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Life Cycle Assessment of Li-Sulphur Batteries for Electric Vehicles

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Summary

Lithium-Sulphur (Li-S) batteries have emerged as a promising battery technology, with a higher theoretical capacity and energy density than Lithium-ion (Li-ion) batteries used today. Moreover, due to their chemical composition, Li-S batteries presumably present a lower environmental profile compared to Li-ion ones. To verify this statement, this study performs life cycle assessment (LCA) analyses on Li-S battery coin cells to be further scaled up in order to estimate their performance as a battery for electric vehicles (EVs).

Keywords: battery cycle life, energy storage, environment, EV (electric vehicle), LCA (Life Cycle Assessment)

1 Introduction

The continuous and planned increase of the electrification in the transport sector is one of the main drivers of advances in energy storage for electric vehicle (EV) propulsion and present technological challenges to achieve the expected requirements. The implementation of the EVs on our roads remains a challenge and it is below the expected figures. The elevated costs of the batteries and thus the EV cost are the main barriers that slow down the massive depletion of this technology. With the aim of reaching a range field of 500 kilometres autonomy in the short term, it is necessary to investigate new materials and configurations of EV batteries. To this end, lithium-sulphur (Li-S) batteries are the closest battery technology capable of meeting these expectations [1]. Although Li-S batteries can overcome most of the technical issues, this solution still needs to demonstrate how the socio-economic-environmental barriers associated are solved, above all when considering their fitting in a circular economy society. There is no clear evidence of the environmental benefits due to the use of Li-S batteries as an alternative to Li-ion batteries. In order to cover this gap, this work aims at performing the environmental assessment of Li-S cells by using Life Cycle Assessment (LCA) methodology.

1.1 Li-S batteries description

Li-S technology differs substantially from Li-ion chemistries; in fact, the use of sulphur as a main metal in the cathode leads to specific chemical reactions that do not occur in Li-ion ones. In particular, in Li-S cells, sulphur reacts with lithium ions when reduced from the elemental state S8, via the intermediates Li2S8, Li2S4, Li2S2, to lithium sulphide Li2S depending on the State of Charge (SOC) [2], [3].

Nowadays, the practical energy density of Li-S batteries is considered to be between 200 and 500 Wh where the lower limit is within the current values obtained for high performance packs [4].

From an environmental perspective, the use of sulphur as a replacement of different metals is supposed to lead to lower impacts because this is an abundant and easy-to-extract material (or even recoverd from industrial waste). However, while there have been many LCAs performed on various types of Li-ion batteries, Li-S batteries are a new technology and since they are not yet commercialised, LCA studies are lacking. The first article on performing a LCA on a Li-S battery was just published this past March, 2017 [5]. A hybrid LCA model was developed for a Li-S battery pack using a lithium metal anode, graphene-sulphur cathode, and LiTFSI electrolyte for the final application in EVs [5].

In our case, the assessment has been done using a Li-S coin cell with a sulphur-carbon composite cathode and lithium metal anode developed within the H2020 HELIS project [6]. This cell uses a cathode binder, two of which were tested here: the first one is styrene-butadiene-rubber (SBR) and carboxymethyl cellulose (CMC) in water and the second one is polyvinylidene fluoride (PVDF) in N-methyl-2-pyrrolidone (NMP). The cell materials also include a polypropylene separator, a cathode connect and anode connect, and Al-PET-PP composite cell casing.

2 Methodology

The environmental assessment of the Li-S battery has been carried out using Life Cycle Assessment methodology. This section describes this methodology and the main hypothesis that have been considered, together with the data employed in the assessment..

2.1 Life Cycle Assessment

Life Cycle Assessment (LCA) is an analysis of the environmental impact of a product, process, or activity over the course of its lifetime by identifying and quantifying the energy and materials used and wastes released to the environment [5]. There are two standards for LCA created by the International Organisation for Standardisation (ISO): ISO 14040 (Environmental management - Life cycle assessment - Principles and framework) and ISO 14044 (Environmental management - Life cycle assessment - Requirements and guidelines) [10]. LCAs have four distinct steps, shown in Figure 1 below.

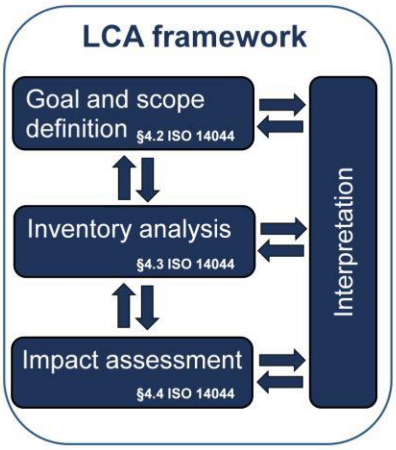

Figure 1 LCA Framework as per ISO 14040

LCA is a proven methodology that enables the quantification of the environmental impacts of a product or service over the course of its lifetime by identifying and quantifying the energy and materials used and wastes released to the environment. According to these standards, LCA studies shall indicate the goal and scope, the boundaries of the system under study, the inventory phase that covers all inputs and outputs of the processes included within the boundaries, the quantification of the environmental impacts and the results discussion.

2.1.1 Goal and Scope

This study has two main purposes. The first one is to analyse the environmental impacts due to the production of the coin cells. As a second purpose, after an adequate scaling to virtually build a 22kWh vehicle battery pack, made using the active material from the Li-S coin cell, the environmental impacts of this battery pack are assessed.

For this second exercise, the full life cycle has been considered and the circuit board (PCB) and battery casing have been considered. The assessment does not include the full battery management system (BMS).

2.1.2 System boundaries and functional unit

There are two functional units used here for the two objectives of the study. For the analysis of the impact of one coin cell, the functional unit used is one Li-S battery cell from “cradle to gate”. For the assessment of the environmental impacts of the full life of the battery in the “cradle to grave” approach, the functional unit used is a 22 kWh Li-S battery system that runs 1000 cycles which would carry out around 150.000 km. The reason for the different functional units is because in the first objective of the study, the impact of one coin cell is determined and thus, it makes the most sense to have the functional unit be that one cell. However, when enlarging the scope to a “cradle to grave” assessment, it is necessary to identify an appropriate function, and this can only be given considering a vehicle battery.

2.1.3 Impact categories

The CML 2001 method [9] was used to evaluate the impact categories in the GaBi Professional software [10]. This impact assessment method was developed by Leiden University’s Institute of Environmental Sciences in Leiden, The Netherlands. CML 2001 limits uncertainties by restricting quantitative modelling to early stages in the cause-effect chain. The selected impact categories are listed below:

- **Acidification Potential (AP) [kg SO2 eq**]: Acidification is caused by release of protons in the terrestrial or aquatic ecosystems. In the terrestrial ecosystem the effects are seen in softwood forests (e.g. spruce) as inefficient growth and as a final consequence dieback of the forest. The substances contributing to acidification can be transported across boundaries via air. Sulphur oxides, nitrogen oxides, inorganic acids (hydrochloric acid, nitric acid, sulphuric acid, phosphoric acid, hydrofluoric acid, hydrogen sulphide), and ammonia are substances contributing to acidification

- **Eutrophication Potential (EP) [kg Phosphate eq]**: Eutrophication can be defined as the enrichment of aquatic ecosystems with nutrients leading to increased production of plankton, algae and higher aquatic plants leading to a deterioration of the water quality and a reduction in the value of the utilisation of the aquatic ecosystem. Nitrogen and phosphorous compounds are mentioned as the main origin of nutrient enrichment.

- **Global Warming Potential (GWP) [kg CO2-eq.]:** Global warming - or the “greenhouse effect” - is the effect of increasing temperature in the lower atmosphere. The lower atmosphere is normally heated by incoming radiation from the outer atmosphere (from the sun). A part of the radiation is normally reflected by the soil surface but the content of carbon dioxide (CO2) and other "greenhouse" gasses (e.g. methane (CH4), nitrogen dioxide (NO2), chlorofluorocarbons etc.) in the atmosphere absorb the IR-radiation. This results in the greenhouse effect e.g. an increase of temperature in the lower atmosphere to a level above normal.

- **Ozone Depletion Potential (ODP) [kg CFC-11 eq]:** Decomposition of the stratospheric ozone layer is causing increased incoming UV-radiation that leads to impacts on humans, natural organisms and ecosystems. Contributors to this decomposition are halocarbons (CFCs, HCFCs, halons, etc.)

- **Photochemical Ozone formation Potential (POCP) [kg ethane eq]:** Photochemical ozone formation is caused by degradation of volatile organic compounds (VOC) in the presence of light and nitrogen oxide (NOx) ("smog" as a local impact and "tropospheric ozone" as a regional impact). The biological effects of photochemical ozone can be attributed to biochemical effects of reactive ozone compounds.

- **Abiotic Resource Depletion Potential, non-fossil (ADP) [kg Sb eq]:** assessment of the scarcity of a given material resource, using a scarcity index.

- **Abiotic Resource Depletion Potential (ADP-fossil) [MJ]:** assessment of the scarcity of a given energetic resource, using a scarcity index.

2.1.4 Main assumptions and data sources

Data for the assessment has been collected from IREC's own laboratory facilities during the manufacturing of the coin cell. Background data has been used using literature research, BATPac [11], and from GaBi Professional [10] and Ecoinvent [12] databases.
The energy consumption of the cell production is assumed for an industrialised process, thus producing material for many more cells than are currently produced. Since Li-S batteries are still in research, data concerning EOL is yet to be established. Thus, the approach of open-loop recycling has been chosen; this means that the recycling processes are not considered in the assessment. For the EOL phase of the life cycle, it was assumed that metals and plastics not coming into contact with hazardous materials could be recycled (e.g. casing materials), and anything within the electrodes and other parts that contained a hazardous material would be considered as hazardous as well.
Finally, almost all transportation in the LCA was assumed due to not having the sufficient data. For the shipment of materials for production purposes, providers were researched and the most appropriate transport was chosen for these shipments. In the HELIS project, shipment of cell parts between partners of the project were also estimated to find the most appropriate modes of transport. In the EOL phase, the transport of materials to a sorting facility was estimated at 500 km and the transport of the recycled materials to a recycling facility was estimated at 200 km. These were most likely overestimations to be sure that we cover the transportation impact as appropriately as possible.

When it came to sizing the battery systems, there was a lack of data since we only have data on the cells and not the battery systems that they would be scaled to. Characteristics such as battery efficiency, new battery energy density, and accurate battery casing information were not provided and thus this study was accommodated accordingly. Data from literature was used for the sizing of the battery system. The LCA study on Li-S batteries that Deng, et. al. [7] performed was used as a guideline in the sizing of the battery system. Additionally, since the battery efficiency was unknown, a rudimentary approach was taken to calculate the electricity usage in the charging of the battery.

2.2 Inventory

This section includes the inventory of the materials used in the coin cells. Additionally, the characteristics of the cells are given, including cell weight, gravimetric energy density, and cycle life. A complete inventory of the materials used in the coin cell is given in Table 1 along with their weight in grams, their weight ratio (% of total weight), and any comments deemed necessary. Li-S cells are coin cells with a sulphur-carbon composite and lithium metal anode, however the carbon is produced in-house by way of carbon nanofibers that endure a long, energy-intensive process. Additionally, these cells differ in the casing, which is all stainless steel, provided by a coin cell part manufacturer in Japan [13]. The electrolyte is a tetraethylene glycol dimethyl ether (TEGDME, also known as tetraglyme)/dioxane mix; since TEGDME is not in the GaBi or Ecoinvent databases, ethylene glycol dimethyl ether (also known as glyme) was used instead since they are produced by the same reaction route. The separator is again a membrane made from PP. A part from the standard electrodes, electrolyte, separator, and casing, these cells also contain additional parts since they are coin cells: a gasket made from PP, a spacer made from stainless steel, and a spring made from stainless steel so that the coin cell can be pressed by a crimping machine to the same measurements every time. Photos of the cells were taken after production and before testing, displayed in Figure 2.

Figure 2 Photos of the cells manufactured by IREC (left) and their individual parts (right).

Table 1 Inventory of the coin cell

Part material	Weight (g)	Weight ratio (%)	Comment
Positive Electrode	**0,0007**	**0,02**	
Sulphur	0,00021	0,006	Active material
Carbon nanofibers	0,00049	0,014	Active material
Polyacrylonitrile	0,0018		Production of carbon nanofibers
N,N-dimethylformamide	0,017	-	Production of carbon nanofibers
High-density polyethylene	0,0098	-	Syringe used for production of nanofibers
Aluminium foil	0,0021	-	Used in production of nanofibers
Tap water	0,044	-	Used in production of nanofibers
Nitrogen gas	2,35E-06	-	Used in production of nanofibers
Compressed air [Nm3]	0,11E-05	-	Used in production of nanofibers
Electricity [MJ]	3,45E-01	-	
Negative Electrode	**0,015**	**0,44**	
Lithium	0,015	0,44	Active material
Separator	**0,006**	**0,17**	
Polypropylene	0,006	0,17	
Electrolyte	**0,045**	**1,28**	
Dioxane	0,0206	0,58	Active material
Ethylene glycol dimethyl ether	0,0196	0,56	Used instead of TEGDME

Ethylene carbonate	0,0024	0,069	Used in production of LiF6P
Dimethyl carbonate 0	0,0024	0,069	Used in production of LiF6P
Lithium hexafluorophosphate	0,0007	0,021	
Lithium carbonate	0,00017	0,0048	Production of lithium nitrate
Nitric acid	0,00029	0,0082	Production of lithium nitrate
Spacer	**1,59**	**45,07**	
Stainless steel	1,59	45,07	
Spring	**0,167**	**4,74**	
Stainless steel	0,167	4,74	
Gasket	**0,099**	**2,81**	
Polypropylene	0,099	2,81	
Cell Casing	**1,70**	**48,02**	
Stainless steel	1,70	48,02	
Total	**3,53**		

The parameters of the coin cell are given below in Table 2, including gravimetric energy density and cycle life.

Table 2 Parameters of the coin cell

Parameter	Quantity
Gravimetric energy density (kWh/kg)	1,05
Mass of coin cell (g)	3,53
Number of cycles achieved	40
Target number of cycles	100

In order to assess the full life cycle of the coin cell, it has been sized up to battery system that could be used in EVs: 22 kWh battery systems that would run 1000 cycles, allowing an EV to travel approximately 150.000 km over its lifetime. The battery system was chosen to be 22 kWh since it is a median power for modern EVs and is the power for the BMW i3 battery system (for reference, the Toyota Prius uses a 4,4 kWh battery pack, the Chevy Volt uses a 16 kWh battery pack, the Nissan Leaf uses a 30 kWh battery pack, and the Tesla Model S uses a 60 kWh battery pack) [14].

Coin cells are not used in EV applications since they are too small and a huge amount of them would be needed in the battery pack. Thus, an intermediate size up has been done to obtain cylindrical cells, keeping the proportion of the required active material. Therefore, the parts pertaining to the coin cell were removed (gasket, spacer, and spring) and were replaced with the electrode connects used in D-cell type (cylindrical cell) (Table 3).

Table 3 Casing for a D-cell (cylindrical cell)

Component	Weight (g)
Positive Electrode Connect	**2,40**
Aluminium foil	2,40
Negative Electrode Connect	**7,90**
Copper	7,90

Cell Casing	**26,00**
Aluminium foil	21,32
Polyethylene terephthalate	3,38
Polypropylene	1,30

To determine the number of cells needed for each battery system, the gravimetric energy density was used to find the energy density per cell and then the energy density per cell was used to find the number of cells required to have a 22 kWh battery system. Table 4 on the next page gives the parameters used in these calculations to show clearly how the number of cells was determined, along with the total mass of the cells in one battery.

Table 4 Parameters for a battery pack

Parameter	Quantity
Gravimetric energy densitiy (kWh/kg)	1,05
Mass of cell (kg)	0,287
Energy density per cell (kWh/cell)	0,301
Number of cells needed for a 22kWh system	73,1
Total mass of cells in one battery (kg)	20,95

Battery pack inventory was taken from literature since battery packs are not currently being manufactured by IREC or for the HELIS project [11]. Table 5 below shows the inventory for the battery pack with the respective weights for the HELIS battery and IREC battery. To find the total weight of the battery pack, the weight ratio of cells to total battery was taken from literature (specifically Deng, et. al. since they also performed a LCA on Li-S batteries so this seemed the most appropriate data to use) [7]. Then, the software BatPac was used to determine the weight ratios of the battery pack materials [11]

Table 5 Battery pack components weight

Material	Weight (kg)
Battery Pack	**10,82**
Stainless steel	6,91
Aluminium foil	2,26
Aluminium extrusión profile	0,97
Printed wiring board	0,66
Copper	0,012
Copper sheet	1,46E-04

A summation of the mass of the cells for each battery and the mass of the battery pack results in the total mass of the battery system which is given in Table 6 below. The table also summarises the characteristics of the battery systems. The energy density of the IREC cell, going from a coin cell to a cylindrical form, will most certainly decrease.

Table 6 Total weight of the battery pack

Parameter	Battery Pack
Mass of cells (kg)	20,95
Mass of the battery pack (kg)	10,82
Total mass of battery system (kg)	31,77
Gravimetric energy density (Wh/kg)	1050

3 Results and discussion

The LCA results for the cradle to gate analysis of the coin cell (solely cell production) are shown in Table 7 where they are categorised by cell part (cathode, anode, electrolyte,etc.).

Table 7: LCA results for cradle to gate analysis

Impact Category	GWP [kg CO2-eq.]	ADP [MJ]	AP [kg SO2-eq.]	EP [kg PO4-eq.]	ODP [kg CFC 11-eq.]	POCP [kg C2H4-eq.]	PED [MJ]
TOTAL	**4,89E-01**	**1,69E+00**	**7,25E-04**	**1,04E-04**	**1,03E+00**	**1,62E-02**	**7,69E+02**
Anode	3,29E-02	3,79E-01	8,81E-05	9,89E-06	1,80E-03	8,52E-05	3,02E+00
Cathode	9,16E-04	9,27E-03	5,32E-06	2,90E-06	5,85E-04	3,64E-04	1,30E+00
Electrolyte	1,73E-04	3,54E-03	8,77E-07	2,88E-07	7,19E-04	4,90E-05	4,01E-01
Separator	9,89E-06	2,54E-04	4,84E-08	3,71E-09	8,58E-08	3,14E-09	7,07E-04
Spacer	1,58E-01	5,07E-01	2,50E-04	3,33E-05	3,53E-01	5,28E-03	2,56E+02
Spring	1,37E-01	2,48E-01	1,18E-04	2,30E-05	3,17E-01	5,10E-03	2,51E+02
Gasket	8,59E-04	1,61E-02	2,32E-06	4,18E-07	1,99E-05	3,96E-06	2,11E-02
Casing+Current Collector	1,60E-01	5,28E-01	2,61E-04	3,42E-05	3,57E-01	5,31E-03	2,57E+02

From Table 7 above, the part of the cell production which contributes most to the impact categories can be seen. The anode (lithium metal) has the majority effect on all impact categories except for human toxicity where the cathode and electrolyte share the effects with the anode. In the rest of the impact categories though, the anode ranges from having 51% contribution to abiotic depletion and primary energy up to 92% contribution to ozone layer depletion potential. This is because lithium metal is a very highly intensive metal to extract and refine for use in products.

The LCA results for the cradle to grave analysis of the HELIS battery (from battery production through the use of the battery in an EV all the way to EOL) are shown in Table 8 where they are categorised by phase of life.

Table 8: LCA results for the cradle to gate analysis

Impact Category	Total	Battery Production	Use	End of Life
GWP [kg CO2-eq.]	1,46E+04	3,81E+03	1,08E+04	1,13E+01
ADP [MJ]	1,59E+05	4,41E+04	1,15E+05	5,53E+02
AP [kg SO2-eq.]	4,32E+01	1,23E+01	3,08E+01	1,87E-02
EP [kg PO4-eq.]	7,73E+01	4,54E+01	2,79E+00	4,02E-02
ODP [kg CFC 11-eq.]	5,09E-05	5,03E-06	4,79E-07	1,52E-11

POCP [kg C2H4-eq.]	2,81E+00	8,50E-01	1,97E+00	-1,63E-03
PED [MJ]	3,63E+05	1,09E+05	2,63E+06	6,55E+01

The use phase dominates the GWP, ADP, AP, POCP, and primary energy demand categories while the battery production dominates the EP and ODP categories. The material extraction for the battery production would have higher effects on the eutrophication potentials while electricity production would have a higher effect on carbon footprint due to the amount of electricity consumed over the lifetime of the EV and battery.

4 Conclusions

A LCA study has been successfully performed on the HELIS project Li-S coin cell and the sized up battery pack system. Various materials have been pinpointed in the battery cells that have higher impacts and which battery ultimately would be more sustainable in the application of electromobility.

Regarding the first analysis, a cradle to gate analysis of the cell production, it was seen that the materials with the highest environmental impacts were shown to be lithium, stainless steel, and aluminium. Regarding the second analysis, a cradle to grave analysis, it has been shown that for now, the battery pack materials were among the most environmentally intensive materials in the cradle to grave study.

Since these batteries are still very much in the research phase, a completely adequate LCA is impossible at this stage. However, this LCA study provides a good basis for when the batteries have matured.

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