LIFE CYCLE ASSESSMENT OF SILICON ALLOY-BASED LITHIUM-ION BATTERY FOR ELECTRIC VEHICLES

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ABSTRACT

Battery Electric Vehicles (BEV) are seen as a solution for cleaner mobility, due to their ability to reduce air emissions in cities. Batteries are key components that have a large influence on performances of EVs. Energy density is an important requirement from automotive industry, therefore the goal of this study is to assess the impact of a traction battery with new cells containing a high voltage NMC cathode and silicon alloy based anode on climate change. Silicon is a promising material for traction batteries, considering its high energy density. The scope of the paper is the manufacturing. This study uses the life cycle assessment method. Setting coherent system boundaries and functional units is essential and literature regarding these choices is reviewed. Site-specific data from industrial partners is collected as much as possible. The uncertainty of the results is then assessed thanks to a Monte Carlo simulation. The main contributor to climate change is cell manufacturing due to the use of fossil resources for electricity generation. The next big contributor is the cathode paste, half of the cathode paste emissions occurring in the nickel sulphate manufacturing. Note that nickel sulphate is the main precursor in the cathode. Substrates, electrolytes and separators do not represent high shares of emissions, even though they represent almost 40% of the cell mass. To evaluate the robustness of the conclusions, a sensitivity analysis is performed. Today, most of batteries are manufactured in China and the European Commission is pushing toward a more local production. The sensitivity of the results is tested by replacing the original mix by the Chinese average mix and by renewable energy sources. In conclusion, manufacturing in Europe can reduce the impact on climate change and using hydropower and/or photovoltaic panels can even improve the environmental performances of manufacturing of this battery. Keywords: battery manufacturing, electric vehicle, life cycle assessment, GHG emissions, silicon lithium ion battery, NMC battery, silicon anode, Cradle to Gate.

1 INTRODUCTION

There is a growing concern about climate change and transport sector. It seems that low carbon mobility can be reached with electric and hybrid vehicles charged with electricity with low GHG (Greenhouse Gas) emissions [1]. Electric powertrains are efficient during use stage but manufacturing of batteries can be energy intensive. It is therefore interesting to focus on GHG emissions of battery manufacturing. This can be performed through a Life Cycle Assessment (LCA), which is a recognized and standardized method to assess environmental impacts of products or services [2].

Several chemistries for batteries are commercially available today and others are still in development [3]. Increasing the energy density of traction batteries is possible using new materials such as silicon for anode active material [4]. Li et al. [5] studied the LCA of a lithium ion battery with a silicon nanowires anode and NMC 111 cathode (lithium Nickel Manganese Cobalt oxide cathode that contains ca. the same amount of nickel, manganese and cobalt). These authors reported that this new anode generated most of the GHG emissions of the battery manufacturing. In our study, nevertheless, the anode is composed of silicon-based alloy, not on nanowires. We focus expressly on manufacturing stage instead of considering also the use stage which might be more difficult to evaluate with new battery technologies that have not yet reached maturity.



WIT Transactions on The Built Environment, Vol 182, © 2019 WIT Press www.witpress.com, ISSN 1743-3509 (on-line) doi:10.2495/UT180131 Environmental performances of LIBs (Lithium Ion Battery) have been the subject of research for several years. Peters et al. [6] found 79 studies on lithium ion batteries and 34 on traction batteries between 2010 and 2016. Among all these publications, the differences in goal and scope bring different boundaries, FUs (Functional Unit) and modelling approaches. There are mainly 4 types of FUs used in literature: measured in battery weight, in energy content, in delivered energy, and in distance. It should be noted, though, that FUs of the same type are not necessarily equivalent and that comparing LCAs that have apparently the same FU is not straight forward. For instance, if the FU is measured in distance, the parameters of the car such as power electronics efficiency and the drivetrain must be the same for the results to be comparable. When focusing on manufacturing, it is more suitable to use a FU based on characteristics of the battery that are not dependent of the use stage.

Fossil fuels generate most of the impact on climate change whether they are used to generate electricity for use stage or for manufacturing [6]. To have robust results, sensitivity should be addressed [2] in order to understand the relative importance of parameters. Electricity mix is often a relevant parameter assessed during sensitivity analysis [7]–[9]. Reliability can also be attained thanks to a range-based analysis [10] or uncertainty quantification [7], [11].

This manuscript begins with the methodology in Section 2, where the first step of the ISO standard, goal and scope definition, is addressed. In Section 3, the inventory is detailed. Section 4 includes the results of the impact assessment, interpretation, sensitivity and uncertainty analysis. Finally, Section 5 describes the conclusions of this research.

2 METHODOLOGY

Life Cycle Assessment (LCA) is a tool that assesses environmental performance all along the life cycle of a product: from raw material extraction to recycling and final disposal. LCA has been standardized [2] and the procedure is divided into 4 steps: goal and scope definition, inventory analysis, impact assessment and interpretation. Definition of the goal and scope should address the context, the intended audience, the objectives, the system boundaries, the functional unit and the modelling choices. Afterwards all relevant material and energy flows are inventoried. To establish a good inventory, the quality of the data is essential. The next step is translating inputs and outputs of elementary flows into impact indicators and interpret the results.

2.1 Goal and scope definition

We developed a new cell technology for NMC traction batteries with high capacity anode, high voltage cathode and new electrolytes. This study will then focus on the manufacturing of the developed technology in Europe. The objective of this study is to answer four questions: 1) What is the influence of nickel content on GHG (Greenhouse Gas) emissions of manufacturing this cell and a pack containing these cells? 2) What is the influence of silicon based anode on GHG emissions of manufacturing this cell and a pack containing these cells? 3) Is the manufacturing of this new battery a good alternative to current batteries in terms of GHG emissions? and 4) How can the manufacturing of this new technology achieve lower GHG emissions?

To answer these questions, the manuscript considers raw materials production, transport and manufacturing of the cells and battery pack. It is a Cradle to Gate (CtG) analysis. First, we focus on the cell manufacturing (CtG Cell in Fig. 1) and in a second time, on the whole battery pack manufacturing (CtG Battery in Fig. 1), including battery housing, cooling system, Battery Management System (BMS) and module packaging. The battery has been





Figure 1: System boundaries of battery LCA.

assessed using attributional process based LCA. The Functional Unit (FU) is the quantified performance of the studied system that serves as the reference unit to which all the inventory and impact assessment are reported. The FU is 1 kWh energy content of a cell or of a 30-kWh battery pack.

2.2 Inventory and data quality

The important processes in battery manufacturing LCA are: production of the electrodes, of the electrolyte, of the separator, of the case, of the BMS and assembly. The best data quality is obtained using site-specific manufacturing data. This kind of information has therefore been gathered as much as possible from project partners for foreground processes. For background processes, such as raw material extractions and electricity generation, the database Ecoinvent 3.3 is used. The modelling is carried out with the LCA software Simapro 8.4. The data quality of the project will be assessed using a Pedigree matrix [12].

2.3 Impact assessment and interpretation

GHG emissions lead to climate change that may have a broad range of impacts on ecosystems. GHG exhibit different behavior over time, the characterization factors depend on the chosen time-horizon. The time horizon for this study is 100 years and the characterization factors are those of the IPCC 2013 method V1.03.



2.4 Sensitivity and uncertainty analysis

Sensitivity of the results to key parameters and uncertainty need to be assessed to better understand the reliability of the results. In this study, sensitivity analysis is performed by assessing the influence of silicon manufacturing and energy source for manufacturing on the results. This analysis helps in evaluating the robustness of the conclusions. After assessing the data quality, the uncertainty is quantified through a Monte Carlo simulation, assuming a lognormal distribution for all gathered data. 1000 runs will be performed. This uncertainty quantification focuses on parameter uncertainty.

3 LIFE CYCLE INVENTORY

3.1 Battery characteristics

The new cells developed are prismatic cells composed of NMC 622 cathode and silicon alloy based anode, in an aluminum hard case. Table 1 shows the inventory of the cells. The higher energy density of silicon compared to graphite, usually used in battery anodes, allows to decrease the quantity of anode paste [4]. The cycle life expectation for such a chemistry is 1000 cycles (100% DoD, C/3).

A module is composed of 12 cells and a pack is composed of 24 modules which leads to a 30-kWh pack (Table 2). The energy density is increased by 15% compared to the same battery with graphite anode. This new technology in a pouch cell would have an energy density of almost 240 Wh/kg which is at the upper limit of today's LIBs [13].

The module pack has been designed and the total mass of the battery is calculated assuming that the cells represent 70% of the total mass (Table 3).

Component	%w
Positive electrode paste	28%
Negative electrode paste	12%
Separator	5%
Substrate, positive electrode	5%
Substrate, negative electrode	9%
Electrolyte	20%
Cell container	21%

Table 1: Life cycle inventory of the silicon based cell.

Table 2: Battery characteristics.

Cell weight [kg]	0.55
Module Energy [kWh]	1.24
Module Weight [kg]	8.22
Pack Weight [kg]	226.3
Pack Energy [kWh]	30
Energy density [Wh/kg]	131
Cell voltage [V]	3.6



Component	%w
Cells	70%
Module packaging	17%
Battery tray and battery retention	6%
BMS	5%
Cooling system	2%

Table 3: Mass repartition of the battery pack.

3.2 Manufacturing

3.2.1 Cell and pack manufacturing process

The facility for cell and battery manufacturing is located in Germany. The manufacturing process is similar for different lithium ion battery chemistries: mixing electrode pastes, coating on current collectors, drying, stacking, filling of electrolyte, sealing and testing. Several steps of this process happen in dry rooms that are known to be energy intensive. The cells are manufactured in a pilot scale facility but no data was available on energy consumption. Sanfélix [14] gathered data from a cell manufacturer and found that cell assembly requires an average of 18 kWh/kg of cell (assuming that all heating and cooling is produced by electricity, assumption made by the manufacturer). The module and battery pack manufacturing consists of assembly and welding, and also testing of the packs. The energy required for assembly is evaluated to 4E-4 kWh/kg [8]. This energy is low, compared to the manufacturing energy of the cells, as the battery assembly is mainly performed manually. The battery pack quality testing and validation consumes 6.4E-3 kWh/kg [5].

3.2.2 Cathode

In the NMC family, the proportion of nickel, manganese and cobalt have an impact on battery properties: more nickel results in a higher capacity, while higher manganese content results in a higher safety and higher cobalt results in a better reversibility. The cathode active material is NMC622 containing ca. 60% nickel, ca. 20% manganese and ca. 20% cobalt. Considering the costs, an NMC 622 battery with silicon alloy-based anode could cost 30% less than an NMC 622 battery with graphite anode [3]. As cobalt is considered a critical raw material for Europe [15], decreasing its use in batteries is interesting to decrease dependence on foreign suppliers. The oxide is manufactured in China and in Korea. Data for the active material is gathered directly from the manufacturer. During the mixing, N-methyl-2-pyrrolidone (NMP) is added as a solvent and we assume that all this solvent evaporates during drying. The cathode paste is coated on a 20 µm thick aluminum foil.

3.2.3 Anode

Silicon has a higher energy density than graphite generally used in LIB anodes (3579 mAh/g for silicon and 372 mAh/g for graphite [4]). The energy density increases with increasing silicon alloy content, but cycling stability is challenged due to side reactions and volume changes. Natural graphite is considered as a critical raw material for Europe [15] and it cannot be recovered through battery recycling. Reducing the quantity of natural graphite in batteries is therefore interesting from the point of view of supply risk. The silicon alloy content in the anode paste is 27% and graphite only 16%, much lower than other NMC batteries [8], [16].

The silicon alloy contains silicon, iron and carbon according to [17]. The silicon powder used in the alloy manufacturing is pure at 99.9%. In the Ecoinvent database, the purity of the



metallurgical grade silicon lies between 98.5% and 99.5% [18]. Using metallurgical grade might underestimate environmental impacts of the material. Nevertheless, the solar grade impurity tolerances are not greater than 0.01 ppmw (parts per million weight), choosing this dataset should increase environmental impacts of the silicon alloy; this choice will be tested during sensitivity analysis.

The anode slurry is aqueous, no NMP is used. Zackrisson et al. [19] showed that waterbased slurries for cathode and anode have lower GHG emissions than NMP containing slurries. This slurry is coated on a 10 μ m thick copper foil.

3.2.4 Electrolyte

The electrolyte is a mixture of LiPF₆ and lithium 4,5-dicyano-2-(trifluoromethyl) imidazolide (LiTDI) in solvents. LiTDI has several advantages over LiPF₆: thermal stability up to 250°C, protection of aluminum against corrosion, and oxidation stability at 4.6V versus Li+/Li. With LiMn₂O₄ cathode, this salt produces good cycling behaviour and good power capability. Nevertheless, this LiTDI has a lower conductivity which can be optimized with a mixture of several carbonates. LiPF₆ is modelled according to data provided by the manufacturer. The data for LiTDI manufacturing is confidential, the proxy used is the data for lithium bis (trifluoromethylsulfonyl) imide from [20]. According to the manufacturer, this is a good proxy.

3.2.5 Separator, BMS, cell container, module, battery housing and cooling system

The separator is a porous polymer layer placed between anode and cathode. It is a three layers separator modeled with data from Ecoinvent for plastics granulate and injection molding. The cell containers are aluminium hard case with aluminium and copper current collectors. Aluminium represents 70% of the mass of the container. The module packaging is composed at 54% of aluminium. The BMS, battery tray, battery retention and cooling system have not been designed in this project. Data from [8] is then scaled to the total mass of the battery obtained by considering that 70% of the total weight is composed of the cells.

4 LIFE CYCLE IMPACT ASSESSMENT

4.1 Total impacts of manufacturing of the cells and of the battery pack

The contribution of electrode pastes, separator, substrates, electrolyte, cell container and cell manufacturing are shown on the left column in Fig. 2. Each process (except cell manufacturing) that contributes to more than 2% of the total GHG emissions is detailed on the middle column. The right column represents the mass composition of the cell.

The main contributor is the manufacturing stage of the cell, which mainly consists of electricity from Germany. We do not have details on energy consumption during the manufacturing stage, but it is reasonable to assume that the drying is the most intensive process. The next big contributor is the cathode paste, 40% of the cathode paste emissions occurring in the nickel sulfate manufacturing process. Note that nickel sulfate is the main precursor as the active material is NMC 622 and the ore extraction is energy intensive. The anode paste emits ca. 6 times less GHG than the cathode paste but the aircraft transport of the silicon alloy contributes to 20% of the anode paste impact. In the anode paste, the US electricity mix shows a relatively high share, but energy intensity for the silicon alloy manufacturing is a data for lab scale. The silicon itself represents 24% of the anode paste emissions, in the sensitivity analysis, we will see how much higher this share is with a higher-grade silicon. The aluminum cell container is also a significant contributor.



electrolyte and separator do not represent high shares of GHG emissions, even though they represent almost 40% of the mass share of the cell.

Considering the whole battery pack (Fig. 3), the CtG GHG emissions reach 163 kgCO₂eq/kWh, calculated with IPCC 2013 method V1.03. Note that, if calculated with IPCC 2007 V 1.02, the GHG emissions are 160 kgCO₂eq/kWh. The values found in [6] lie between 35 kg CO₂eq/kWh and 356 CO₂eq/kWh for NMC batteries (mean value 160 kg CO₂eq/kWh). Many of those values found in literature may be based on IPCC 2007.

Even at battery pack level, cell manufacturing and cathode paste are predominant on the impact on climate change. Nevertheless, the hard case is not negligible as it consists of aluminum. The high share of this component shows the energy intensity of aluminum processing. The emissions of the module and battery packaging mainly originate from the aluminum present in the module packaging.

4.2 Sensitivity

4.2.1 Scenario analysis

As previously mentioned, there is no silicon dataset in Ecoinvent that matches the requirements for the silicon alloy manufacturing. Metallurgical grade has been chosen for the



Figure 2: GHG emissions of manufacturing 1 kWh energy content cell.



Figure 3: GHG emissions of manufacturing 1 kWh energy content battery pack.

base case, and, according to [21], polysilicon solar grade is suitable for battery anodes. It is a metallurgical grade silicon that follows a modified Siemens process. The impact on climate change at the cell level is higher if the silicon is a solar grade, and the relative difference is 2.6%.

The manufacturing facility of the cells and the battery is in Germany for the base case, where electricity generation is mainly based on fossil resources. Today, most of the battery are manufactured in China and the European Commission is pushing toward a more local production. In this section, the German electricity mix is then replaced by 2015 Chinese average, 2015 European average and 2015 Norwegian electricity mix. Norwegian electricity mix is chosen because it is based on renewable energy sources: hydropower (95%). The manufacturing electricity will also be provided by photovoltaic panels (100%PV and 50% PV + 50% German electricity mix) and wind turbines (100% wind energy and 50% wind energy + 50% German electricity mix) to account for the intermittent nature of these energy sources.

Renewable energies allow to decrease the impact on climate change up to 37% (Fig. 4). Ellingsen et al. [8] found a decrease of more than 60% on the impact on climate change using electricity based on hydroelectric power for manufacturing.

4.3 Uncertainty

To quantify the uncertainty of the previous results, 1000 runs of a Monte Carlo simulation are performed and the distribution of the results is shown in Fig. 5. The 95% confidence interval is [140; 194] kgCO₂eq/kWh. The coefficient of variation, defined as the ratio of the standard deviation to the mean is 8%. This coefficient of variation shows the reliability of the results of this study.





Figure 4: GHG emissions of the manufacturing of 1 kWh battery pack with German electricity mix (DE), Chinese electricity mix (CN), European average electricity mix (EU), only photovoltaic energy (100% PV), half photovoltaic energy (50% PV), only wind energy (100% wind) and half wind energy (50% wind).



=Mean =Lower bound of the 95% confidence interval =Upper bound of the 95% confidence interval

Figure 5: Distribution of GHG emissions of manufacturing 1kWh energy content pack.

5 CONCLUSION

Energy density of batteries is a key issue for automotive industry. Silicon is a promising material to increase this density. In this study, the GHG emissions of manufacturing an NMC battery with a silicon based anode are evaluated. The key parameters for environmental



performances of this new battery pack are the energy consumption for cell manufacturing and the cathode paste materials.

Four questions were to be answered in the objectives. First, on a cell level, nickel is the material that contributes more to the impact on climate change, due to the energy intensiveness of its mining and refining process. Secondly, silicon has a smaller influence on the manufacturing GHG emissions of the cell. Thirdly, the manufacturing of this new cell technology seems to be a good alternative to current batteries. Lastly, it is even more true if the energy source includes renewable energy sources such as hydropower, solar energy or wind energy.

This study only focuses on manufacturing stage but as LCA has the power to assess the entire life cycle, with information on the use stage and the end of life, the new pack could be assessed.

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