Life Cycle Assessment of Lithium-Sulphur Batteries

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Abstract

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. However, Li-S batteries have yet to be commercialised, as achieving the theoretical capacity and energy density has proven quite difficult. This study performs life cycle assessment (LCA) analyses on two Li-S battery cells being researched for the final aim of being applied in electric vehicles (EVs). One of the Li-S battery cells comes from the investigation of the EU-funded HELIS project, a consortium of 14 partners across Europe and Israel, with the aim of bringing a competitive Li-S battery to market. The other Li-S battery cell comes from IRECs (Catalonia Institute for Energy Research) own research lab. The first objective of the study is to perform a cradle to gate LCA on just the cell production to evaluate which parts of the cells have the highest environmental impact. The second objective of the study is to perform a cradle to grave LCA on two battery systems for use in EVs where all phases from the extraction of raw materials to the end of life of the battery are considered. This required the scaling up of the cells to battery systems, where the functional unit was decided as a 22 kWh battery that would run 1000 cycles and allow the EV to go a distance of 150.000 km. The results showed that lithium, stainless steel, and aluminium were the highest impact materials in the cell production and that the battery pack materials are highly intensive as well. Thus, the BMS should be investigated to involve less-intensive materials. While the HELIS battery had a 12% lower carbon footprint than the IREC battery, the IREC battery had lower impacts in many categories such as human toxicity (66% lower), ecotoxicity (60-82% lower), and ozone depletion (64% lower). If the energy consumption to produce the cathode in the IREC battery were decreased to industrial levels, then the IREC battery would be the more sustainable battery to use in EVs. This study provided an additional LCA on Li-S batteries and a good basis for future LCA studies when these batteries have matured.

Keywords: lithium-sulphur battery, life cycle assessment, electric vehicles, HELIS project, sustainability

1. Introduction

This study was performed for the purposes of the HELIS project which receives funding from the European Union's Horizon 2020 research and innovation program under Grant Agreement No 666221. The HELIS project aims to develop three different series of Li-S cell prototypes to be tested for use in EVs [6]. By comparing the chemistry of the first Li-S cell prototype with Li-S cells already tested and proven in the IREC laboratories, the environmental impacts can be analysed.

LCA research on Li-S batteries is lacking since these batteries have yet to be commercialised. The first article published performing a LCA on these batteries was in March of 2017 so there is not enough research yet on the sustainability of these batteries [5]. By performing this study on two different types of Li-S battery cells currently being researched, the goal is that more awareness is brought to these types of batteries and that they are shown to be more sustainable than batteries used today.

While not much LCA research currently exists on Li-S batteries, the field of electromobility has received much attention and research globally to discover innovative ways of reducing the environmental impact of conventional vehicles. Along with EVs comes energy storage and the motivation to find clean and proper electricity storage systems. While EV sales increase every year, there still remain two key issues with the widespread use of EVs. The first issue is the limited range due to low energy density of the battery. The second issue is the high cost of batteries; the most expensive part of the EV is the battery, thus making the batteries cheaper is intrinsic to making the cost of the vehicle cheaper [1]. LCA and other life cycle tools such as life cycle costing (LCC) help improve upon these batteries by identifying which materials and processes have higher impacts environmentally and economically.

Much of literature in the electromobility field when it comes to energy storage is dedicated to the second life of these EV batteries. Once they have lost 20% of their capacity, EV batteries are no longer considered useful for traction purposes. But these batteries still have 80% of their capacity and thus can be used for other stationary purposes [2]. LCA can be a very useful tool for identifying these possible applications since it assesses the end of life (EOL) of the battery.

Various motivations lie behind this study on Li-S batteries and hopefully this research can shed more light on the situation and propel these types of batteries to the forefront of energy storage research as a viable option in the electromobility field and elsewhere.

2. Background

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 [17]. 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].

2.2. Li-S Batteries

In the world of energy storage, specifically battery technology, Li-S batteries have emerged as quite promising due to the replacement of sulphur for the metals in the cathode of typical Li-ion batteries. Sulphur is one of the most abundant elements on earth and due to it being an electrochemically active material that can accept up to two electrons per atom at 2,1 V versus Li/Li+, sulphur cathode materials have a very high theoretical capacity of 1672 mAh/g [11]. Consequently, Li-S batteries have a theoretical energy density of around 2600 Wh/kg, an entire magnitude of order higher than typical Li-ion batteries [13].

Li-S batteries actually came on to the scene in the late 1960s when the first configuration was presented. This configuration had the positive electrode comprised of elemental sulphur, electronic conductors (carbon or metal powder), and binders, the negative electrode comprised of metallic lithium, and an organic electrolyte separating the two electrodes. This set the base for which Li-S batteries are configured today, typically having a lithium metal anode, an organic liquid electrolyte, and a sulphur composite cathode. The overall redox couple is described by the reaction 1 below [11]:

$$\mathrm{S_8 + 16Li^+ + 16e^- \longleftrightarrow 8Li_2S} \tag{1}$$

In addition to the higher theoretical capacity and energy density, Li-S batteries are supposed to be more environmentally and economically sustainable than Li-ion batteries (given they have good performance). Sulphur replaces toxic transition metals found in the cathodes of Li-ion batteries such as cobalt and manganese, and sulphur is cheaper and more abundant than these heavy metals [13]. If Li-S batteries can eventually attain higher performance than Li-ion batteries, then this also translates to the batteries lasting longer and less material being wasted in the long run.

3. Implementation

This study has two main objectives. The first is to analyse the environmental impacts due to the production of the coin cells from IREC and the cells from the HELIS project. As a second objective, after an adequate scaling to make both devices equivalent, the cells themselves can be compared; the different ways of manufacturing Li-S battery cells are compared to find the optimal type, chemistry, and materials of the cells that maintain high performance and are as environmentally sustainable as possible. In order to withdraw more conclusions about each battery according to the mentioned purposes, several sensitivity analyses are performed.

In the first objective, the system only consists of the cell of the battery; this is what is manufactured currently and the impacts of the process to make just the cell are an important aspect of the study. A cradle to gate approach is taken here, meaning from the raw material extraction to the production of the battery cells to find the impacts of the individual cells. The functional unit used is one Li-S battery cell. Then for the second objective, the battery pack is included to be able to compare the two battery cells within the context of a larger application. The pack includes the circuit board (PCB) and battery casing but does not include the full battery management system (BMS) which includes the cooling technology needed. A cradle to grave approach is taken here, analysing the entire life cycle of the battery, from raw material extraction through production and use of the battery in an EV and finally EOL. 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 two battery systems were scaled to this metric, determining the number of cells and battery packs needed to fulfil the 1000 cycles. The inventory for the battery packs was taken from literature and ratios of the materials were determined based on the performance and parameters of the cells.

GaBi Professional software was used to perform the LCA of the Li-S batteries. The GaBi software is a LCA modelling software created by the German company thinkstep, originally PE International [18]. The CML 2001 method was used to evaluate the impact categories in the GaBi Professional software. This impact assessment method was developed by Leiden Universitys Institute of Environmental Sciences in Leiden, The Netherlands. CML 2001 limits uncertainties by restricting quantitative modelling to early stages in the cause-effect chain [12].

3.1. Limitations and Assumptions

Various limitations were present in this study, most of which were due to lack of sufficient data.

Data was provided for the HELIS project cells in the form of an Excel file listing all the various inputs for the GaBi software. Unfortunately, no processes were explained in detail and thus energy inputs were entered as they were given to us, rather than knowing exactly where these inputs came from. So while we were able to give an accurate estimation of the energy consumption in the production of the IREC cells since we had access to the machinery and all details of the processes used, this same detail in data was unavailable for the HELIS cells.

Since only the battery cells are being researched thus far, no data was provided on the battery pack for the overall system and likewise, no current methods of recycling or waste disposal exist for these types of batteries.

Finally, not all data was available for providers of the materials used in the batteries, especially for the HELIS batteries. To be able to include this transport data in the LCA, many assumptions were made.

For the energy consumption of the cell production, it was assumed that the values provided from the HELIS data were on an industrial scale since the values were quite low. Thus, the energy consumption calculated for the IREC coin cells is assumed for an industrialised process, thus producing material for many more cells than are currently produced. This gave energy inputs on a similar scale for both cells; otherwise the energy consumption of the IREC cells would produce results giving IREC cells a much larger environmental impact than the HELIS cells. However, for the IREC cylindrical cells used in the battery system, where the surface area of the electrodes is much greater than for the coin cells, the energy consumption calculated had to be assumed for only one cylindrical cell at a time. Since this is not optimal, a sensitivity analysis on this energy consumption was performed where the energy consumption was decreased to industrial levels.

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 accounted for as they are allocated in the life cycle of the future product that is produced from the recycled material. The analysis then reflects the benefit of using a material that can be and is recycled and no environmental burdens are allocated in that case [8]. 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 that transportation impact as appropriately as possible.

3.2. HELIS Battery Cell

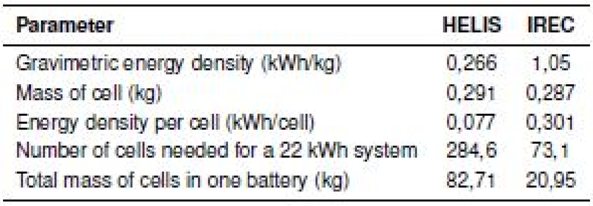
As can be seen it is a typical Li-S cylindrical cell with a sulphur-carbon composite cathode and lithium metal anode. It uses a cathode binder, two of which were tested here: the first one is styrene-butadiene-rubber (SBR) and carboxymethyl cellulose (CMC) in water and the second one is polyvinylidene fluoride (PVDF) in N-methyl-2-pyrrolidone (NMP). PVDF is not in the GaBi or Ecoinvent databases and thus polyvinyl fluoride (PVF) from the Ecoinvent database was used instead as this was the closest material to PVDF available in the databases accessible. A sensitivity analysis was performed on these two binders in Section to see which is more sustainable. 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 cell materials also include a polypropylene separator, a cathode connect and anode connect, and a Al-PET-PP composite cell casing [16].

3.3. IREC Battery Cell

In contrast to the HELIS battery cell which is cylindrical, the IREC 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 [3]. The electrolyte used is the same as in the HELIS cells and the separator is again a membrane made from PP. Apart 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 [7].

3.4. Parameters

The parameters of both cells are given below in Figure 1, including gravimetric energy density and cycle life. As can be seen, they are two very different cells made for different applications. One is a cylindrical cell made for mobile applications such as EVs while the other is a coin cell made for stationary applications. Thus, on this scale they are not comparable.



Parameter	HELIS	IREC
Gravimetric energy density (kWh/kg)	0,266	1,05
Mass of cell (kg)	0,291	0,287
Energy density per cell (kWh/cell)	0,077	0,301
Number of cells needed for a 22 kWh system	284,6	73,1
Total mass of cells in one battery (kg)	82,71	20,95

Figure 1: Parameters of the two battery cells [16][7].

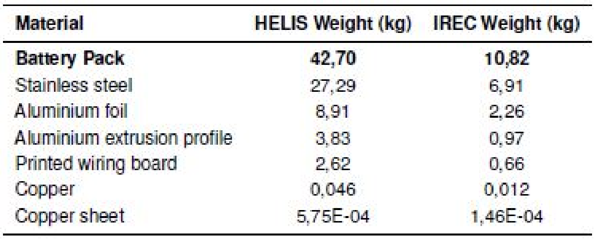
3.5. Equivalency for Comparison

To be able to compare the two battery cells, they were sized up to battery systems 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) [19].

To be able to compare the two cells for EV application, they had to both be in cylindrical form (or pouch form, but since the HELIS cell is already in cylindrical form, this makes the most sense). 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, the chemistry of the IREC cell was taken and used in a cylindrical cell. The electrodes, electrolyte, and membrane were scaled up to have the same weight as these same parts in the HELIS cylindrical cell but still having the same ratio of weight as in the IREC coin cell. The parts pertaining to the coin cell were removed (gasket, spacer, and spring) and were replaced with the electrode connects used in the HELIS cell. The cell casing from the HELIS cell was used for the IREC cylindrical cell since they will be the same form and weight (just differing chemistry).

3.6. Battery Pack

Battery pack inventory was taken from literature since battery packs are not currently being manufactured by IREC or for the HELIS project. Figure 2 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) [5]. Then, the software BatPac was used to determine the weight ratios of the battery pack materials [14].

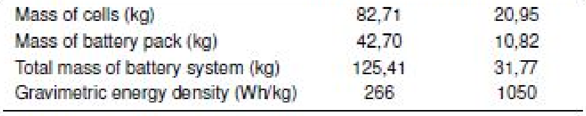


Material	HELIS Weight (kg)	IREC Weight (kg)
Battery Pack	**42,70**	**10,82**
Stainless steel	27,29	6,91
Aluminium foil	8,91	2,26
Aluminium extrusion profile	3,83	0,97
Printed wiring board	2,62	0,66
Copper	0,046	0,012
Copper sheet	5,75E-04	1,46E-04

Figure 2: Material inputs inventory for the battery pack for the two battery systems [14].

3.7. Equivalency Parameters

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 shown in Figure 3 below. A summary of the characteristics of the battery systems is also displayed.



Parameter	HELIS Battery	IREC Battery
Mass of cells (kg)	82,71	20,95
Mass of battery pack (kg)	42,70	10,82
Total mass of battery system (kg)	125,41	31,77
Gravimetric energy density (Wh/kg)	266	1050

Figure 3: Parameters of the equivalency of the two batteries.

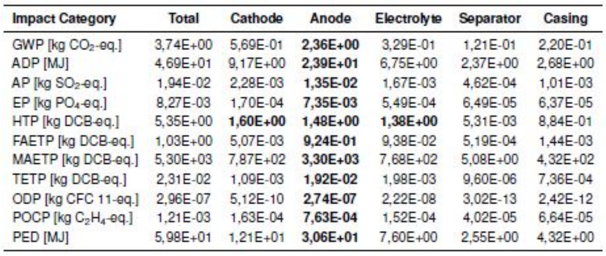
3.8. Use Phase

The process of calculating the electricity consumption for the use phase in the LCA had to be simplified due to the lack of data on the battery systems that were composed (battery efficiency as well as discharged energy are unknown). Thus, a fuel consumption rate was taken from literature. The value of 0,586 MJ/km was used since this was used in the LCA of Li-S batteries [4]. This seems an appropriate value to take since there is a range in literature from 0,48 MJ/km to 0,623 MJ/km [9]. In fact, the electricity consumption is most likely very conservative since the Li-S batteries studied in the LCA published had an energy of 61,3 kWh and in this study the batteries are set to 22 kWh [5]. The electricity mix used was the average European (EU-28) mix.

4. Results

4.1. HELIS Battery Cell

The LCIA results for the cradle to gate analysis of the HELIS battery cell (solely cell production) are shown in Figure 4 where they are categorised by cell part (cathode, anode, electrolyte, etc.) and the part of the cell production which contributes most to the impact categories can be seen (highlighted in bold). 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 due to the fact that lithium metal is a very highly intensive metal to extract and refine for use in products. While lithium is obviously a necessary material in the production of Li-S batteries, the amount of lithium these batteries contain can be decreased.



Impact Category	Total	Cathode	Anode	Electrolyte	Separator	Casing
GWP [kg CO_2-eq.]	3,74E+00	5,69E-01	**2,36E+00**	3,29E-01	1,21E-01	2,20E-01
ADP [MJ]	4,69E+01	9,17E+00	**2,39E+01**	6,75E+00	2,37E+00	2,68E+00
AP [kg SO_2-eq.]	1,94E-02	2,28E-03	**1,35E-02**	1,67E-03	4,62E-04	1,01E-03
EP [kg PO_4-eq.]	8,27E-03	1,70E-04	**7,35E-03**	5,49E-04	6,49E-05	6,37E-05
HTP [kg DCB-eq.]	5,35E+00	**1,60E+00**	**1,48E+00**	**1,38E+00**	5,31E-03	8,84E-01
FAETP [kg DCB-eq.]	1,03E+00	5,07E-03	**9,24E-01**	9,38E-02	5,19E-04	1,44E-03
MAETP [kg DCB-eq.]	5,30E+03	7,87E+02	**3,30E+03**	7,68E+02	5,08E+00	4,32E+02
TETP [kg DCB-eq.]	2,31E-02	1,09E-03	**1,92E-02**	1,98E-03	9,60E-06	7,36E-04
ODP [kg CFC 11-eq.]	2,96E-07	5,12E-10	**2,74E-07**	2,22E-08	3,02E-13	2,42E-12
POCP [kg C_2H_4-eq.]	1,21E-03	1,63E-04	**7,63E-04**	1,52E-04	4,02E-05	6,64E-05
PED [MJ]	5,98E+01	1,21E+01	**3,06E+01**	7,60E+00	2,55E+00	4,32E+00

Figure 4: LCIA results for the HELIS battery cell (cradle to gate analysis) categorised by cell part.

The pie chart given in Figure 5 below shows the effects of the cell parts on the global warming potential in a more visual and clear way.

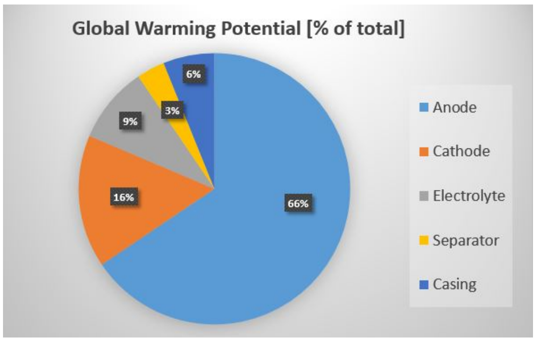
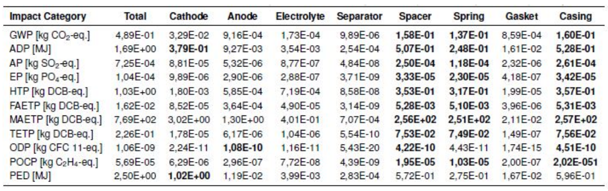


Figure 5: Pie chart displaying the contributions of each part of the HELIS cell production to global warming potential in percentages.

The anode dominates with a 66% contribution, with the cathode next, contributing 16%, and the electrolyte contributing 9%. The casing and separator have the lowest contributions to the GWP. Lithium metal has a value of 59,4 kg CO_2-eq. per kg of material (the majority of which comes from the emission of 53,8 kg CO_2) whereas sulphur has a value of 0,655 kg CO_2-eq. per kg of material (again the majority of which comes from the emission of 0,563 kg CO_2). It can be seen from this almost 100X difference why the anode has such high effects in this impact category.

4.2. IREC Battery Cell

The LCIA results for the cradle to gate analysis of the IREC battery cell (solely cell production) are shown in Figure 6 where they are categorised by cell part (cathode, anode, electrolyte, etc.) and the parts of the cell production which contribute most to the impact categories can be seen (highlighted in bold). Mostly the stainless steel parts - spacer, spring, and casing - have the highest effects on all impact categories except for ODP where the anode has a high impact and primary energy where the cathode has a high impact as well. Steel is a highly intensive metal to extract and refine for use in products, like lithium. In a coin cell, the use of steel is unavoidable and since it is easily recyclable it is a desirable product to use, but in batteries for use in EVs, the use of steel can be minimised as much as possible.



Impact Category	Total	Cathode	Anode	Electrolyte	Separator	Spacer	Spring	Gasket	Casing
GWP [kg CO_2-eq.]	4,89E-01	3,29E-02	9,16E-04	1,73E-04	9,89E-06	**1,58E-01**	**1,37E-01**	8,59E-04	**1,60E-01**
ADP [MJ]	1,69E+00	**3,79E-01**	9,27E-03	3,54E-03	2,54E-04	**5,07E-01**	**2,48E-01**	1,61E-02	**5,28E-01**
AP [kg SO_2-eq.]	7,25E-04	8,81E-05	5,32E-06	8,77E-07	4,84E-08	**2,50E-04**	**1,18E-04**	2,32E-06	**2,61E-04**
EP [kg PO_4-eq.]	1,04E-04	9,89E-06	2,90E-06	2,88E-07	3,71E-09	**3,33E-05**	**2,30E-05**	4,18E-07	**3,42E-05**
HTP [kg DCB-eq.]	1,03E+00	1,80E-03	5,85E-04	7,19E-04	8,58E-08	**3,53E-01**	**3,17E-01**	1,99E-05	**3,57E-01**
FAETP [kg DCB-eq.]	1,62E-02	8,52E-05	3,64E-04	4,90E-05	3,14E-09	**5,28E-03**	**5,10E-03**	3,96E-06	**5,31E-03**
MAETP [kg DCB-eq.]	7,69E+02	3,02E+00	1,30E+00	4,01E-01	7,07E-04	**2,56E+02**	**2,51E+02**	2,11E-02	**2,57E+02**
TETP [kg DCB-eq.]	2,26E-01	1,78E-05	6,17E-06	1,04E-06	5,54E-10	**7,53E-02**	**7,49E-02**	1,49E-07	**7,56E-02**
ODP [kg CFC 11-eq.]	1,06E-09	2,24E-11	**1,08E-10**	1,16E-11	5,43E-20	**4,22E-10**	4,43E-11	1,74E-15	**4,51E-10**
POCP [kg C_2H_4-eq.]	5,69E-05	6,29E-06	2,96E-07	7,72E-08	4,39E-09	**1,95E-05**	**1,03E-05**	2,00E-07	**2,02E-051**
PED [MJ]	2,50E+00	**1,02E+00**	1,19E-02	3,99E-03	2,83E-04	5,72E-01	2,75E-01	1,67E-02	5,96E-01

Figure 6: LCIA results for the IREC battery cell (cradle to gate analysis) categorised by cell part.

The pie chart given in Figure 7 below shows the effects of the cell parts on the global warming potential in a more visual and clear way. In contrast to the HELIS cell, the IREC cell has more of a division of the effects among the different parts. The three parts made of stainless steel - spring, spacer, and casing - dominate with 28%, 32,2%, and 32,7% contributions. The cathode is next with a 6,7% contribution. The anode, electrolyte, and separator have the smallest effects. Whereas the anode has an almost 15% weight ratio in the HELIS cell, the anode has a much smaller weight ratio in the IREC cell, due to the domination of the weight coming from the steel parts, and this is why the anode has such a small effect on the impact categories for the IREC cell. Stainless steel has a value of 3,16E+03 kg CO_2-eq. per kg of material (the majority of which comes from the emission of 2,95E+03 kg CO_2). This is over 50X that of lithium and almost 5000X that of sulphur - so it is quite obvious why the steel parts would have the highest carbon footprint impacts.

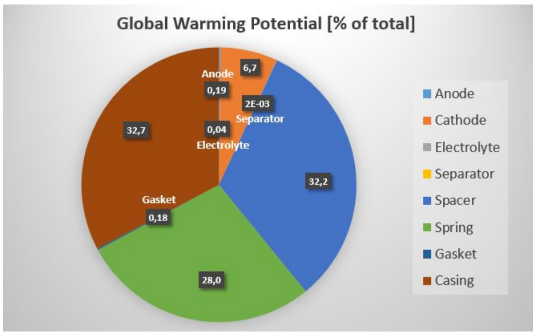
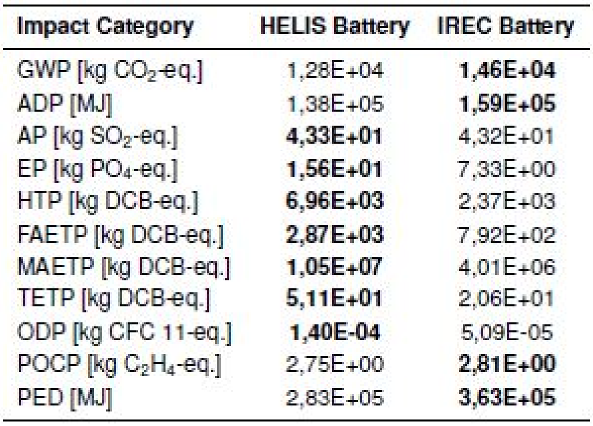


Figure 7: Pie chart displaying the contributions of each part of the IREC cell production to global warming potential in percentages.

4.3. HELIS and IREC Battery Systems

Figure 8 below displays the total impacts for the two batteries to show the differences between them. The higher impacts are put in bold to clearly show in which categories which battery has more of an effect. As can be seen, the IREC battery has higher impacts in GWP, ADP, POCP, and primary energy. The HELIS battery has higher impacts in AP (although it's almost the same between the batteries), EP, HTP, FAETP, MAETP, TETP, and ODP. The differences between the batteries in the categories where the IREC battery has a higher impact are much smaller than the differences between the batteries in the categories where the HELIS battery has a higher impact. Thus, when the HELIS battery has a higher impact, it is a more significant difference. Since many of the parts are the same (anode, electrolyte, casing), these differences arise from the difference in cathodes and from different weights of the materials they do have in common.



Impact Category	HELIS Battery	IREC Battery
GWP [kg CO_2-eq.]	1,28E+04	**1,46E+04**
ADP [MJ]	1,38E+05	**1,59E+05**
AP [kg SO_2-eq.]	**4,33E+01**	4,32E+01
EP [kg PO_4-eq.]	**1,56E+01**	7,33E+00
HTP [kg DCB-eq.]	**6,96E+03**	2,37E+03
FAETP [kg DCB-eq.]	**2,87E+03**	7,92E+02
MAETP [kg DCB-eq.]	**1,05E+07**	4,01E+06
TETP [kg DCB-eq.]	**5,11E+01**	2,06E+01
ODP [kg CFC 11-eq.]	**1,40E-04**	5,09E-05
POCP [kg C_2H_4-eq.]	2,75E+00	**2,81E+00**
PED [MJ]	2,83E+05	**3,63E+05**

Figure 8: LCIA results for the HELIS and IREC battery systems (cradle to grave analysis).

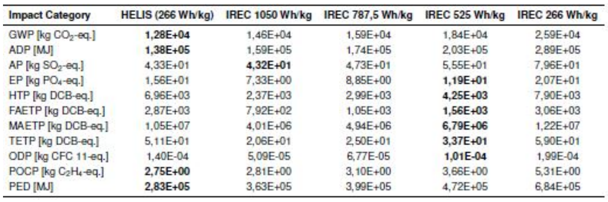
The differences in GWP, ADP, POCP, and primary energy are caused by the higher energy consumption the cathode production uses in the IREC battery. For example, in GWP, the IREC cathode contributes 22% to the overall impact whereas in the HELIS battery, the cathode only contributes 1%. Since the impacts of the individual materials in the cathodes are mostly equivalent (although the polyacrylonitrile and N,N-dimethylformamide in the IREC cathode have a bit higher impacts than the SBR and CMC in the HELIS cathode), these large differences are due to the vast difference in energy consumption of the cathodes.

The differences in AP, EP, HTP, FAETP, MAETP, TETP, and ODP are caused by the difference in battery pack material weights. In all of these impact categories, the battery pack was one of the major contributors, along with the electricity consumption during the use phase (which is the same between the two batteries because they are both 22 kWh batteries). Within the battery pack, the PCB has the highest effects, with steel and then aluminium coming afterward. Since the battery pack of the HELIS battery is four times greater than the mass of the IREC battery, these categories have higher impacts from the HELIS battery. These are all due in the end to the lower energy density the HELIS cells perform at in comparison to the IREC cells.

As can be seen in Figure ??, MAETP has the highest impact out of any of the categories. This is mainly due to the battery pack materials which have high effects on marine ecotoxicity. Just the PCB has a value of 2,83E+06 kg DCB-eq. per kg material (for comparison it has a value of 972 kg DCB-eq. per kg material for FAETP). The majority of this effect on MAETP comes from the emission of beryllium (1,86E+06 kg DCB-eq.) in addition to selenium (3,12E+05 kg DCB-eq.). Stainless steel, which has been shown already to be a high-impact metal to extract and refine for use in products, also has an exceptionally high value of 3,71E+06 kg DCB-eq. per kg steel, mostly coming from the emission of hydrogen sulfide (2,78E+06) and also coming from the emission of molybdenum (6,42E+05). Again, in comparison stainless steel has a value of 250 kg DCB-eq. per kg material for FAETP. To decrease the MAETP impact, the battery pack could be reconfigured with more environmental metals, although nothing can be done about the PCB as it is an integral part of the battery system.

4.4. Sensitivity Analysis: Energy Density

A sensitivity analysis was performed on the energy density of the IREC cylindrical battery since this energy density was not known and was subject to many assumptions and uncertainties. Thus, here the results are displayed for three energy densities tested: 787,5 Wh/kg (a 25% decrease in energy density), 525 Wh/kg (a 50% decrease from original), and 266 Wh/kg (the energy density of the HELIS cells and consequently almost exactly a 75% decrease in energy density from the original density). The results of these three new tests are displayed with the results of the original energy density tested (1050 Wh/kg) and with the HELIS battery results in Figure 9 below and graphically in Figure ??. The impacts which remain lower than the HELIS battery impacts are bolded to highlight how low the energy density can go without having higher impacts than the HELIS battery.



Impact Category	HELIS (266 Wh/kg)	IREC 1050 Wh/kg	IREC 787,5 Wh/kg	IREC 525 Wh/kg	IREC 266 Wh/kg
GWP [kg CO_2-eq.]	**1,28E+04**	1,46E+04	1,59E+04	1,84E+04	2,59E+04
ADP [MJ]	**1,38E+05**	1,59E+05	1,74E+05	2,03E+05	2,89E+05
AP [kg SO_2-eq.]	4,33E+01	**4,32E+01**	4,73E+01	5,55E+01	7,96E+01
EP [kg PO_4-eq.]	1,56E+01	7,33E+00	8,85E+00	**1,19E+01**	2,07E+01
HTP [kg DCB-eq.]	6,96E+03	2,37E+03	2,99E+03	**4,25E+03**	7,90E+03
FAETP [kg DCB-eq.]	2,87E+03	7,92E+02	1,05E+03	**1,56E+03**	3,06E+03
MAETP [kg DCB-eq.]	1,05E+07	4,01E+06	4,94E+06	**6,79E+06**	1,22E+07
TETP [kg DCB-eq.]	5,11E+01	2,06E+01	2,50E+01	**3,37E+01**	5,90E+01
ODP [kg CFC 11-eq.]	1,40E-04	5,09E-05	6,77E-05	**1,01E-04**	1,99E-04
POCP [kg C_2H_4-eq.]	**2,75E+00**	2,81E+00	3,10E+00	3,66E+00	5,31E+00
PED [MJ]	**2,83E+05**	3,63E+05	3,99E+05	4,72E+05	6,84E+05

Figure 9: Results for the sensitivity analysis on energy density of the IREC cylindrical battery.

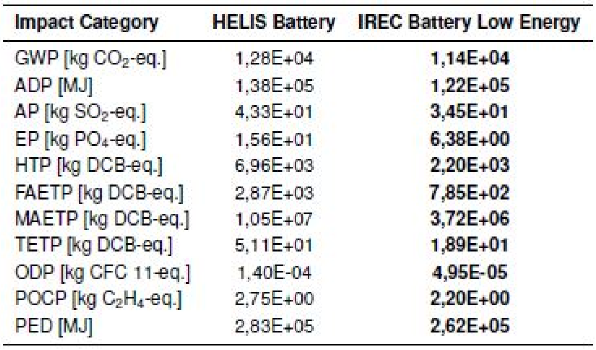
As can be seen, there is a more or less proportionate increase in the impacts as the energy density decreases (due to the increase in material needed for the battery pack to reach 22 kWh). Some of the impact categories stay lower for the IREC battery as long as the energy density does not go down to 266 Wh/kg. EP, HTP, FAETP, MAETP, TETP, and ODP all are lower for the IREC battery at 525 Wh/kg than for the HELIS battery. From extrapolation, it was found that the energy density could decrease to 416 Wh/kg for the IREC battery to continue having a lower effect on EP than the HELIS battery and to 333 Wh/kg for the IREC battery to continue having a lower effect on HTP than the HELIS battery. But if the energy density of the IREC battery decreases until 266 Wh/kg (the same as the HELIS battery), all impacts are higher and there is no incentive to use this battery instead (due to the energy consumption in the cathode production).

4.5. Sensitivity Analysis: Cathode Production Energy Consumption

Since the energy consumption in the production of the cathode of the IREC battery cells is the main factor causing such a large difference between the HELIS and IREC battery impacts, a sensitivity analysis was performed, decreasing the energy consumption of the IREC cathode to be equivalent to the energy consumption of the HELIS cathode (7,01E-02 MJ). Currently, the IREC cathodes made in-house from scratch are produced one at a time, causing the energy consumption per battery cell to be incredibly high. This sensitivity analysis proposes an industrial-scale production process so that many more cathodes can be produced at once and thus the energy consumption per cell decreases drastically. The results, given in the total battery LCA (cradle to grave) are represented below in Figure 10and are also shown graphically in Figure ??.

As can be seen, once the energy consumption is equated for the two batteries, the IREC battery then has lower impacts in all categories, due to the fact that the energy density is higher and thus less material is needed. It is yet to be seen if the energy consumption for the cathode production of the IREC cells could actually be reduced enough to see these kinds of results but if it is possible and the energy density remains higher than the HELIS cells, it makes sense to use the IREC cell chemistry.

Additionally, the HELIS battery uses much more aluminium in its cathode and since aluminium is a very high-impact metal, this contributes to the difference in the two batteries concerning the cathode once the energy consumption is equated. The HELIS battery cell has 36 g of aluminium while the IREC battery cell has less than 8 g of aluminium - this difference of over 4X contributes to a significant difference in cell production impacts.



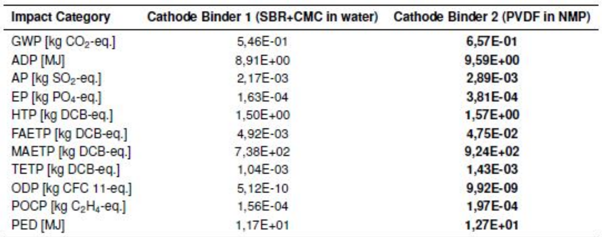
Impact Category	HELIS Battery	IREC Battery Low Energy
GWP [kg CO_2-eq.]	1,28E+04	**1,14E+04**
ADP [MJ]	1,38E+05	**1,22E+05**
AP [kg SO_2-eq.]	4,33E+01	**3,45E+01**
EP [kg PO_4-eq.]	1,56E+01	**6,38E+00**
HTP [kg DCB-eq.]	6,96E+03	**2,20E+03**
FAETP [kg DCB-eq.]	2,87E+03	**7,85E+02**
MAETP [kg DCB-eq.]	1,05E+07	**3,72E+06**
TETP [kg DCB-eq.]	5,11E+01	**1,89E+01**
ODP [kg CFC 11-eq.]	1,40E-04	**4,95E-05**
POCP [kg C_2H_4-eq.]	2,75E+00	**2,20E+00**
PED [MJ]	2,83E+05	**2,62E+05**

Figure 10: Results for the sensitivity analysis on cathode production energy consumption.

4.6. Sensitivity Analysis: Cathode Binders

Although cathode binders are not used in the IREC battery cells, the HELIS cells do use them and they are a point of investigation in the project. Thus, a sensitivity analysis was performed on two cathode binders that have been used in the cell prototypes: SBR and CMC in water and PVDF in NMP. The comparison of these two binders has been performed in other studies as well and the results here were compared with those in literature - in this way, it also assured that the results coming from GaBi Professional are in line with results found in other studies. The results are shown below in Figure 11 and graphically in Figure **??**.

As can be seen, cathode binder 2 of PVDF in NMP has higher impacts in all categories. The all-water-based binder provides a 17% reduction in GWP and a 95% reduction in ODP from the organic binder - Peters, et. al. got similar results of a 8.6% reduction in GWP and almost one order of magnitude change in ODP [15]. However, while Peters, et. al. saw relatively little changes in the other impact categories, here there is a 57% decrease in EP as well as 89% in FAETP [15]. Thus it is proven that SBR and CMC in water is a more environmental choice of cathode binder.



Impact Category	Cathode Binder 1 (SBR+CMC in water)	Cathode Binder 2 (PVDF in NMP)
GWP [kg CO_2-eq.]	5,46E-01	**6,57E-01**
ADP [MJ]	8,91E+00	**9,59E+00**
AP [kg SO_2-eq.]	2,17E-03	**2,89E-03**
EP [kg PO_4-eq.]	1,63E-04	**3,81E-04**
HTP [kg DCB-eq.]	1,50E+00	**1,57E+00**
FAETP [kg DCB-eq.]	4,92E-03	**4,75E-02**
MAETP [kg DCB-eq.]	7,38E+02	**9,24E+02**
TETP [kg DCB-eq.]	1,04E-03	**1,43E-03**
ODP [kg CFC 11-eq.]	5,12E-10	**9,92E-09**
POCP [kg C_2H_4-eq.]	1,56E-04	**1,97E-04**
PED [MJ]	1,17E+01	**1,27E+01**

Figure 11: Results for the sensitivity analysis on cathode production energy consumption.

5. Conclusions

A LCA study has been successfully performed on two different Li-S cells and battery systems. 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 objective, 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. If these materials can be decreased in mass or even replaced with more environmental materials, the batteries would have fewer impacts.

Regarding the second objective, a cradle to grave analysis to compare the two battery systems through their production, use in an EV, and EOL, it has been shown that for now, the HELIS battery has a lower carbon footprint although the IREC battery is more sustainable regarding other impact categories such as human toxicity, ecotoxicity, and ozone depletion. However, if the IREC battery can achieve lower energy consumption for the production of the cathode, it would become the superior battery chemistry for all impact categories as long as the energy density stays higher than the HELIS battery energy density.

When the two batteries were compared, the HELIS battery had a lower GWP as well as lower ADP, POCP, and PED (due to the higher enery consumption in the cathode production process for the IREC battery), but the IREC battery had lower effects on AP, EP, HTP, FAETP, MAETP, TETP, and ODP (due to the difference in battery pack material weights). Since the differences in GWP, ADP, POCP, and PED are caused by the higher energy consumption in the cathode production process for the IREC battery, a sensitivity analysis was performed on decreasing this energy consumption.

The category with the highest impacts was found to be MAETP due to the battery pack materials, like PCB and stainless steel which have much higher effects on marine ecotoxicity than on freshwater ecotoxicity or any other impact category.

From the sensitivity analyses performed, it was found that the energy density of the IREC battery could decrease to 525 Wh/kg or even a bit lower and still maintain lower impacts in many categories such as EP, HTP, and ODP than the HELIS battery but that if the IREC battery's energy density decreased to 266 Wh/kg (that of the HELIS battery), its impacts would be higher in every category (due to the energy consumption in the cathode). Additionally, if the energy consumption of the cathode production process for the IREC battery were decreased to be equivalent to that of the HELIS battery, then the IREC battery would have lower impacts in all categories, from a mere 7% decrease in primary energy up to a 73% decrease in FAETP. Finally, it was proven that SBR and CMC in water is a more sustainable binder to use than PVDF in NMP, providing reductions of up to 95% in ODP.

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 and performance is proven.

5.1. Future Work

There is much future work that can be done here. For one, more sensitivity analyses could be performed, some of which could include varying the battery power capacity (22 kWh, 50 kWh, 60 kWh, etc.), varying the country of production and use (China and Sweden for example, in addition to the European average), and changing battery pack materials. Also, the sensitivity analyses performed on the IREC batteries here (energy density and cathode production energy consumption) could be combined to see the results when the energy consumption is optimised but the energy density decreases.

Additionally, a LCC analysis could be performed to see which battery is more economically sustainable. While there was not adequate financial data to perform it here, it would be an interesting study to pair with the LCA to see if the battery that is environmentally superior is also financially superior.

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