integrated national energy and climate plan (INECP) of Italy has set forth particular objectives to be fulfilled by 2030, such as targets for energy efficiency, the utilization of renewable energy sources, and the reduction of GHGs emission[1]. The world of portable devices has already seen a well-known transformation thanks to rechargeable batteries. Secondary lithium-ion batteries (LIBs), which were first made commercially available by Sony in 1991, have dominated the market for rechargeable batteries. However, LIBs are barely able to reach an energy density of 250 $Wh.kg^{-1}$, which indicates that they are approaching their theoretical limit. The increased demand for electrified transportation cannot be met with this energy density (for instance in plug-in battery electric cars, EVs) and is a barrier to the development of clean stationary energy storage systems. EVs can have further good effects since, in contrast to traditional vehicles, they can be charged at home by just plugging them in, minimizing the overconsumption of petroleum and the pollution relater to petroleum or being exposed to viruses like Covid-19[22]. As a result, significant academic and industrial attention is being paid to the design and production of battery cathodes that efficiently store energy. Compared to conventional LIB cathodes, which primarily use lithium cobalt oxide (LiCoO2), lithium manganese oxide (LiMn2O4), lithium iron phosphate (LiFePO4), or lithium-nickel-manganese-cobalt-oxide (NMC), along with carbon black and a polymeric binder as cathode materials, the ability to store lithium using naturally abundant elemental sulfur cathodes is greater. Lithium-sulfur (Li-S) batteries are therefore desirable to replace LIBs because they have a theoretical specific capacity of 1.672 $mA.hg^{-1}$[5]. When used with a metallic Li as the anode, Li-S batteries are able to give a phenomenal theoretical specific energy density of 2.600 Wh.kg^{-1}, which is far more than the 250 Wh.kg^{-1}offered by traditional LIBs. Moreover, compared to the components required in typical LIB cathodes, sulfur is a more abundant element. For instance, cobalt only makes up 0.003% of the Earth's crust while sulfur makes up 0.042%. In compared to the heavy metals used in LIBs, sulfur is thought to be more ecologically friendly, and Li-S batteries pose fewer safety risks[46]. There are severe obstacles to the development of Li-S batteries, however, will ultimately reduce their energy density and cycling life.

As a result, a thorough analysis of the environmental effects linked to the production of Li-S cathodes should be done in order to gain a whole picture and lessen the strain on ecosystems and natural resources. Thus, LCA, a comprehensive technique, offers a systematic framework for quantifying the environmental impacts associated with a technology or product from cradle to gate. In the case of Li-S batteries, which have the potential to transform industries ranging from electric automobiles to grid energy storage, this analytic method is especially pertinent. It is crucial to evaluate these batteries' environmental performance in relation to current technologies before fully accepting them as an eco-friendly alternative. This essay sets out on a quest to analyse the different environmental impacts of Li-S battery cathodes via the lens of LCA and then compare them with conventional and resent technology like lithium-ion and sodium-ion batteries. We want to provide information on both the possible advantages and disadvantages connected with this developing technology by investigating the intricate details of raw material extraction, manufacturing processes, energy usage, and emissions. By doing this, this thesis seek to advance knowledge about Li-S batteries' function in an effort to create a cleaner and greener energy environment.

1.2 Methodology

The LCA is a standardised methodology for holistic whole system environmental impact assessment [2] Also, LCA is an analysis of the environmental impact of a product, process, or service over the whole lifetime by identifying and quantifying the energy and materials utilized and wastes released to the environment [3]. This means that LCA evaluates the environmental impact of a product from the extraction of raw materials (Cradle) to production, use phase, transportations and end of life processes. The International Organisation for Standardisation (ISO) has established two LCA (Life Cycle Assessment) standards: ISO 14040, which deals with the principles and framework of environmental management, and LCA, also, ISO14044, which focuses on the requirements and guidelines for conducting life cycle assessments within environmental management[4]. Generally, performing LCA as a tool in Life Cycle Thinking is the great assist to define the alternatives and more sustainable scenarios in the production, use, and disposal of production or services to have more environmentally friendly practices.

The LCA methodology is defined in four steps:

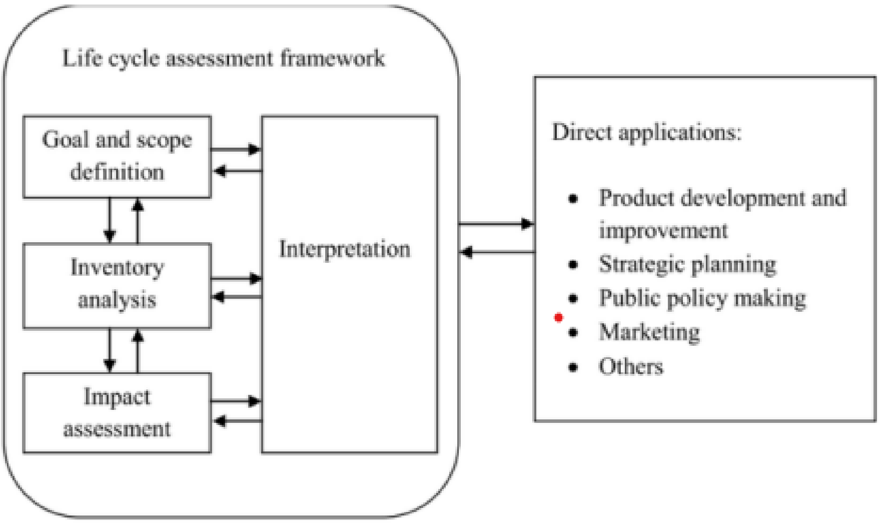


Figure 1.1: LCA framework, Figure taken by ISO 14040:2006:E

Figure 1.1 is the simple definition of the Life Cycle Assessment (LCA) framework which is so comprehensive approach that encourage to evaluate the environmental impacts of the products and all processes of the system.LCA is a methodology that allow designers and engineers to implement the best options which the improvements can be made to decrease the environmental impacts of a product or service[51].

1.2.1 LCI, ILCD and PEF principles

The International Organization for Standardization (ISO) 14040/44 (2006) standard on Environmental Management is the most significant source and set of guidelines for LCI when performing a Life Cycle Assessment (LCA). ISO provides all necessary information on the principles and framework, guidelines, and requirements for performing an LCA for all business sectors. The joint research center of the European Commission created the international reference Life Cycle Data System (ILCD) manual to offer technical guidelines and specialized information for LCA investigation. This manual assures the accuracy and reliability of the information, techniques, and evaluations required by organizations, corporations, and institutions. Additionally, the EU created the Product Environmental Footprint (PEF) methodology framework to address and quantify the environmental performance of the product throughout the course of its full life. This framework's objective is to offer a consistent method for assessing how a product's manufacture, usage, and disposal affect the environment. The PEF talks about things that affect the environment, like greenhouse gas emissions, resource depletion, energy use, water use, and many kinds of pollution. Governments, businesses, legislators, and consumers can utilize the PEF principles to demonstrate how environmentally friendly a product is. It takes exceptional and exact data, time, and knowledge to perform an LCA, which may be a restriction or a lack of data for some firms. The limitations of LCA can have an impact on the results, so LCA should incorporate many assumptions and uncertainties into data collection and modeling. In order to address these issues, the right data sources should be used, uncertainties should be taken into account, and sensitivity analysis should be used to assess how robust the results are. Another restriction is the LCA's diminished effectiveness when downscaling environmental problems from a global to a local level. The causes are the local scale conditions, which are more important and dependent on particular contexts or production processes. also, Using regional data and considering the local context is important for improving LCA results [6].

1.2.2 Goal and scope definition

The first phase in a Life Cycle Assessment (LCA) is the specification of the aim and the system. The decisions made during this phase virtually entirely determine the outcomes of LCA. The goal and scope definition phase is what the International Organization for Standardization (ISO) norm 14040 refers to.The initial step in this phase is to give a description of the goals. The life cycle assessment's (LCA) goal, the intended use of the data, the target market, and the parties involved are all identified here. The system's function is examined in the second stage in order to choose a suitable unit to represent it[7]. After the objective has been established, the scope of an LCA must take into account and precisely outline the following components (ISO 14044, Section 4.2.3.1):

- The product system to be studied (in this work, we refer to this as the system rather than the product system term used by ISO, because the system can also be used to analyse services)
- The function of the system, or of the systems in the case of comparative studies [7].

1.2.2.1 Functional unit

The Functional unit must be quantifiable and specific[7]. Analysing one component of a large system is based on the FU of the system; however, when it comes to comparative studies, the functional unit is the requirement, therefore a particular FU refers to the amount of goods or services required to fulfill the function. This unit should be the same for all products or services being evaluated, it can be define as a quantity that all products can be provide it in different units.

1.2.2.2 System boundary

The modules that are included or omitted throughout the modelling process are determined by the system boundaries. They are designed to include all steps required to complete the specified function, from beginning to end. Even though it may sound simple, in practical situations, it can easily become complicated. Coverage and modelling of all global industrial activities occurring at any point in the supply, demand, or disposal chain would be necessary for an exhaustive LCA[7].According to ISO 14044, the system boundary is the “set of criteria specifying which unit processes are part of a product system”

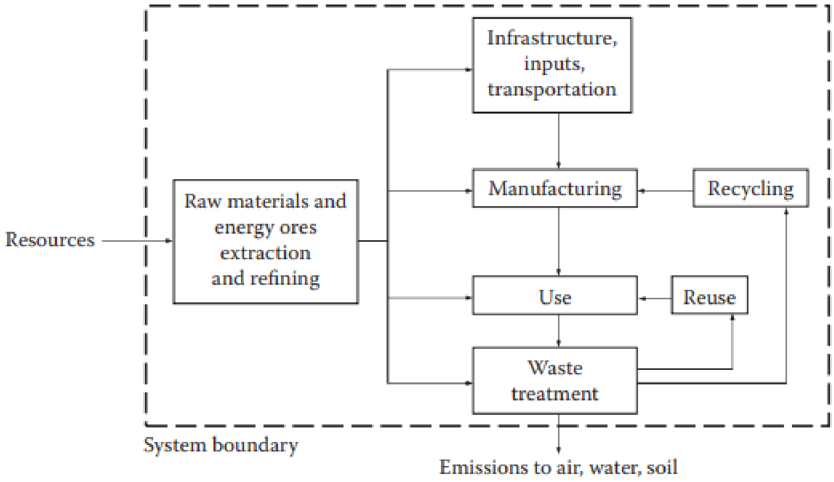


Figure 1.2: System boundary of major process and stages in life cycle of a product

There are some criteria and rules for defining the system boundary which are crucial for the degree of confidence in the results of a study and the possibility of reaching the study goal.

Rule 1 The system boundaries must cover the same functional unit in all scenarios.

Rule 2 states that the criteria for deciding which processes are included within the system boundary must be clearly explained, covering assumptions, reasoning, and the impact on study outcomes. Processes should only be excluded if they contribute less than the predetermined cut-off percentages (e.g., 1%) to factors such as product mass, system energy consumption, or environmental impacts like pollutant emissions (as per ISO 14044, 2006). These cut-off criteria are established in advance and remain fixed[7].

Rule 3 Processes that are identical in the different scenarios can only be excluded if the reference and intermediary flows affected by these processes are strictly equal (i.e., the intermediary flows of each excluded process per FU are exactly the same for the different scenarios) [7].

1.2.3 Inventory analysis

LCI is one of the steps in the performing of LCA methodology that involves combining and quantifying inputs and outputs for the goods or services across the course of their life cycles. The inventory of elementary flows or emissions and extractions can be defined as a measurable account of the movement of matter, energy, and pollutants across the system boundary. It encompasses the release of polluting substances into the environment, along with the quantities of resources extracted from the environment (such as minerals, energy carriers, soil surface area, etc.) throughout the entire life cycle of the analysed product or service. To achieve the process approach, the inventory is calculated by multiplying the reference flows and corresponding intermediary flows per FU by the direct emission or extraction factors of each unit process. There are several databases that provide the quantities material extraction and pollutant emissions that is contributed to each unit process[7].

1.2.3.1 Process-based Inventory Analysis

1. Defining the reference flows that correlate to the FU is the first stage. The design of the flowchart for the central process in the system, the inclusion of the intermediary flows of materials and processes related to the reference flow, and the identification of the upstream and downstream processes based on the reference flows offered.

2. For each unit process, total inputs (quantified intermediary flows) and direct emissions (elementary flows) must be given. By measuring or speaking directly with businesses, these emissions and extraction variables and intermediary flows are made available in databases.

3. Document the data on a flowchart or in the software, describing the source of information used.

4. The emissions of each unit process are calculated by multiplying the amount of each unit process per FU by its elementary flows, emission, and extraction factors[7].

1.2.3.2 Data collection

The collection of data is a necessary step of the inventory phase, the information for each unit process could be categorized into groupings, such as inputs for energy, raw materials, supplementary inputs, transportation, products, coproducts, waste, emissions to the (air, soil and water), and other environmental information. All the data should be defined for the aspect of the functional unit of the product system. The data modelling for performing LCA must be validated, tied to unit operations, and related to the functional unit's reference flow in order to produce trustworthy data.

1.2.4 Life cycle Impact assessment (LCIA)

The life impact assessment phase of a life cycle assessment (LCA) begins after data on the raw material extractions and substance emissions associated with a product's life cycle were gathered. The inventory phase identifies the quantities of materials and energy consumed as well as the emissions to soil, air, and water. However, the impact assessment phase deals with the interpretation of inventory data and compares and links inventory values to their environmental implications. There are various impact categories that are categorized in various steps, such as the characterization of the midpoint impact and the characterization of the damage (endpoint).

1.2.4.1 Purpose of impact assessment

During the inventory phase, data is typically collected and consolidated by summing up the emissions of individual substances and resource extractions throughout the entire life cycle. Processing the inventory table that shows the total emissions for each chemical and resource is the goal of impact assessment. Although it is possible that one scenario will result in fewer effects from the substances, it frequently results in higher emissions for a number of other scenarios. It is important to evaluate the significance of the effects brought on by each chemical in order to choose the optimal scenario

1.2.4.2 Principles of impact assessment

When doing an LCA, environmental consequences are the primary focus. Energy and material inputs should be compared for their potential to harm the environment and human health. When pollutants are released into the environment, their concentration rises through the ambient and frequently spreads to other environmental media (air, water, or soil), where they bioaccumulate and affect ecological life and, ultimately, either human health or environmental quality.

To connect each inventory data to its potential environmental harm, life cycle impact assessment techniques predict the impact pathways of various compounds..[7]

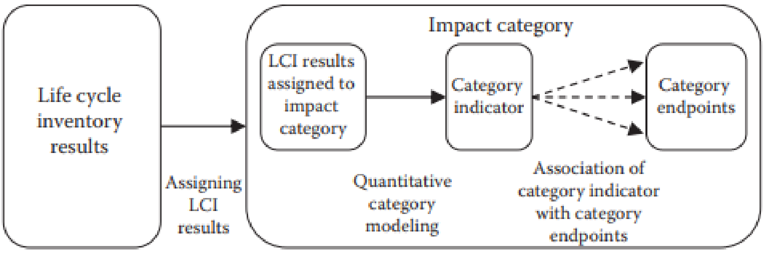


Figure 1.3: The impact assessment scheme establishes a connection between the inventory results and the specific impacts or damages associated with different areas of production. (ISO, ISO 14040 Environmental management—Life cycle assessment—Principles and framework, 2006. With permission.)

1.2.4.3 LCIA Methodological framework

The Life Cycle Initiative has created a methodological framework to connect inventory data to environmental harm. At the intermediate level, all the findings must be categorized into an impact category known as the midpoint category. By multiplying a characterization factor by the relevant flow, one can calculate the contribution of each inventory flow to a certain midpoint category. The idea of a midpoint implies that it is a location along the impact pathway, midpoint between the results of the inventory and the actual damages. For instance, the impact brought on by greenhouse gases is captured by the midpoint category known as global warming. The harm to several areas of protection, such as HH and ecosystems, is then addressed in one or more damage categories, which are assigned to each midway category. A damage indicator, also known as an endpoint indicator, is used to depict the damage category[7].

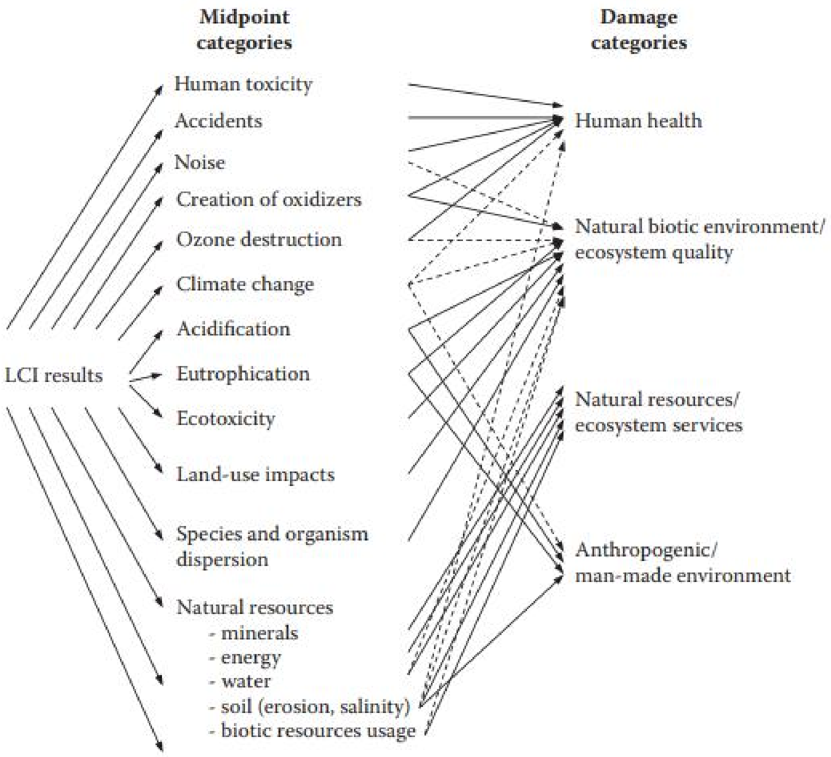


Figure 1.3: The overall framework of the UNEP-SETAC impact assessment is depicted by the general structure. In this structure, the dotted arrows symbolize the conversions from midpoint categories to damage categories, highlighting those areas where uncertainties are particularly prominent.

1.2.5 Interpretation

Examining the various approaches for reducing environmental impact is one of the goals of the interpretation of the assessment's findings. The identification of crucial product or service life cycle points—where the majority of the impact occurs—as well as the quality assessment and robustness of results using a number of checks, including quality control, sensitivity analysis, and uncertainty analysis—are all steps in the interpretation phase that help achieve these goals. This stage's top aim is to concentrate on the life cycles of the products, services, and practices that have the biggest effects. another crucial point in the life cycle stage is the highest potential to decrease impact by limited investment. The importance of interpretation is made clear by the fact that businesses frequently analyse and devote resources to changing their own operations, even if the majority of environmental effects occur upstream or downstream of these activities. [7]

1.2.6 Sensitivity analysis and allocation

The purpose of conducting a sensitivity analysis is to evaluate the strength and vulnerability of outcomes in response to variations in data, assumption, and method. The objective is to identify the critical variables that have the biggest impact on the outcomes. An approach often used consists in making the quantities of specific inputs/outputs vary in a range of uncertainty, and evaluate how this variation affects the impact results. In many industrial operations, it is customary to encounter multiple outputs or non-linear correlations between inputs of raw materials and outputs. In practice, most industries generate multiple products and use recycled intermediate or discarded products as raw materials. The allocation is a crucial procedure that should be considered when dealing with systems that involve multiple products and recycling, because of accurately measuring and accounting for environmental impacts.

1.3 OpenLCA software & related Database

OpenLCA is an open-source software that allows users to model and analyse the environmental impacts of products, processes, and services throughout their entire life cycle. Moreover, the comparison analysis can be done by this software between different scenarios. There are many activities included in this platform, such as inventory data management, impact assessment, interpretation, and reporting. It can assist the analyser to quantify and evaluate the environmental performance of systems and explore potential improvement strategies. In this research the OpenLCA software is used in combination with Ecoinvent 3.6 database, the aim is to model the impacts of Li-S batteries with different inventory data for the cathode structure.

Chapter 2: Li-S, NIB ans LIB batteries

2.1 Lithium-sulphur batteries

Recently, lithium-sulfur batteries have emerged as a promising alternative to other types of energy resource. These types of batteries provide specific capacity (1675 mA h.g^{-1}) and energy density (2600 Wh kg^{-1}) which has the potential of being reasonably beneficial production and environmentally friendly[8].

A sulfur cathode, a lithium (Li) metal anode, and an organic electrolyte typically make up a basic Li-S battery [8]. Depicts the design of coin and pouch cells as well as the variation in some operational parameters. Cathodes based on sulfur in Li-S batteries, lithium-metal anodes have typically been used in conjunction. Because they offer extremely high capacity in Li-S batteries as it is mentioned in comparison to other type of batteries. Additionally, the abundance of natural reserves around the world, the most competitive pricing, and sulfur's lower environmental effect have made Li-S batteries attractive. However, because sulfur has weak electrical conductivity as a cathodic material, additional conductive elements, such as carbon additions, have been added to the cathode structure to increase electrical conductivity and encourage optimal electron flow[8]. First off, sulfur's full potential as an active material is constrained by its ability to behave as an electrical insulator. Early attempts therefore concentrated on combining sulfur with carbonaceous conductive fillers. Contrary to conventional insertion cathode materials, sulfur experiences structural and compositional changes during cycling, resulting in the formation of soluble lithium polysulfide intermediates (Li2Sx, 4 <x< 8), which contaminate the battery and reduce its stability and performance[31]. Different cathode topologies, separator formulations, and electrolyte chemistries have been investigated in order to reduce this shuttle mechanism, improve cycle stability, and boost system efficiency. Other factors causing capacity decline include the volumetric change during continuous cycling and the unstable solid-electrolyte interphase (SEI).

2.1.1 Structure

An organic electrolyte, a lithium (Li) metal anode and a sulfur cathode typically make up a basic lithium-sulfur battery(figure 1.4). [9] Due to their high capacity and energy density when compared to other similar batteries, sulfur-based cathodes, and lithium-metal anodes are typically used in Li-S batteries. Due to the abundance of sulfur resources worldwide, its affordability, and its potentially favourable and low hazardous properties, sulfur has grown more and more alluring for use in Li-S batteries. Sulfur, when employed as a cathodic substance, has limited electrical conductivity; nevertheless, further steps have been taken to improve electrical conductivity and promote the movement of electrons. This required incorporating conductive additives, such as carbon, into the cathode structure[10].

Figure 1.4: Li-S coin-shaped cell structure[8]

2.1.2 Cathode

Sulfur is the main constituent of Li-S cathode. Due to the nature of the sulfur, Li-S cathodes usually need a conductive host such as carbonaceous materials to collaborate with sulfur in order to improve the electronic conductivity and provide enough electron flows in the electrode. Recent developments have concentrated on combining nanocomposites made of metal-organic frameworks (MOF), metal oxides, and organosulfur compounds in order to reduce the drawbacks of cathodes and increase the effectiveness of Li2S batteries[11].

2.1.3 Anode

the best choice for the Li-S batteries manufacturing is the lithium-based anodes due to its eminent characteristics regarding redox potential, gravimetric density, and specific capacity which is the excellent option for energy storing[12].

2.1.4 Electrolytes

Because they offer the ion transit cycles between two electrodes, electrodes play a substantial and sensitive function in Li-S batteries. Effective ionic conductivity, steady chemical reactivity, and strong affinity with both electrodes are desirable properties of an ideal electrolyte. For polysulfide species, it should also have a low solubility to avoid the undesirable shuttle effect inside the cells[13]. The most prevalent type of electrolytes that have been demonstrated as the typical material of Li-S battery electrodes is lithium salts, such as LiTFSI mixed with dimethoxyethane(DME) and dioxolane(DOL).

2.1.5 Separator

An insulator and an ionic conductor, a separator acts as a physical barrier between a battery's anode and cathode. Its purpose is to reduce the shuttle effect, prevent short circuits, and improve battery stability by maintaining PS (polysulfide) species. Due to their advantageous properties like electrochemical and mechanical stability, adequate porosity, superior electrolytic wettability, and cost-effectiveness, polyolefin-based membranes, such as PP and PE membranes, have significantly increased in use as separators for Li2S batteries. Recent studies have summarized the most recent developments utilizing separators in Li2S batteries [14].

2.1.6 Binder

Binders are essential in Li2S batteries because they make it easier for carbon and sulfur to join together and keep the cathode's structural integrity. However, some binders may cause the development of inactive areas, which would result in poor battery performance. Therefore, proper binder selection is necessary to guarantee top performance. Although they have been widely utilized, conventional binders like poly(tetrafluoroethylene) and polyvinylidene fluoride (PVDF) have only been somewhat successful. In recent years, it has been reported that the creation of innovative binders and binder-free techniques has improved battery performance [13,15].

2.2 2BoSS project

the project Toward sustainable batteries based on silicon, sulfur and biomass derived carbon (2BoSS) will develop an innovative, durable and more circular battery technology, the processing of part of the required raw materials, and the associated recycling strategies to minimize the use of critical raw materials. 2BoSS will turn commercial batteries compatible with a more circular economy, enhancing their performance, extending their service life, and assuring a more sustainable production and entire lifecycle. Prof Andreu Cabot from the "Functional Nanomaterials" at IREC is the coordinator of this project. It partners with the "Nanoionics and Fuel Cells" and "Energy Storage, Harvesting and Catalysis" groups of the same institute, together with CEA (France), Politecnico di Torino (Italy) and Cleopa GmbH (Germany). The role of IREC in 2BoSS is to obtain biomass-derived carbon to be used at the cathode, to produce the cathode electrodes and to assemble and test the batteries. IREC's developing battery is a coin cell battery with a sulfur cathode and a lithium anode and Lithium salt electrolyte. This project is very comparable to the cathode kinds studied in this thesis.

Figure 1.5: Li-S coin-shaped cell structure by IREC

** the inventory data is provided in appendix at the end of study

2.3 Five cathode types of Lithium-sulfur batteries

This study is about five cathodes which are listed as follows; 1-the first cathode is contain a small amount of sodium carboxymethylcellulose (NaCMC) binder by the simple fabrication process. NaCMC performs as a glue, creating rigid connections between adjacent particles without enveloping them. This allowed for unobstructed electrochemical reactions and ion mobility to take place. This strategy is based on using the environmentally friendly and non-toxic NaCMC binder instead of conventional PVDF binder. By mixing NaCMC, a cathode with a sulfur loading of 15 $\mathrm{mg\,cm^{-1}}$capable of delivering over 1200 $\mathrm{mA\,g^{-1}}$ can be achieved. The benefit of this strategy is to eliminate the environmental damage associated with PVDF and develop sustainability[17]. 2-The second cathode consist of graphene, carbon nanotubes (CNTs) and cobalt nanoparticles with 3d structure which also known as graphene-CNT-Co-sulfur. This cathode able to capture lithium polysulfides due to the existence of cobalt nanoparticles. In addition, its highly porous structure allows for favourable interaction with the electrolyte, thus, cathode exhibits minimal capacity degradation, with only a 0.09% decrease after 500 cycles at a 1C rate. (1C refers to a current that can discharge the fully charged battery in 1 hour, equivalent to 1.675 $\mathrm{mA\,h.g^{-1}}$in this case)[18]. 3-The third cathode, is developed by a composite material called Li2S-graphene, where crystalline Li2S nanoparticles are enveloped by graphene. This innovative cathode design aims to achieve rapid electronic and ionic transport while minimizing volumetric changes[19]. 4-The group develops the poor sulfur conductivity and polysulfide shuttling using a lightweight and high-surface area MgB2 metallic cathode which well known as MgB2-sulfur[20]. 5-The final type of cathode prepared an electrically conducting $\mathrm{Co_9S_8}$ material linked with graphene in order to create a Li2S cathode that effectively mitigates LiPS (lithium polysulfide) shuttling, resulting in a capacity degradation of less than 0.045% per cycle over 1500 cycles at a 2C rate. This achievement represents a tenfold enhancement compared to standard porous carbon materials [21]. The LCA methodology will be performed for these five cathodes to identify the best inventory that quantifies the lowest potential environmental impacts associated with Li-S batteries and their performance.

2.4 Sodium-ion battery’s definition

Sodium-ion batteries (NIBs) are emerging as potential alternatives to lithium-ion batteries (LIBs). The possible environmental effects of NIB production, however, have not been quantified. This work fills in this gap by providing a future life cycle evaluation for the manufacture of a sodium-ion battery using hard carbon as the negative electrode material and layered transition metal oxide as the positive electrode material. Environmentally, Na-ion batteries are found to be promising, with environmental impacts per kWh of storage capacity that are at the lower end of the range given for existing Li-ion batteries. Significant improvement potential remains, particularly by minimizing the environmental consequences associated with the anode's hard carbon synthesis and by lowering the nickel level of the cathode active material. The use of organic waste for hard carbons can be considered promising in this regard. In terms of energy storage capacity across lifespan, obtaining a long cycle life is one of the most significant characteristics when striving to provide environmental alternatives to LIBs. Similarly, internal charge/discharge efficiency is important, and even marginally higher efficiency than contemporary LIBs can bring significant benefits over time[16].

2.4.1 Sodium-ion batteries modelling

The Na-ion battery under consideration is built with a layered oxide cathode and a hard carbon anode, the most widely researched and currently most promising material combination for such batteries. A layered oxide in combination with an organic binder (polyvinylidene fluoride; PVdF) is utilized as a composite cathode. The composite anode is made up of a hard carbon active material made from a carbohydrate precursor (sugar) and a water-based binder, styrene-butadiene rubber (SBR) combined with sodium carboxymethylcellulose (CMC).[16] Aluminium is utilized as a current collector foil for both electrodes since it does not alloy with sodium at low potentials. The electrolyte is a sodium hexafluorophosphate (NaPF6) salt in an organic solvent, and the separator is a standard polyethylene/polypropylene porous sheet similar to those used in Li-ion batteries. The battery has an energy density of 128 $Wh.kg^{-1}$. Similarly to this investigation, the NIB's impacts were determined utilizing a cradle-to-gate approach, making the comparison valid [16]. NIBs are anticipated as a sustainable and cost-competitive alternative to lithium batteries, their environmental implications are also compared. As a result of sodium's abundance (2.36 wt% of the Earth's crust), inexpensive cost, and high redox potential (2.71 V vs. E^0), NIBs have a good capacity for storing energy, with energy densities of 90e120 $Wh.kg^{-1}$.[34] NIBs are therefore advantageous for large-scale energy storage systems where stringent weight constraints are not necessary.

2.5 Lithium-ion battery

Rechargeable batteries have already triggered a well-known revolution in the world of portable electronics Secondary lithium-ion batteries (LIBs) have dominated the rechargeable battery market since their introduction by Sony in 1991[52]. However, LIBs are approaching their theoretical limit with an energy density that hardly goes beyond 250 $Wh.kg^{-1}$. Traditional LIB cathodes mostly use lithium cobalt oxide (LiCoO2), lithium manganese oxide (LiMn2O4), lithium iron phosphate (LiFePO4), or lithium-nickel-manganese-cobalt-oxide (NMC).

The fabrication of 14 single cells, a battery management system, a steel box, and cables are all part of the reference battery dataset. Additionally, Ecoinvent database was used for the cathode (LiMn2O4), separator (polyethylene fleece processed with liquid acetone, hexafluoroethane, PVDF, and silica sand), anode (graphite), and electrolyte (LiPF6 in ethylene carbonate) in order to perform this analysis regarding the LIB reference case[24].

Chapter 3: LCA of LI-S batteries

3.1 Goal and Scope

The purpose of this study is to examine the associated environmental impacts during the manufacturing process by analysing the life cycle inventory of lithium-sulfur batteries cathode. The chosen cathodes use various techniques to include sulfur into the cathode structure to get the highest energy densities possible. However, all 5 battery types exhibit acceptable cycle stability, reducing their adverse effects on the environment [16]. The goal of performing LCA is to analyse five recently developed high-performance lithium-sulfur battery cathodes with high sulfur loadings to provide well developed energy storage alternatives with reduced environmental impact. In additional, these five types of batteries will be compared with lithium-ion and sodium-ion batteries to illustrate the environmental impact differences.

3.1.1 Definition of the system

Depending on the goal of this investigation the system in this analysis will be related to Li-s battery packs, although, the main study only consists of the battery cell. The battery cell is now produced, and the main focus of the researchers is the environmental effects of the processes including in producing the cell. In order to compare the two battery cells in the context of a major application, the battery pack is included. The inventory for the battery packs was created using information from the literature, and the ratios of the components were established using the characteristics and performance data of the cells. The creation of a battery management system (BMS) for these cells is still being researched. Our battery packs were modelled on the basis that each cell needed to produce (60 A h)[23]. The modelled battery packs have 432 cells with a power capacity of 57 kWh to 62 kWh, and the cells have a performance range of roughly 132-144 Wh[33].

3.1.2 system boundaries

The life-cycle assessment (LCA) performed for this investigation takes a cradle-to-gate approach and considers both the primary production procedures for the Li-S batteries and manufacturing phase. The batteries use phase is not taken into account due to the fact that there is not enough data about emissions and energy consumption or materials. Due to a paucity of data, the argument is also predicated on a number of assumptions. It's also critical to recognize the study's constraints and any potential sources of uncertainty that might have an impact on the outcomes.

Secondary data for some components of the study was taken from the cathode production literature, which also had statistics on emissions and energy use. The Ecoinvent database was utilized as a source of secondary data when the Environmental Footprint database lacked pertinent information.

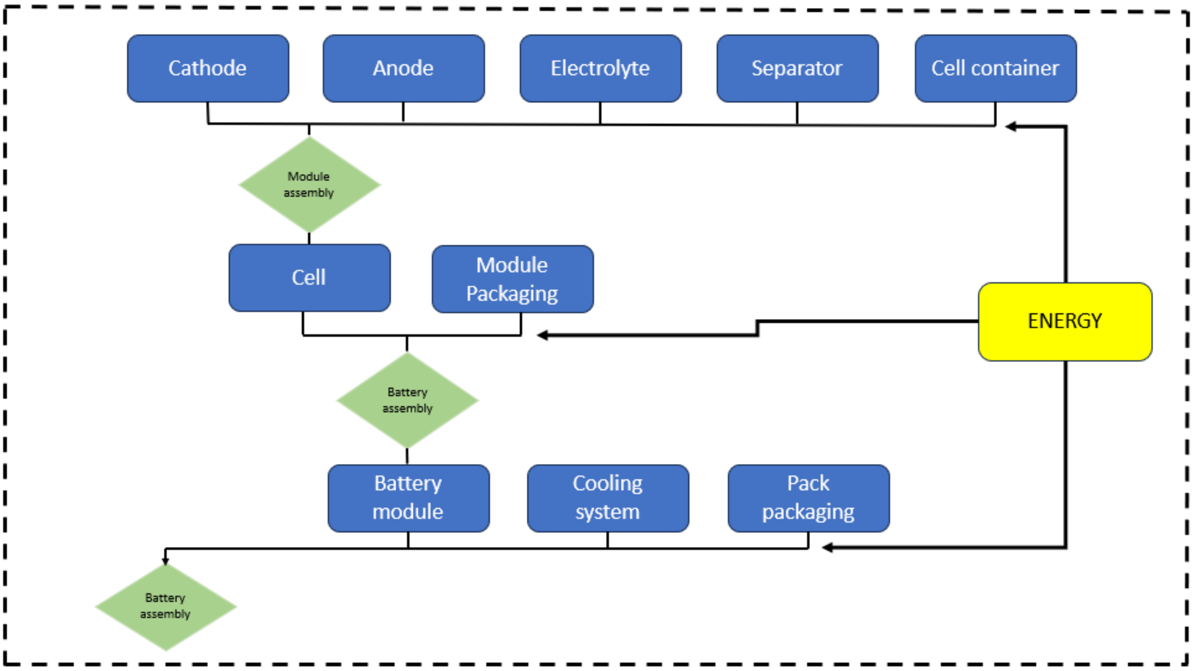


Figure 2.1: boundary of the LCA for the 5 analysed Li-S batteries [24].

Due to the existing lack of data when describing the recycling procedures of Li-S batteries, the boundary system has been described as cradle-to-gate in all batteries.

3.1.3 Functional unit

In our study, we compare the cradle-to-gate manufacture of five Li-S batteries. This decision was made on the grounds that its inclusion could make it difficult to properly compare the environmental analysis of Li-S batteries. Regarding the Functional Unit (FU), it is expected that the modelled batteries will have the unique quantity in order to compare the results between the examined Li-S batteries, reference lithium-ion (LIB), and sodium-ion (NIB). With the help of the Ecoinvent database. A FU of 1 kWh of storage capacity has also been used to standardize batteries with a range of storage capacities (from 29.9 to 62.0 kWh). This standardization enables us to compare the effects of Li-S, LIB, and NIB batteries on the environment [16].

3.1.4 Selection of the impacts category

Through the CML-baseline technique, eleven impact categories—hereafter referred to as impact indicators—have been investigated. [25] The following are the CML-baseline standardized categories

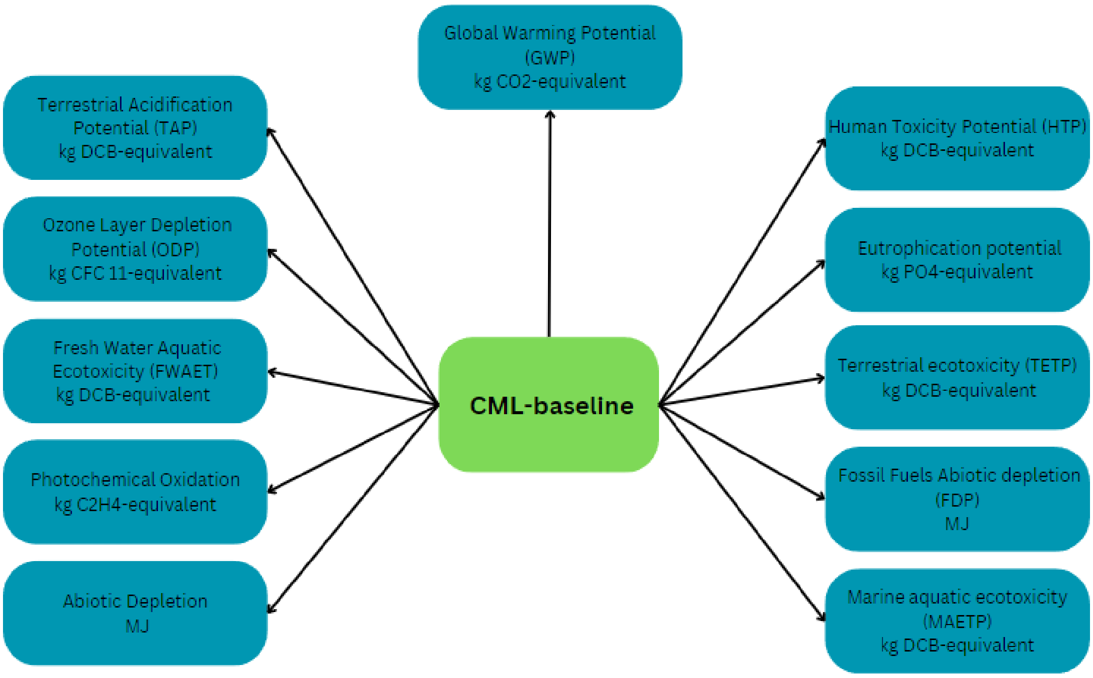


Figure 2.2: Impact categories according to the CML-baseline method

The University of Leiden developed the eleven baseline indicators used by the CML technique in 2001, and they give a common framework for comparing the many impact categories used in LCA. [25] All of the analysed indicators are midpoint (directly associated with chemical compounds), showing a lower level of uncertainty than endpoint indicators, as they are not connected to a cause-and-effect framework, such as the impacts on human health (measured as Disability Adjusted Life Years or DALYs), or biodiversity loss (species disappeared annually). Global Warming Potential (GWP) in kg CO2-eq has received particular attention since it allows for an easy comparison of the environmental effects of various energy storage options. [26] Due to the environmental costs involved in producing batteries, the production of EVs has a double insist on global warming potential (GWP) when compared to cars powered by combustion engines. We, therefore, believe that supplying the GWP of Li-S batteries will produce the most interesting findings.

3.1.5 Limitation and Main assumptions

This study had a number of drawbacks, most of which were brought on by insufficient data. An Excel file with a list of all the different inputs for the OpenLCA software containing data from publications and experiments was provided. Unfortunately, no specific details about the processes were provided, therefore energy inputs were supplied without any knowledge of where they came from. Since access to the machinery and all information regarding the procedures utilized made it possible to estimate the energy consumption in the production of cells, this information was not available for other types of batteries. Thus the energy consumption for these type of batteries are mostly assumed by the letritures.

In an effort to give the best conclusion for the study, assumptions were made based on the numerous restrictions listed above. Because the estimates for the energy consumption of cell manufacture were fairly low, it was thought that the values provided by the data were on an industrial scale. As a result, the amount of electricity consumed during battery production has been determined based on the weight of the batteries. In this investigation, a value of 17,204.32 Wh.kg-1 was chosen as a reference[28].

Furthermore, the model involves the utilization of an argon-filled glove box to provide a moisture-free inert environment (H2O and O2 1 ppm) during the Li-S cell assembly process. Furthermore, the effects of metal and chemical factories have been incorporated into the cell's assembly process, with "item" serving as the unit of measurement.

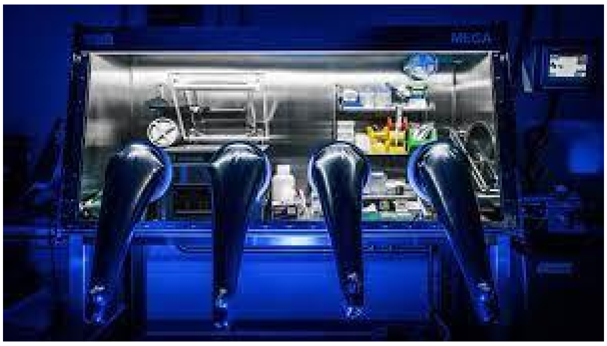
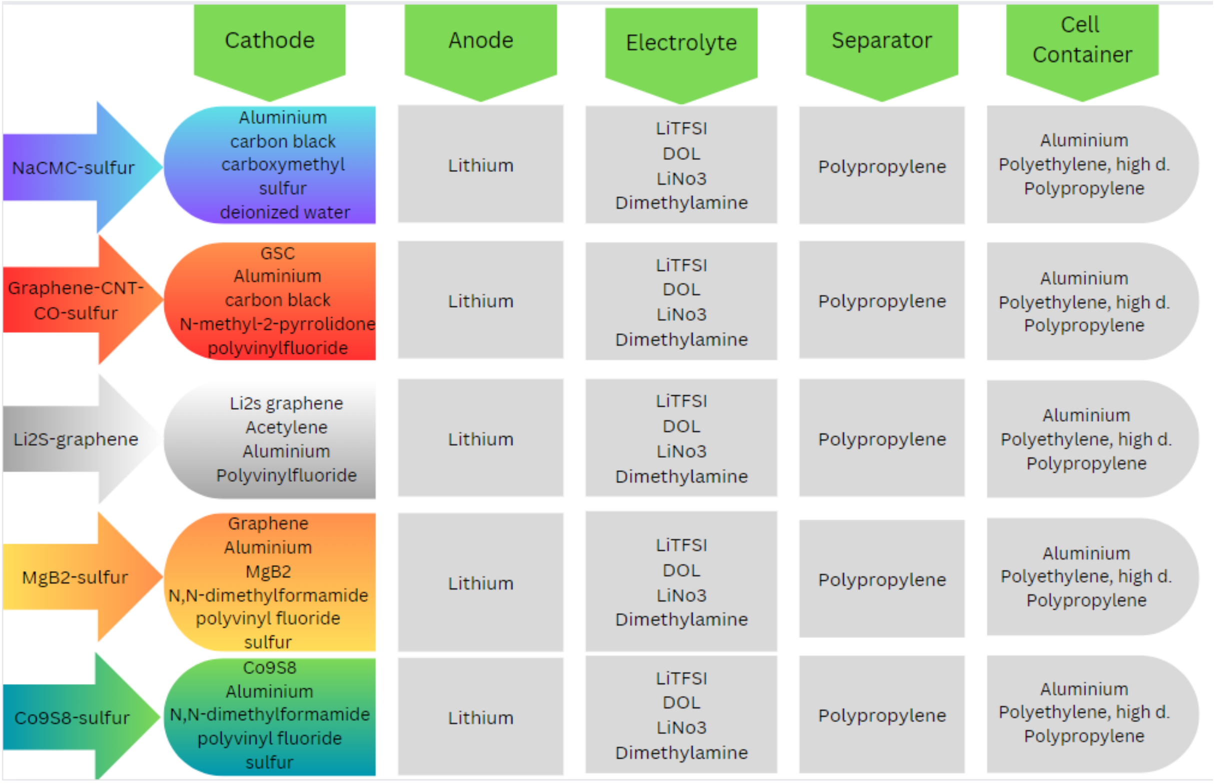


Figure 2.3: the image of argon-filled glove box

Furthermore, the data related to Transportation is not included in this investigation and the reason is both the lack of available data from reliable sources and the purpose of this thesis, because the main goal is to compare the materials and manufacturing processes of the different type of Cathode materials in battery, so in this part there is not any requirement for the transportation data.

3.2 Life cycle Inventory (LCI)

The LCA's Life Cycle Inventory section according to ISO 14040 (Section 1.4.2) is where the data analysis and validation are carried out. These sentences provide a thorough explanation of every action that has been done on data, from data collection to data validation and model aggregation. The usage of specialized tools for modelling and computing environmental findings is reminded. While certain cell portions are similar, the majority of the cell's parts are very dissimilar. For a conventional 60 kWh EV battery pack as a functional unit (depending on the applied technology, the capacity varies from 57 to 62 kWh), material and energy input inventories for all the examined Li-S cathodes are provided. There is a table below included all inventory details for the Lithium-sulfur battery types [24].



	Cathode	Anode	Electrolyte	Separator	Cell Container
NaCMC-sulfur	Aluminium carbon black carboxymethyl sulfur deionized water	Lithium	LiTFSI DOL LiNo3 Dimethylamine	Polypropylene	Aluminium Polyethylene, high d. Polypropylene
Graphene-CNT-CO-sulfur	GSC Aluminium carbon black N-methyl-2-pyrrolidone polyvinylfluoride	Lithium	LiTFSI DOL LiNo3 Dimethylamine	Polypropylene	Aluminium Polyethylene, high d. Polypropylene
Li2S-graphene	Li2s graphene Acetylene Aluminium Polyvinylfluoride	Lithium	LiTFSI DOL LiNo3 Dimethylamine	Polypropylene	Aluminium Polyethylene, high d. Polypropylene
MgB2-sulfur	Graphene Aluminium MgB2 N,N-dimethylformamide polyvinyl fluoride sulfur	Lithium	LiTFSI DOL LiNo3 Dimethylamine	Polypropylene	Aluminium Polyethylene, high d. Polypropylene
Co9S8-sulfur	Co9S8 Aluminium N,N-dimethylformamide polyvinyl fluoride sulfur	Lithium	LiTFSI DOL LiNo3 Dimethylamine	Polypropylene	Aluminium Polyethylene, high d. Polypropylene

Figure 3.4: Scope of followed LCA for 5 types of lithium-sulfur batteries

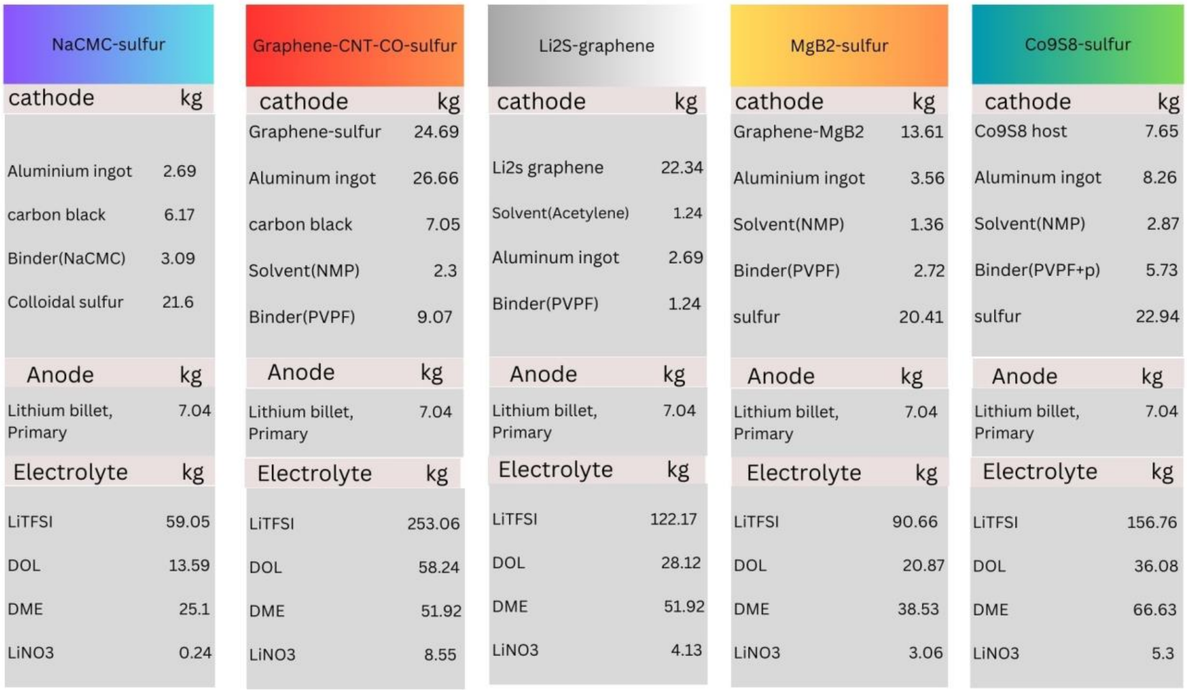
3.2.1 Inventory analysis for Lithium-sulfur batteries

An overview of the energy and material inputs for an inventory of the Li-S battery packs is given in Table 1. The outputs from the Battery pack method are used to build inventories for the inventory analysis of items such cell containers, cooling systems, modules, and pack-level packaging. We have created process-based inventory models for the GSC, lithium film, electrolyte (LiTFSI, DOL, LiNO3), and Li-S cell manufacturing, which are described below. Moreover, Table 1 shows that the capacity ranges from 57 to 62 kWh depending on the technology employed[24].

The specific types of materials in table 1 are included as Polyvinylidene fluoride (PVDF), dimethylformamide (DMF), n-methyl-2-pyrrolidone (NMP), sodium carboxymethylcellulose (NaCMC), dioxolane (DOL), dimethoxyethane (DME), lithium nitrate (LiNO3), polypropylene (PP), polyethylene (PE), and acrylonitrile butadiene styrene (ABS).

In order to assemble the inventory data for Li-S battery materials, a hybrid inventory analysis model is built in this study integrating the lab experiments and theoretical modelling methods. By simulating their unit production processes, inventories of the lithium metal anode and the LiTFSI electrolyte were built, and relevant information was then gathered from the literature and the Ecoinvent database.

The unit processes of producing lithium films and the subsequent surface treatment for building a protective layer are included in the inventory of the lithium metal anode. Extruding lithium metal via a slit is the method used to create lithium film in the commercial sector[30]. Based on the mechanical model used in this study, the extrusion process was modelled, and the cold sheet rolling of steel found in the Ecoinvent database was converted into cold rolling of lithium based on the relative densities of the two materials.



NaCMC-sulfur	
cathode	**kg**
Aluminium ingot	2.69
carbon black	6.17
Binder(NaCMC)	3.09
Colloidal sulfur	21.6
Anode	**kg**
Lithium billet, Primary	7.04
Electrolyte	**kg**
LiTFSI	59.05
DOL	13.59
DME	25.1
LiNO3	0.24

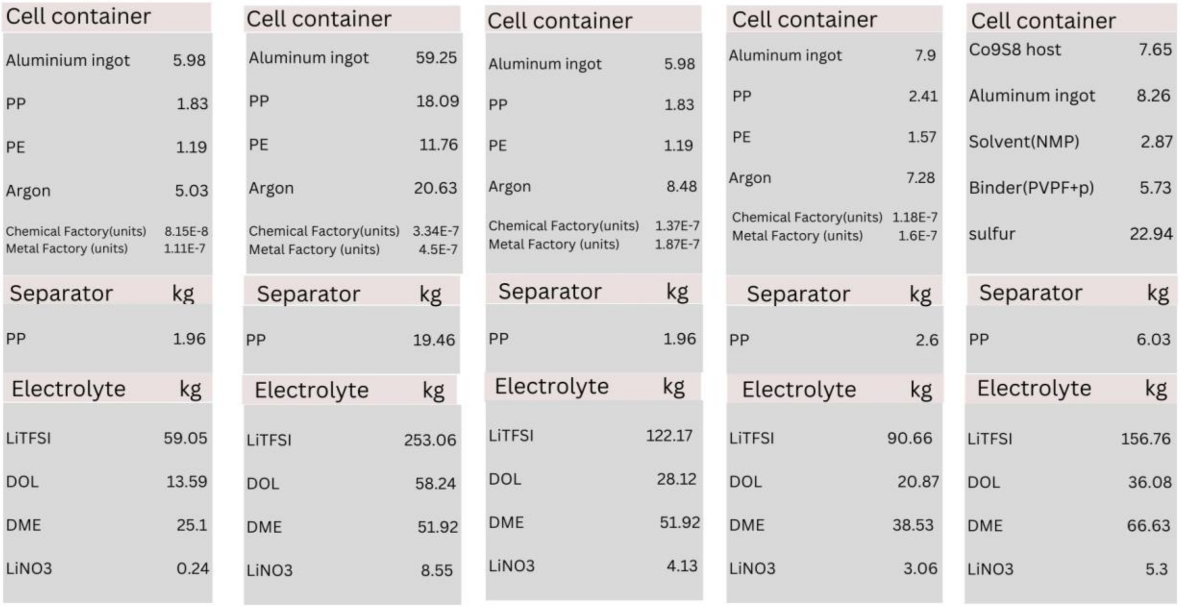
Graphene-CNT-CO-sulfur	
cathode	**kg**
Graphene-sulfur	24.69
Aluminum ingot	26.66
carbon black	7.05
Solvent(NMP)	2.3
Binder(PVPF)	9.07
Anode	**kg**
Lithium billet, Primary	7.04
Electrolyte	**kg**
LiTFSI	253.06
DOL	58.24
DME	51.92
LiNO3	8.55

Li2S-graphene	
cathode	**kg**
Li2s graphene	22.34
Solvent(Acetylene)	1.24
Aluminum ingot	2.69
Binder(PVPF)	1.24
Anode	**kg**
Lithium billet, Primary	7.04
Electrolyte	**kg**
LiTFSI	122.17
DOL	28.12
DME	51.92
LiNO3	4.13

MgB2-sulfur	
cathode	**kg**
Graphene-MgB2	13.61
Aluminium ingot	3.56
Solvent(NMP)	1.36
Binder(PVPF)	2.72
sulfur	20.41
Anode	**kg**
Lithium billet, Primary	7.04
Electrolyte	**kg**
LiTFSI	90.66
DOL	20.87
DME	38.53
LiNO3	3.06

Co9S8-sulfur	
cathode	**kg**
Co9S8 host	7.65
Aluminum ingot	8.26
Solvent(NMP)	2.87
Binder(PVPF+p)	5.73
sulfur	22.94
Anode	**kg**
Lithium billet, Primary	7.04
Electrolyte	**kg**
LiTFSI	156.76
DOL	36.08
DME	66.63
LiNO3	5.3

Table 1A: Materials and energy inputs inventory[24]



Cell container	
Aluminium ingot	5.98
PP	1.83
PE	1.19
Argon	5.03
Chemical Factory(units)	8.15E-8
Metal Factory (units)	1.11E-7
Separator	**kg**
PP	1.96
Electrolyte	**kg**
LiTFSI	59.05
DOL	13.59
DME	25.1
LiNO3	0.24

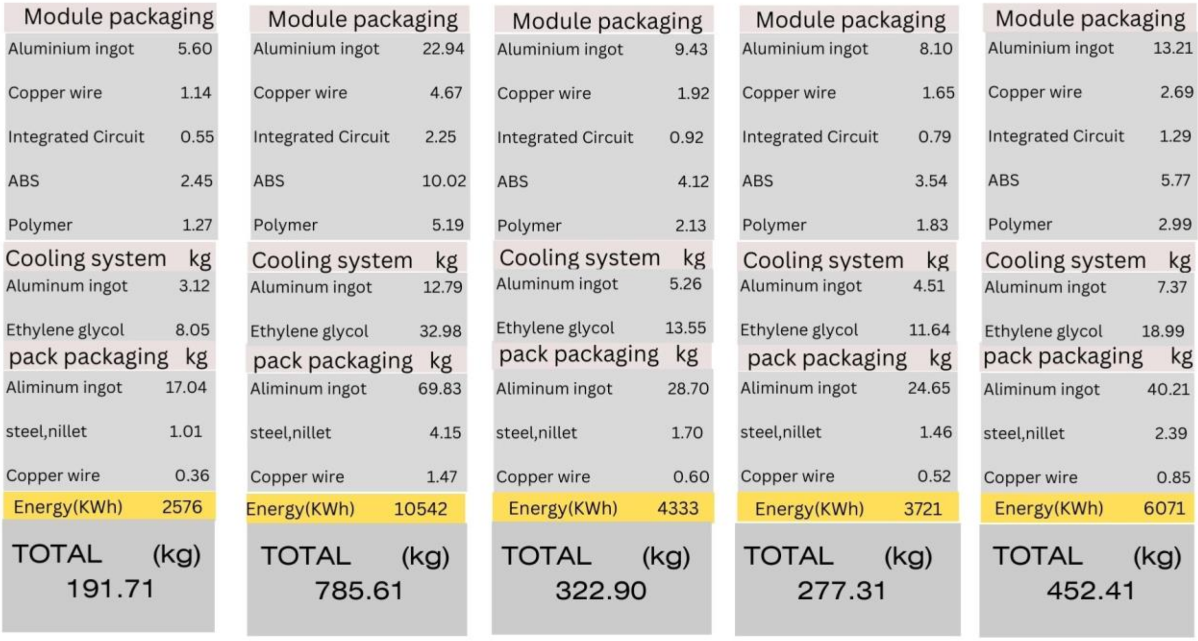
Cell container	
Aluminum ingot	59.25
PP	18.09
PE	11.76
Argon	20.63
Chemical Factory(units)	3.34E-7
Metal Factory (units)	4.5E-7
Separator	**kg**
PP	19.46
Electrolyte	**kg**
LiTFSI	253.06
DOL	58.24
DME	51.92
LiNO3	8.55

Cell container	
Aluminum ingot	5.98
PP	1.83
PE	1.19
Argon	8.48
Chemical Factory(units)	1.37E-7
Metal Factory (units)	1.87E-7
Separator	**kg**
PP	1.96
Electrolyte	**kg**
LiTFSI	122.17
DOL	28.12
DME	51.92
LiNO3	4.13

Cell container	
Aluminum ingot	7.9
PP	2.41
PE	1.57
Argon	7.28
Chemical Factory(units)	1.18E-7
Metal Factory (units)	1.6E-7
Separator	**kg**
PP	2.6
Electrolyte	**kg**
LiTFSI	90.66
DOL	20.87
DME	38.53
LiNO3	3.06

Cell container	
Co9S8 host	7.65
Aluminum ingot	8.26
Solvent(NMP)	2.87
Binder(PVPF+p)	5.73
sulfur	22.94
Separator	**kg**
PP	6.03
Electrolyte	**kg**
LiTFSI	156.76
DOL	36.08
DME	66.63
LiNO3	5.3

Table 1B: Materials and energy inputs inventory[24]



Module packaging	Module packaging	Module packaging	Module packaging	Module packaging	Module packaging
Aluminium ingot	5.60	22.94	9.43	8.10	13.21
Copper wire	1.14	4.67	1.92	1.65	2.69
Integrated Circuit	0.55	2.25	0.92	0.79	1.29
ABS	2.45	10.02	4.12	3.54	5.77
Polymer	1.27	5.19	2.13	1.83	2.99
Cooling system	kg	kg	kg	kg	kg
Aluminum ingot	3.12	12.79	5.26	4.51	7.37
Ethylene glycol	8.05	32.98	13.55	11.64	18.99
pack packaging	kg	kg	kg	kg	kg
Aliminum ingot	17.04	69.83	28.70	24.65	40.21
steel,nillet	1.01	4.15	1.70	1.46	2.39
Copper wire	0.36	1.47	0.60	0.52	0.85
Energy(KWh)	2576	10542	4333	3721	6071
TOTAL (kg)	191.71	785.61	322.90	277.31	452.41

Table 1C: Materials and energy inputs inventory[24]

Small scale production can be used to predict the status of Li-S battery manufacture in the near future because Li-S batteries are still in the early stages of commercialization. Energy usage will be considerably lower when producing Li-S batteries on a large scale for industrial use in the future. Here, the Li-S battery manufacturing is broken down into unit manufacturing processes, such as active material mixing, slurry coating, drying, calendaring, notching, stacking, filling, welding, degassing, and packaging, in order to evaluate and benchmark the energy use of Li-S battery production at both pilot scale and industrial scale. Based on relevant industrial production statistics from the literature, the precise energy consumption of each unit manufacturing process at an industrial scale is compiled. Finally, it is anticipated that producing Li-S batteries on an industrial scale requires between 11.3-22.8 kWh of energy for each Li-S cell[28].

3.3 Equivalency for comparison

Our battery packs were modelled using the approximate reference of the Audi Etron [33] and in accordance with the models replicated by [28] assuming that each cell must generate 60 A h. The modelled battery packs have 432 cells (Table 1) with a power capacity of 57 kWh to 62 kWh, and the cells have a performance capacity of about 132-144 Wh.

Chapter 4: Results and discussion

4.1 Life cycle impact Assessment from cradle to gate analysis

Fig 3.1 shows the environmental impacts of Li-S batteries per kWh of storage capacity. Results are presented in 11 impact indicators that can be easily identified by colour from the life cycle impact assessment (LCIA) for the five Li-S batteries under study. The graphene-CNT-Co-sulfur battery, which has a cathode based on graphene nanosheets, CNTs, Co nanoparticles, sulfur, super P carbon, and PVDF, has the highest environmental burdens. At first glance, the NaCMC-sulfur battery, which has a cathode composed of 70% colloidal sulfur, 20% activated carbon, and 10% NaCMC, has the lowest environmental impact of all the studied categories. The MgB2-sulfur cathode, which contains metallic MgB2, is the second battery with a lower environmental impact in the assessed impact indicators[20].

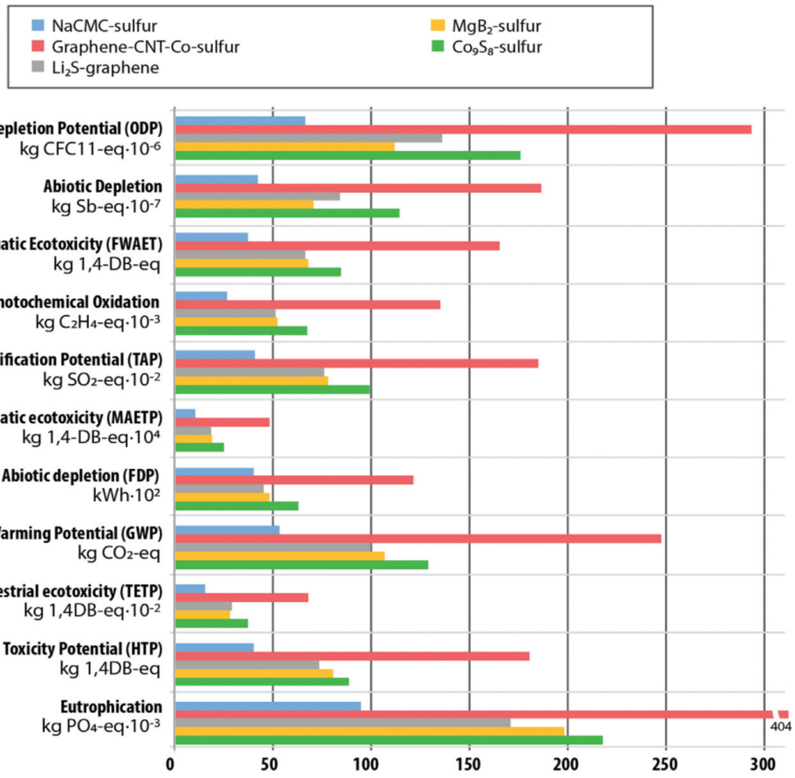


Figure 4.1: Environmental effects of the five original Li-S batteries chosen, each with a storage capacity of 1 kWh

These variations are more pronounced in impact measures like ODP, AP, and GWP, where increases up to a factor of 4.5 are seen. It should be noted that as Li-S cathodes are often made to perform better in terms of energy density, tactics that trap lithium polysulfides are frequently attempted. Green chemistry principles receive less attention because this performance enhancement sacrifices resource/energy efficiency and process simplicity.

We attribute this increased environmental impact to the cathode's complex multicomponent nature and the several synthetic methods used to produce it, including calcinations at 900 C in an argon atmosphere and the use of hydrochloric acid. These findings emphasize the critical need of avoiding cathodes, which are made up of numerous components created by time- and energy-consuming multistage synthetic processes.

In addition, Renewable materials, such those made from cellulose, are favoured over PVDF made from petroleum for use as a binder. Therefore, straightforward one-pot batch syntheses and the utilization of renewable resources are advised in order to reduce the environmental effect connected with the fabrication of Li-S batteries.

4.1.1 Global warming potential of Li-S batteries

The distribution of GWP for each battery component has been determined with the goal of providing guidance to reduce environmental impacts during Li-S battery design, as shown in Fig. 3 (the impact has been adjusted so that in all situations the GWP is 100%). For each of the five batteries under study, the electrolyte makes a significant contribution to the GWP (ranging from 35% for the MgB2-sulfur battery to 47% for the Li2S-graphene battery). This considerable contribution results from the significant volume of electrolyte utilized in such batteries, contributing 73 6% of the cell's weight overall.

Because there is a significant amount of non-renewable energy in the mix of power used in Europe, the electricity needed for material processing and cell-pack production also contributes 20 to 25% of the overall impact in this category, making it an important driver for the global warming problem. As they are based on aluminium cell containers and contribute between 8% and 10% of the overall impact, pack packing, cell container, and assembly also have a significant role. The cathode contributes, on average, only 2.3% of the overall GWP, which is far less than the 20% reported for NIBs [16].

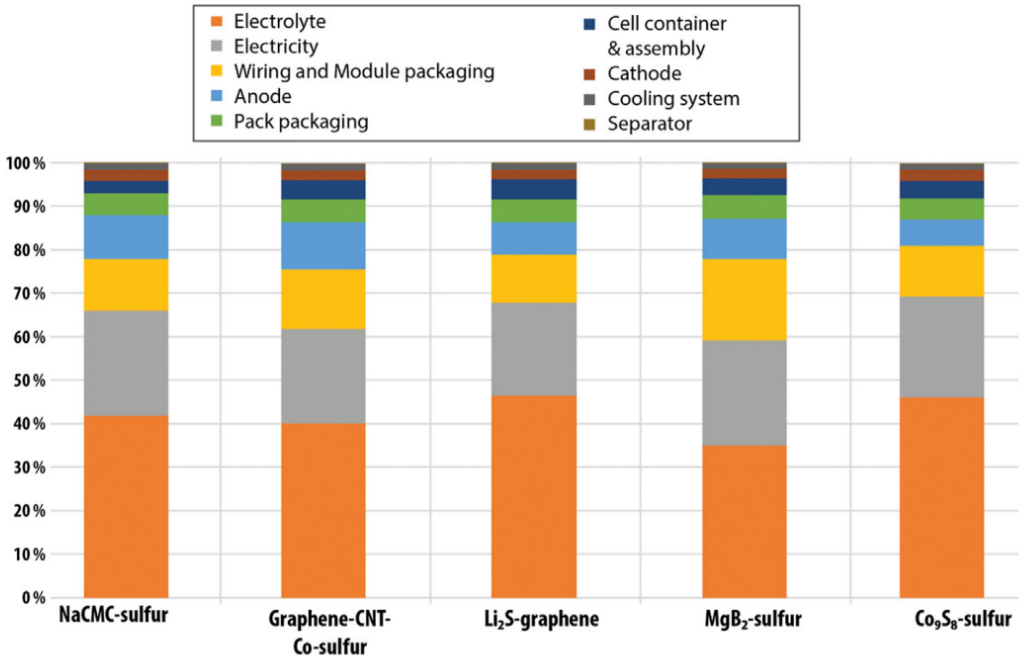


Figure 4.2: comparing the relative contributions of each battery component to the GWP regarding to FU.

4.2 Comparison with Lithium ion and Sodium ion batteries

The resulting LCA findings are compared with the LIB reference case using the same 1 kWh of storage capacity as a FU to provide further insight into the possibilities of Li-S batteries for more sustainable energy storage applications (see Table 2).

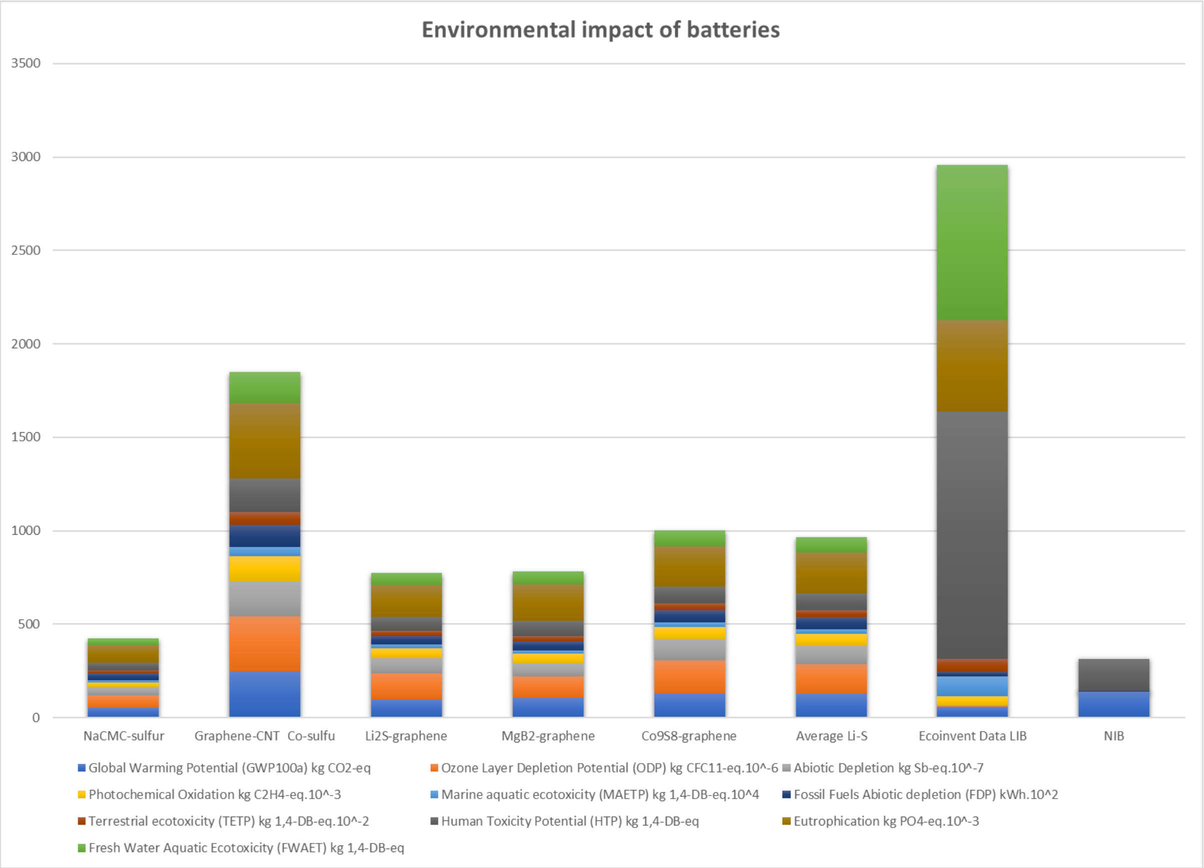
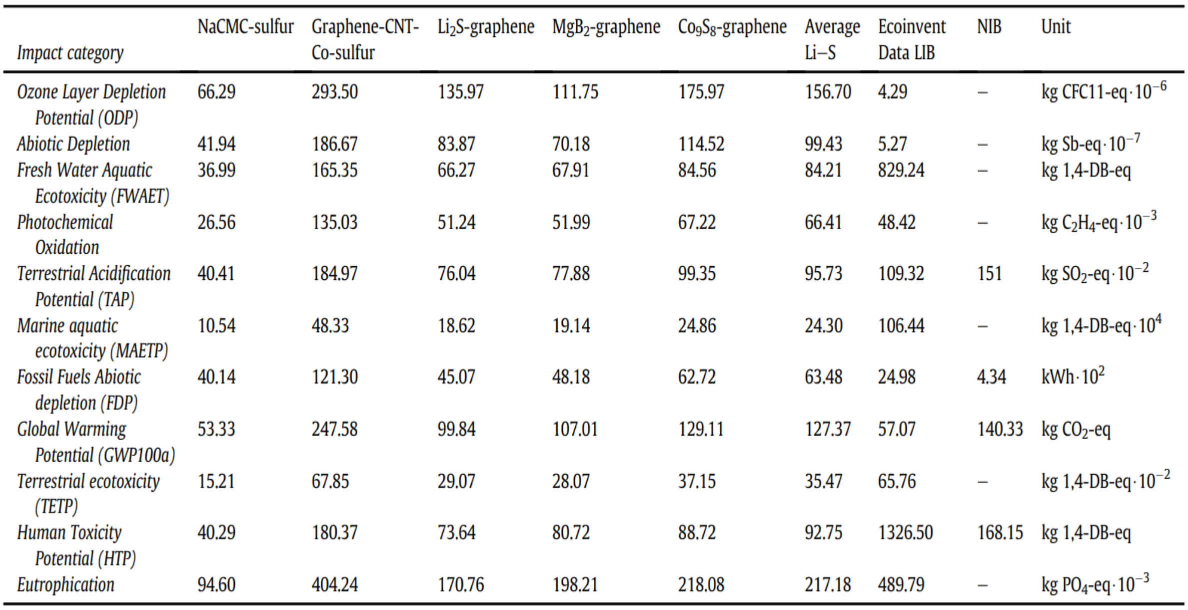


Figure 4.3: Environmental impacts of Lithium-Sulfur batteries, LIB and NIB

The environmental impacts for each of the Li-S cathodes under study. Data for the LIB reference battery was collected from the Ecoinvent database, whilst the impacts of NIB cells were taken from the reference [16]. Due to variations in the LCA analysis, several effect categories for NIB cannot be obtained. Every battery's FU has been kept, and cradle-to-gate boundary system analysis has been used for all analyses.



Impact category	NaCMC-sulfur	Graphene-CNT-Co-sulfur	Li_2S-graphene	MgB_2-graphene	Co_9S_8-graphene	Average Li–S	Ecoinvent Data LIB	NIB	Unit
Ozone Layer Depletion Potential (ODP)	66.29	293.50	135.97	111.75	175.97	156.70	4.29	–	kg CFC11-eq $\cdot 10^{-6}$
Abiotic Depletion	41.94	186.67	83.87	70.18	114.52	99.43	5.27	–	kg Sb-eq $\cdot 10^{-7}$
Fresh Water Aquatic Ecotoxicity (FWAET)	36.99	165.35	66.27	67.91	84.56	84.21	829.24	–	kg 1,4-DB-eq
Photochemical Oxidation	26.56	135.03	51.24	51.99	67.22	66.41	48.42	–	kg C_2H_4-eq $\cdot 10^{-3}$
Terrestrial Acidification Potential (TAP)	40.41	184.97	76.04	77.88	99.35	95.73	109.32	151	kg SO_2-eq $\cdot 10^{-2}$
Marine aquatic ecotoxicity (MAETP)	10.54	48.33	18.62	19.14	24.86	24.30	106.44	–	kg 1,4-DB-eq $\cdot 10^{4}$
Fossil Fuels Abiotic depletion (FDP)	40.14	121.30	45.07	48.18	62.72	63.48	24.98	4.34	kWh $\cdot 10^{2}$
Global Warming Potential (GWP100a)	53.33	247.58	99.84	107.01	129.11	127.37	57.07	140.33	kg CO_2-eq
Terrestrial ecotoxicity (TETP)	15.21	67.85	29.07	28.07	37.15	35.47	65.76	–	kg 1,4-DB-eq $\cdot 10^{-2}$
Human Toxicity Potential (HTP)	40.29	180.37	73.64	80.72	88.72	92.75	1326.50	168.15	kg 1,4-DB-eq
Eutrophication	94.60	404.24	170.76	198.21	218.08	217.18	489.79	–	kg PO_4-eq $\cdot 10^{-3}$

Table 2 : Environmental impacts of Lithium-Sulfur batteries, LIB and NIB

Environmental effects for each of the Li-S cathodes under study. Data for the LIB reference battery was collected from the Ecoinvent database, whilst the impacts of NIB cells were taken from the reference.[16] Due to variations in the LCA analysis, several effect categories for NIB cannot be obtained. Cradle-to-gate boundary system was used for all analyses and FU was kept constant across all batteries.

4.2.1 Interpretation of Li-S, LIB and NIB batteries

Comparing the 140 kg CO2-eq of an NIB battery with a layered oxide cathode and an anode made of styrene-butadiene rubber, NaCMC binder, and hard carbon (with an electrolyte based on porous polyethylene/polypropylene soaked in an organic solvent containing sodium hexafluorophophate salt), studied Li-S batteries exhibit an improved GWP of 53-247 kg CO2-equivalent and 57 kg CO2-eq of the LIB reference case[16, 35].

The human toxicity potential (HTP) of Li-S batteries, on the other hand, is in the range of 40-180 kg 1,4-DB-eq (mean value 92), which is comparable to the results for NIBs in the worst-case scenario (battery cell 2) and significantly less than the 1326.5 kg 1,4-DB-eq of the LIB reference case. In comparison to NIBs 151 kg SO2-eq. 10^{-2} or the LIB reference case's 109 kg SO2-eq.10^{-2}, the TAP achieves impacts of 40-185 kg SO2-eq. 10^{-2} (mean value 96).

Overall, it is evident that Li-S batteries by storage capacity of 1 kWh as FU, have the ability to beat as environmental performance match better than both LIBs and NIBs for the majority of environmental consequences. The following explanation helps to understand these findings. In comparison to LIB and NIB batteries, Li-S batteries need less hard carbon. Precursors for carbonaceous materials are typically petroleum coke or sugars, which increases the overall environmental effect due to the usage of non-renewable petroleum or the requirement for sugar extraction from sugar beets or sugar cane, which increases water consumption and eutrophication[36].

Additionally, it takes up to 11 kg of sugar to produce 1 kg of hard carbon (Peters et al., 2019), and the carbonization process requires energy (heat and electricity), and nitrogen is needed to maintain an inert atmosphere during manufacturing, all of which have an influence on the environment[37].

Cathode active materials for LIBs include lithium cobalt oxide LiCoO2, lithium manganese oxide LiMn2O4, and lithium iron phosphate LiFePO4, whereas NIBs require nickel hexacyanoferrates (Ni2 [Fe(CN)6]) or sodium vanadium phosphates (Na3V2(PO4)3). In contrast, heavy metals such as cobalt, manganese, or nickel are not required in Li-S batteries, where cathodes have sulfur levels as high as 70% by weight. Because LIBs rely on hazardous cathodes, the fresh water aquatic ecotoxicity and human toxicity potentials associated with Li-S batteries are reduced [40].

Overall, there are three impacts that are clearly shown in this investigation for LIB batteries: the first is freshwater aquatic ecotoxicity (FWAET), which shows nearly 12 times more damage than average Li-S batteries, the second is eutrophication, which shows more than 2 times more damage than average, and the highest is human toxicity potential (HTP), which shows 1326.5 kg 1,4-DB-eq effect. Furthermore, Li-S cathodes are frequently created following the efficient thermal infusion of sulfur into a carbonaceous framework, bypassing labor-intensive, costly, and environmentally destructive synthetic processes for the layered oxides used in LIBs and NIBs[41].Li-S batteries could be a potential long-term energy storage solution. In comparison to the LIB reference scenario, Li-S batteries have a variety of drawbacks, including a higher risk for ozone layer depletion. This could be explained by the fact that sulfur serves as a reactive medium for chlorine gases to destroy ozone at low temperatures (in the atmosphere), with one chlorine atom capable of destroying over 100,000 ozone molecules. In contrast to petroleum-based PVDF, which is the major binder in LIBs and NIBs (accounting for over 20% of the cathode and considerably contributing to greenhouse gas emissions), Li-S batteries can use cellulose-derived binders, yielding positive results. Furthermore, because aluminium is 1200 times more abundant in the Earth's crust than copper, utilizing aluminium as a cathode current collector instead of copper reduces HTP and freshwater eutrophication potential (FEP) while also lowering metal depletion caused by copper mining. These results are congruent with the findings of Ellingsen et al., who discovered that copper current collectors provided more than 60% of the impact indicators of freshwater ecotoxicity, marine ecotoxicity, terrestrial ecotoxicity, and human toxicity[41].

4.3 Sensitivity analysis

In batteries with an electrolyte/sulfur (E/S) ratio greater than $10\ \mathrm{mL\,.\,g^{-1}}$, the electrolyte weighs more than 50% of the total cell weight. Thus, too much electrolyte could make the battery as a whole heavier (and larger), decreasing the energy density. In order to create high-performance Li-S batteries, it has been demonstrated in various publications that lowering the E/S ratio to values below 5 results in a boundary condition.[43] As a result, the E/S ratio was reduced to 4 and the environmental effects of the examined Li-S batteries were once again assessed.

The majority of papers report using large electrolyte volumes, typically expressed as E/S ratios of 1.5-15 $\mathrm{mL\,.\,g^{-1}}$ (see Fig. 3.4), to obtain high-performance Li-S batteries and achieve good electrochemical sulfur utilization. However, the electrolyte contains a high passive weight, which increases the environmental burdens of the battery without making a positive electrochemical contribution[44].

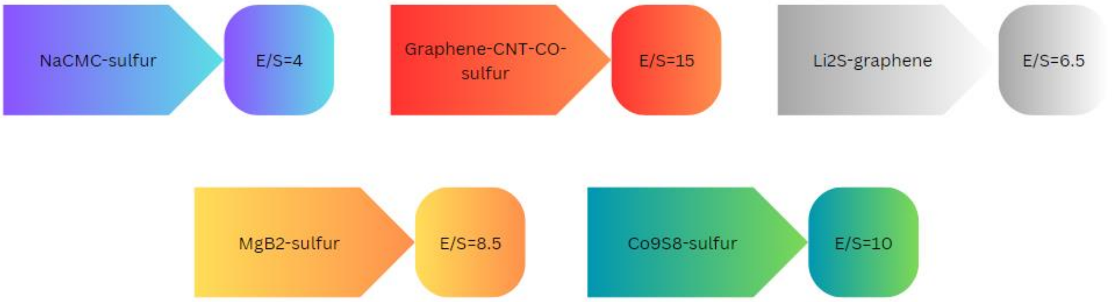


Figure 4.4: electrolyte/sulfur (E/S) ratio for each Li-S battery type

Based on this assumption and research results, which demonstrate that the usage of the electrolyte is largely what causes the environmental impact of Li-S batteries, a sensitivity analysis has been conducted to measure the impact of the liquid volume. Accordingly, the cathodes have been standardized with an E/S ratio of 4, assuming that long-cycling may still be maintained while still maintaining good electrode wetting and assuming future forecasts for the electrochemical stability [45,46].

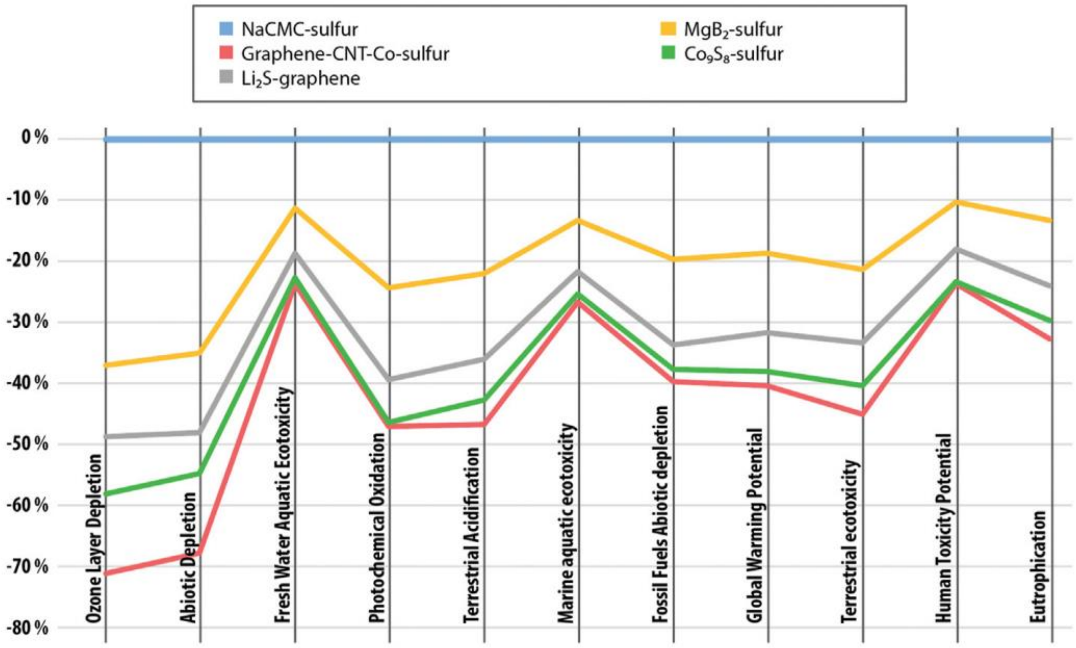


Figure 4.5: Analysis of the impact of the life cycle on each of the 11 impact indicators under different conditions, ranging from the original E/S ratio.

In Fig. 4, which accounts for the relative reduction on each impact indicator, the effect of the electrolyte reduction on the 11 impact indicators in a cradle-to-gate LCA for the five Li-S batteries under study is depicted. The environmental effect of Li-S batteries is demonstrably reduced by an E/S reduction of up to 4. When compared to batteries using the huge electrolyte contents reported in the investigated batteries, the life cycle impacts of Li-S batteries with an E/S ratio of 4 are 11-71% lower. The improvements in ozone layer depletion, abiotic depletion, photochemical oxidation, acidification, and human toxicity, where reductions of over 40% are achieved, are particularly significant. There are various explanations for this. On the one hand, lithium is a very rare element that occurs in nature in low amounts, necessitating extensive soil processing during mining. In order to limit the effects of ozone layer depletion, abiotic depletion, or human toxicity, it may be possible to reduce the amount of lithium salts in the liquid electrolyte (LiTFSI and LiNO3). This would reduce waste generation, water contamination, and transport issues that are caused by brine treatment.[47] On the other hand, a significant amount of methylchloride solvent, which has a high ozone depletion potential, is required for the synthesis of LiTFSI.

Additionally, the use of dioxolane and dimethoxyethane solvents as liquid electrolytes can have negative health effects because they have NFPA 704 (Standard System for the Identification of the Hazards of Materials for Emergency Response) ratings of 1-3-2 and 2-2-0, respectively, for health, flammability, and instability.[48] In addition, dioxolane and dimethoxyethane have relatively low vapour pressures at 20 degrees Celsius (79 and 48 mm Hg, respectively), making them easy to volatilize. Their release into soil or water also exhibits high mobility, as indicated by their estimated KOCs (organic carbon-water partition co-efficients) of 15 and 18, respectively. Finally, ammonia and nitrate are released during the synthesis of dimethoxyethane and dioxolane.[28]

Given that all other factors remain constant, it may be safe to anticipate that lowering the E/S ratio to 4 will result in lower battery delivered capacity, which will reduce energy density and increase the environmental effect per kWh of storage capacity. However, because we aim to emphasize how the electrolyte affects the total environmental impact, we hypothesize that lowering the E/S ratio up to 4 is not linked to a decreased electrochemical performance. Additionally, relatively few research articles thoroughly investigate the drop in electrochemical performance caused by electrolyte decrease, making it difficult to gather this information.

Chapter 5: Lesson learned and Conclusion

5.1 Achievement

The life cycle inventory of five Li-S batteries has been compared in a cradle-to-gate life cycle assessment research with cathodes that have high sulfur loadings in the range of 1.5-15 $mg.cm^{-2}$. Life cycle inventories of the examined batteries, which include battery assembly and component fabrication, are made public to allow for future comparisons. Environmental impact are categorized into 11 standardized CML-baseline indicators, such as the potential for ozone depletion, global warming, or acidification, because they offer more specific information about particular chemical compounds and the associated environmental burdens of using Li-S batteries.

The results show that changing the cathode and the other components in the appropriate ways can reduce the environmental impact of the entire Li-S battery by up to 5 (for example, the global warming potential ranges between 53 and 248 kg CO2-eq per kWh). It's interesting to note that the cathode with the lowest environmental effect was one made up of 70% colloidal sulfur, 20% activated carbon, and 10% NaCMC, highlighting the critical need for using renewable binders and high sulfur loadings. Li-S batteries can have a lower environmental effect per kWh of storage capacity as compared to traditional lithium-ion batteries. Additionally, even though a liquid electrolyte excess is typically considered advantageous for the electrochemical performance, the acquired LCA results unmistakably show that large electrolyte volumes have a detrimental impact on the environmental loads connected with the use of Li-S batteries. As a result, a sensitivity analysis where the amount of electrolyte is decreased was carried out, which revealed that simply restricting the amount of used electrolyte can reduce environmental loads by up to 70%. Given the low technical development of Li-S batteries compared to LIBs, which offers space for significant improvements regarding environmental performance, the obtained results are especially encouraging. Cradle-to-grave LCA studies should be conducted as soon as the data is available to fully understand the environmental effects of Li-S batteries. LIB batteries have an increased modelling capacity of up to 38%, depending on the impact category. In light of the simplicity with which the spent salts and anodes can be recovered using a variety of automated separation techniques, this would highlight the improved recycling potential of Li-S batteries in compared to LIBs.

Overall, this study would encourage more, follow-up research concentrating on the crucial factors that must be taken into account for low environmental effect Li-S batteries, offering recommendations to encourage the commercialization of greener Li-S batteries.

5.1.1 Lessons Learned

Both substantial literature research on different batteries used in the field of energy storage as well as the intensive use of OpenLca Professional Software were part of this study.

The research on batteries that are still very much in the LAB scale helped to understand the process of battery maturity and the eventual release to the market in addition to giving a strong understanding of the most common LCA tools. Although Li-S batteries still have a long way to go before they completely replace Li-ion batteries in EVs or in other industrial equipment, this study has given us another perspective on the research process and highlighted several areas that could use improvement.

5.2 Future improvement potential

This study about Li-S batteries is still in its early stages, as evidenced by the issues that Li-S batteries still have. This has the potential to be advantageous because there is still much space for advancement, both in terms of sustainability and electrochemical performance. In order to create extremely porous and electrically conducting cathode materials, for instance, renewable resources like cellulose, the most prevalent organic substance on Earth, might potentially be used[49]. This would reduce the need for harmful or rare elements. As some impact categories, such as GWP, could be lowered by 13%, scaling up the production of Li-S batteries from laboratory-scale to market (into pouch cells, for example) should be a priority to reduce their associated environmental impact[23]. When evaluating the environmental effects of energy storage devices, battery longevity and internal efficiency are crucial considerations. In the short to medium term, it is anticipated that the environmental costs connected with the production and use of Li-S batteries would decrease because the technology is still in its early stages of development. To that aim, it should be a top priority to develop batteries that can withstand up to 2000 cycles with an internal efficiency of above 90%[16].

Recycling ought to be a fundamental component of any system for storing renewable energy because it can lessen the negative environmental effects of Li-S batteries. For instance, the LiTFSI salt that is frequently utilized in Li-S electrolytes is extremely stable chemically and thermally, allowing for its recovery and generating additional financial benefits[50]. As compared to typical LIBs, Li-S batteries employ solid lithium metal, which can be recovered using automated processes like Foucault's current and density separators[28]. This could lead to future advancement in the field.

Although the combination provides the greatest benefits at the plant level, hybridization can also be implemented at the light level, allowing application in EVs powered by Li-S batteries when space is limited. Recent LCA studies in the field of thermal energy storage have demonstrated that combining diverse energy storage technologies can minimize greenhouse gas emissions while also improving energy source reliability and economic viability. The coupling of Li-S batteries with thermal energy storage should be researched in the near future in order to gain synergistic benefits toward energy storage systems with decreased environmental impact.

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Appendix

** This table illustrate the Inventory data related to the Litium-Sulfur battery from IREC energy institute in Barcelona which investigating lithium-sulfur batteries making use of Si anodes and biomass-derived carbon materials.

Flow	**Quantity**	**Unit of measure**	**Environmental footprint dataset**	**Notes**
OUTPUT				
Biomass based-carbon	1	kg		
INPUTS				
Carbon fibre	0/00015	kg		
Carbon, organic, in soil or biomass stock	0/0035	kg		
Copper sulfate_at plant_EU-28+3_S	0/00005	kg	Ecoinvent database	This flow is exported from Ecoinvent database
De-ionised water	2	kg		
Ethanol	0/01578	kg		
Potassium chloride (agrarian, 60% K2O)	0/001	kg		
Sodium sulphite	0/0045	kg		

Table 3 : inventory data for Biomass based-carbon

Flow	Quantity	Unit of measure	Ecoinvent dataset	Notes
OUTPUT				
Li-s battery from IREC	1	Coin cell		
INPUTS				
Aluminium foil	0,0000044	kg		
Biomass based-carbon	0,00000042	kg		This flow is provided separately from IREC
Carbon black, general purposes	0,00000017	kg		
Dimethyl carbonate	0,00002	kg		
Dioxane	0, 00002	kg	Extracted from Ecoinvent 3.2 database	
Ethylene carbonate	0,00002	kg		
Ethylene glycol dimethyl ether	0,00002	kg	Extracted from Ecoinvent 3.2 database	
lithium	0,0000044	kg		
lithium carbonate	0,00000015	kg		
lithium hydroxide	0,000009	kg		Bistrifluoromethanesulfonimide lithium salt (LiTFSi) has similar chemical structure as lithium hydroxide but there is no clear data in EF database. lithium hydroxide is used instead.
Transportation Ship	0,087233475	kgkm	ransoceanic ship, containers, consumption mix, to consumer, heavy fuel oil driven, cargo, 27.500 dwt payload capacity, ocean going	
Transportation lorry	0,0000024486	kgkm	Articulated lorry transport, Total	20-26t, Euro5

			weight 20-26 t, mix Euro 0-5, consumption mix, to consumer, diesel driven, Euro 0 - 5 mix, cargo, 20 - 26t gross weight / 17,3t payload capacity	
Residual grid mix, consumption mix, to consumer, AC, technology mix, 1kV - 60kV	0,0489	MJ	Electricity, Residual Mix, ES	The electricity which is used for manufacturing and testing (1000 cycle)
Stainless steel (cold rolled)	0/00339	kg		It contains all stainless steel included as casing, spring spacer
Sulphur	0/000001	kg		

Table 4 : inventory data for Li-S battery cell production

the most important point in this inventory data is the energy consumption which is not so reliable due to the lab scale production of battery, there is not clear data and information energy consumption for producing a coin cell of battery in IREC institute and this data is assumed.