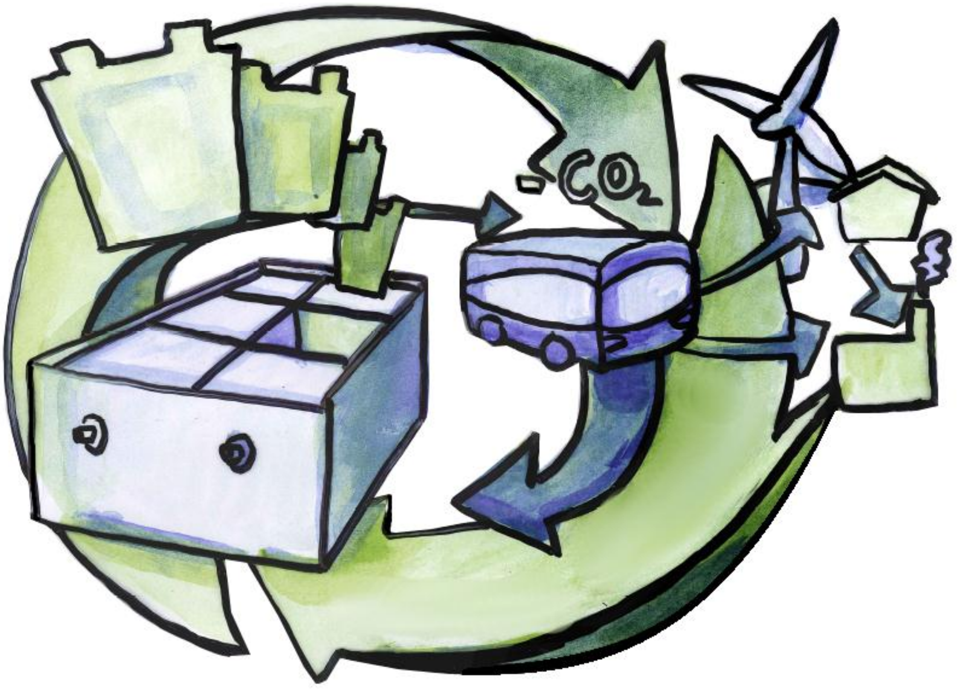

Life Cycle Assessment of Lithium-ion Batteries for Plug-in Hybrid Buses

Master of Science Thesis

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CHALMERS UNIVERSITY OF TECHNOLOGY
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Abstract

Electrified buses are becoming increasingly popular and are labeled less environmental impacting compared to conventional buses thanks to reductions in fuel consumption. It is in light of this, however, important to consider the added environmental burden related to production, use, and end of life of the energy storage system, a fundamental component in the electric drive line.

This thesis investigates the possible gains and losses when using battery cells with a range of different chemistries. The effect of modularization and change in pack design of the system is also assessed in terms of potential gains and environmental burden. The goal has been to determine the steps in the life cycle with most environmental impact by conducting a life cycle analysis on a full energy storage system based on lithium-ion chemistries. Lithium iron phosphate and lithium nickel manganese cobalt oxide are considered for the cradle to gate life cycle assessment. Other current and future chemistries are assessed for reference.

When considering modularization, special focus has been given the environmental impacts related to measures for interoperability of battery module units, as well as effects of reuse and second life. For the use phase, the impacts of the battery related to the number of passengers of the bus are investigated. Also the environmental effect of choosing different battery pack materials is investigated.

Regarding the effects of changing cell chemistry, the results indicate that a transition from materials with scarce constituents to those with more abundant materials can be beneficial for the environmental impact, even if energy consumption is not improved. The assessment also pinpoints aluminum current collectors as a part with large impact. In addition, another large part of the impact from the cells is due to the active materials and their processing, indicating the potential gains associated with improved recycling. It is indicated that different processing alternatives have different benefits depending on whether or not the active materials need to be of nano-size.

In the perspective of the whole battery pack, the cells together with the electronics and control systems have the largest impacts, and this can efficiently be reduced by applying reuse. Through modularization, the battery pack can be prepared for different types of reuse or second life. When using several small packs the impacts are higher than when using one larger pack. The impact of using several smaller packs is also dependent on the placement of control units.

Additional cooling system structure for fast charging has shown to have high significance for the weight of the battery pack, indicating the need of paying high attention to the cooling system design. The electronics and battery monitoring system result in a large impact. The magnitude of this impact is, however, still dependent on the type of printed circuit board used.

In the total life cycle, the energy consumption during the driving related to a typical increase in the battery pack weight is same order of magnitude as the energy needed to produce the battery. Moreover, if a weight increase also leads to a decreased passenger capacity, normalizing with the number of passengers has a great importance for the outcome of the LCA, motivating a thorough allocation method.

In light of the results found in this thesis it is clear that assessing the impacts of using different materials and components in the battery energy storage system is a key in order to design systems with as low environmental impact as possible.

Acknowledgments

We would like to extend a warm thank you to all those who made this thesis possible, both at Chalmers, and through the collaboration with AB Volvo. A big thanks to all of the group at Volvo ATR who were so friendly and always ready to answer any questions, no matter how simple or difficult, and to all of the employees who made our work here as enjoyable as it has been.

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Mia Romare and Ylva Olofsson
Göteborg, 2013

Contents

Acronyms

ADP	Abiotic Depletion Potential
AP	Acidification Potential
BEV	Battery Electric Vehicles
BMS	Battery Management System
CPM	Cells Per Module
DCB	Dichlorobenzene
DMC	Dimethyl Carbonate
EC	Ethylene Carbonate
EI99	Eco-indicator 99
ELU	Environmental Load Units
EOL	End Of Life
EP	Eutrophication Potential
EPS	Environmental Priority Strategies
ESS	Energy Storage System
GWP	Global Warming Potential
HEV	Hybrid Electric Vehicles
HOMO	Highest Occupied Molecular Orbital
HTP	Human Toxicity Potential
LCA	Life Cycle Assessment
LFP	$LiFePO_4$
LFS	Li_2FeSiO_4
Li-S	Lithium-Sulfur
LMO	Lithium Manganese Oxide
LMP	$LiMnPO_4$
LTO	$Li_4Ti_5O_{12}$
LUMO	Lowest Unoccupied Molecular Orbital

NCA	Lithium Nickel Cobalt Aluminium oxide
NiMH	Nickel-Metal Hydride
NMC	$Li(Ni_{1/3}Mn_{1/3}Co_{1/3})O_2$
NMP	N-methyl-2-pyrrolidone
OCV	Open Circuit Voltage
PbA	Lead Acid
PC	Polycarbonate
PCB	Printed Circuit Board
PE	Polyethylene
PET	Polyethylene Terephthalate
PHEV	Plug-in Hybrid Electric Vehicles
POCP	Photochemical Ozone Creation Potential
PP	Polypropylene
PU	Polyurethane
PVC	Polyvinyl Chloride
PVdF	Polyvinylidene Fluoride
RES	Renewable Energy Sources
SEI	Solid Electrolyte Interphase
SOC	State Of Charge
SOH	State Of Health
UPS	Uninterruptible Power Supply

Contribution summary

Mia Romare: Main responsibilities: Sections 3.1, 3.2, 3.5, 4.1, 4.2, 4.6, 5.1, 5.4
Ylva Olofsson: Main responsibilities: Sections 3.3, 3.4, 4.3, 4.4, 4.5, 5.2, 5.3

Introduction

The environmental impact of the transportation sector is an area that has received increasing attention during the past decades. The transportation sector contributes 16% of mankind's total emissions of CO_2 [OICA - International Organization of Motor Vehicle Manufacturers 2013], and is one important sector that needs to reduce its emissions.

Legislations to encourage this reduction are being passed, and further emission reductions will be required after the Euro-6 emission norm for light vehicles, and Euro-VI emission norm for heavy duty vehicles are introduced as standard in 2014 for the new models released focusing on the reduction of NO_x [Volvo Trucks 2013], [Johnson 2008].

Fear of depletion of fossil fuels and fuel security issues are also reasons for the increased interest in alternative fuels. In light of this, the interest in electrified vehicles has increased. In turn, the possibility of using electricity as a propulsion means is dependent on the development of durable, stable and reliable energy storage systems (ESS) to store the energy. Batteries could be an alternative, and therefore the battery concepts and their constituent materials are of interest.

The share of electrified vehicles is already growing. Electrified vehicles started being produced in the early 20th century, but the development of the combustion engine hindered their growth. In the 21st century, interest in electric vehicles is again great. The world stock of electrified vehicles was around 180 000 in 2012. USA, Japan, France and China have the largest electrified vehicle fleet, but other countries like Norway and Ireland are also adopting electric vehicles. Between 2011 and 2012 global sales increased from 43 000 to 113 000 electric vehicles [IEA - International Energy Agency 2013].

Different electrified vehicles exist and require different sizes and design of the batteries. Examples of electrified vehicles are hybrid electric vehicle (HEV), plugin-hybrid electric vehicle (PHEV) or fully electrified battery electric vehicle (BEV or FEV). Hybrids use the battery system to store energy from regenerative braking, while plug in vehicles store electricity supplied from the grid and additionally from regenerative braking. Thus, HEVs need a smaller battery, PHEVs slightly larger, and BEVs need large batteries to sustain full electric driving. If the type of electrified vehicle is generic the system is often labeled xEV. Additionally, different kinds of battery systems and types exist. Currently sold commercial alternatives use lithium-ion chemistries to a large extent. Past alternatives have mostly been nickel metal hydride or lead acid batteries.

The aim of using electrified vehicles is to decrease the environmental impact of the transport sector. When the use of electrified vehicles increases it becomes ever more important to evaluate at what cost the benefits of electric vehicles come. The impact of the batteries themselves, and the environmental load they place on different environmental categories, can determine the net savings when switching from fossil fuels to battery systems. If the battery production uses more energy than what is saved when driving there would be no benefit.

When talking about electrified vehicles, the focus is often on the potential gains in the use phase. This gain must, however, be viewed in light of the added production cost and corresponding environmental impact from adding an electric propulsion system where the battery system usually dominates. Therefore, an environmental assessment is necessary, and can help to give a deeper insight into the impact of the total life cycle, from production to use. In previous thesis work it has been determined that the battery has a large impact for the total electrified drive line [Laudon & Inzunza Soriano 2012]. Therefore further assessment of the battery and its sub-components is necessary to fully determine why the battery plays such a large role in the total drive line and what components should be improved in order to decrease this role. This in order to improve the total environmental benefit of the electrified vehicle.

An important parameter for the introduction of electrified vehicles is the battery cost, as the battery is one of the most expensive components of the vehicle. A reduction of the battery price will facilitate the growth of the xEV fleet. Solutions for such a price reduction related to the pack design and standardization are at present being investigated and a significant decrease is expected in the future from the present approximate 400 $/kWh towards 150 $/kWh [Argonne National Laboratory 2000]. Special focus in this thesis is on the environmental impacts of different possibilities for design, recycling, reuse and second life, possibly leading to battery pack price reduction.

The results from this assessment could serve as a base for introducing the environmental concepts of batteries in product development, purchasing, manufacturing, remanufacturing and contacts between vehicle manufacturer and battery manufacturer. It can also help in decisions making concerning battery end of life (EOL) solutions.

1.1 Goal

The goal of this thesis is to assess the life cycle impacts of lithium-ion batteries for plug-in hybrid buses. The aim is to highlight potential hot-spots in the battery life cycle when choosing different cell chemistries, modularization approaches and pack designs. The results from the report are aimed to guide and recommend the most beneficial current and future solutions. This in the light of both energy consumption and other environmental impact categories.

The assessment is performed with the help of life cycle assessment (LCA) methodology. The life cycle steps included in the assessment range from extraction and production of constituent materials, to assembly, use phase and end of life management. Priority has been given to achieve transparent data. In this way the method used in this thesis can be applied to more case specific life cycle assessments in the future.

For the cell chemistries the extraction and production of active material, along with cell assembly is in focus. Also the potential gains of recycling the cells after use are evaluated. On a higher system level, environmental effects and opportunities for second use and reuse coupled with modularization are assessed. Lastly different materials choices for supporting components in the whole pack are evaluated.

1.2 Scope and limitations

The thesis aims to assess the environmental impacts of different battery components and subsystems. Therefore only the battery system and its casing are included. Other components in the electrical drive line, like the electric motor, are not included. Also supporting components for the battery system, like the battery charger, are omitted from the thesis scope.

The LCA is divided in parts, with separately explained data collection and results, related to the different product life phases and components. The methodology differs from the one in a standard LCA since the full life cycle impact receives less focus than the results from the different phases of product life and the most important results derive from sensitivity analysis of the importance of various components and production process choices.

In this thesis the end of life options for the pack are only included in the total life cycle as decreased extraction of various metals and materials. For the cells, possible end of life process costs are also included in the assessment.

The time frame of the thesis work is set to be present day for all production, assembly and materials extractions. Also the use phase is set to be in present time, with current electricity mixes and fuels. The vehicles are assumed to follow emission limits for vehicles being produced during 2013.

The life cycle assessment only has lithium-ion batteries within its scope. Other possible materials are assessed outside of the LCA methodology. All models are based on literature studies and calculations, and no lab test have been performed to support the data collection. A battery modeling software, BatPaC, has been used to design battery systems.

1.3 Life Cycle Assessment

LCA is a method to evaluate the environmental impact of the complete life cycle of a product or a service [Baumann & Tillman 2004]. The methodology has been in wide practice since the early nineties as a tool to compare different choices of processes and materials. LCA is commonly used in product development, production processes and waste management, and has become important for standardized environmental market communication.

There are international standards for how a LCA study is conducted, the one used in this thesis is ISO 14044. The environmental impacts are measured according to a group of standard indicators, which makes the LCA results comparable between studies. The indicators and other thesis specific choices will be presented in chapter 2.

Life cycle assessment as a tool for product development

Apart from assessing potential hot-spots of the complete life cycle of a product or service, LCA can be a useful tool for environmentally beneficial design, also called ecodesign [Baumann & Tillman 2004]. This gives the opportunity to find the most optimal design even at a conceptual stage. There are a few general rules to follow when aiming to achieve this design:

- Avoid toxic substances.
- Minimize energy and resource use in production, transport and use phase.
- Use structural features and high quality light materials to minimize weight.
- Promote repair and refurbishment to enable reuse.
- Use materials that promote long product life for products with high production and end of life impact.
- Prepare for upgrade, repair, reuse and recycling by using few and simple materials.
- Use joining elements that can easily be removed to facilitate disassembly.

1.4 Software and tools

GaBi software

The GaBi software is a tool to conduct life cycle assessments of products, and it was developed by the Chair for Building Physics, University of Stuttgart in collaboration with PE International. The software provides features to manage the large sets of environmental data associated to the product life cycle, to create balances for different subcomponents and life phases, and to interpret and visualize the impacts [PE International 2013].

GaBi itself does not provide the data sets of specific materials and processes and so databases containing this data are connected independently. The databases are updated regularly with current data about the material production processes, electricity mixes and average data for regions to keep the environmental evaluations up to date with present industry and theory [PE International 2013]. In some cases the data provided by the existing databases needs to be adjusted to represent a very specific process, and such a change should be motivated by calculations or from literature. In this thesis the changes made to the provided datasets are noted in Appendix A and the assumptions are clarified in chapter 4. The version used is GaBi 6, and the databases used are PE International, Plastics Europe and Ecoinvent.

BatPaC

BatPaC is a performance and cost model developed by Argonne National Laboratory [Nelson, Bloom & I Dees 2011]. The name BatPaC stands for Battery pack Performance and Cost. The model contains information and design models for several different lithium-ion battery cells and the resulting modules and packs. There is the opportunity to choose many parameters to get a system that is a good model for the one that is being investigated. Thereby valuable data for modeling can be retrieved, like weight of components and relative contributions. The version used in this thesis was version 2.1. The focus was to a great extent on the performance part of the program and not the cost.

1.5 Rechargeable batteries

The use of batteries to achieve portable and small scale electrical sources is wide-spread in today's society. Depending on size, batteries can power anything from electronics to vehicles. Batteries that cannot be recharged are used to great extent in most households in various electronic devices. Rechargeable batteries are, however, becoming increasingly common. Batteries offer the possibility to store energy in chemical form and retrieve it as electrical energy through an electrochemical reaction. Unlike in non-rechargeable batteries the reaction is reversible in rechargeable batteries and the cell can be cycled from charged to uncharged many times. This comes with higher demands on the materials involved, and thus a higher price. Generally, this type of battery instead provides the opportunity of up to thousands of recharges and thus longer use.

The fundamentals of the battery were discovered early, and realized in the year 1800 by Volta, when he created his voltaic pile. He found that when two materials of different electrochemical potential were connected with an electrolyte between, a current could be collected. The same basic idea exists in current batteries. When the battery cell is coupled to an external circuit, oxidation and reduction reactions occurs at the negative and positive electrodes respectively. The electrons are collected and used in the external circuit and the ions are transported between the electrodes through the electrolyte. Separating the anode and cathode with an electrically

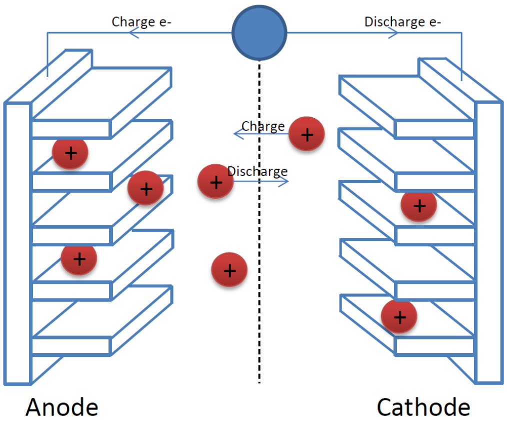

Figure 1.1: Schematic illustration of the workings of a battery cell. All key materials components are shown. The foils supporting the active material (shelves), the separator (dashed line) and mobile charges can all be viewed in the figure. The electrolyte component would be contained between the anode and cathode, and also inside the active materials.

insulating separator ensures that the electrons only can pass through the external circuit, and reaction is limited to when the cell is connected. This basic setup is illustrated in figure 1.1.

When a rechargeable battery is used, it is cycled between different states of charge and discharge. The highest state of charge (SOC) indicates the maximum available energy storage capacity in the battery. The current SOC is the percentage of the highest SOC that is charged at the moment.

The range of charge in which the battery is cycled is called the SOC window. When rechargeable batteries are tested, they are often tested with deep cycles having an 80% SOC window, and the number of available cycles stands in correlation with this. When used in vehicles, a typical SOC window is smaller, around 40% to achieve a greater number of cycles. When comparing battery alternatives it is important to use the same definition of SOC window. In this thesis the total life length of the system in years is used to avoid this confusion.

1.6 Energy storage systems

An automotive energy storage system (ESS) has the function of storing and delivering electric energy, for example to the propulsion of electrified vehicles. The size of the ESS in terms of power and energy is determined by the expected driving pattern, requested range with electric drive, and vehicle weight. An ESS can be designed in a vast amount of ways; from a small system for electronics to large systems with many components for automotive use. For a vehicle size system there are some basic sub-systems that are used to build up the whole battery ESS. The assembly of the sub-systems and their relations to each other are depicted in figure 1.2. These sub-systems comprise:

- The battery cell where the chemical reaction occurs (A).
- The module which stores and manages a certain number of cells (B).
- The pack which contains all modules and all other subcomponents (C).
- The housing which contains one or several packs, creating the outer wall of the ESS (D).
- Subcomponents to control the operation of the battery.

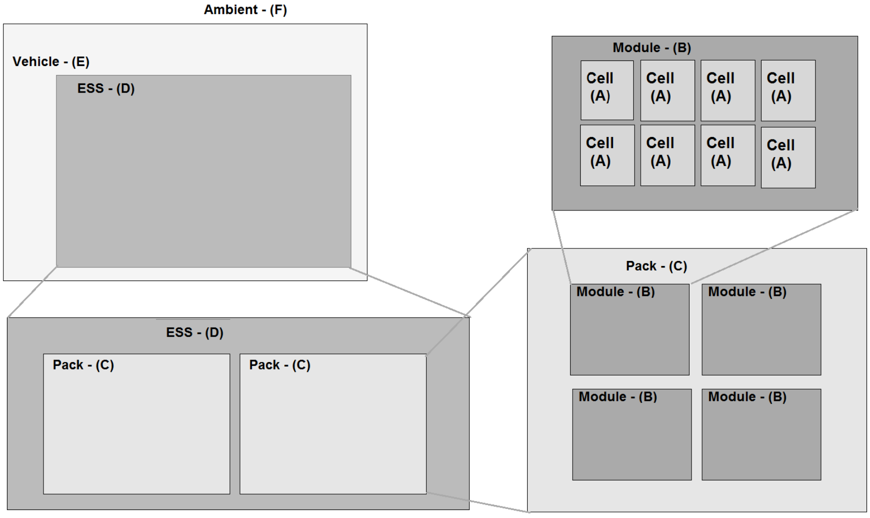

Figure 1.2: The various system boundaries between the subsystems comprising cells, modules, packs, ESS and vehicle are illustrated. The cells are contained in modules, and a number of modules in turn comprise a pack. A full energy storage system is then made up of one of more packs, and placed as a component in the complete vehicle system.

Battery cells

The basic components of a battery cell are a positive and a negative electrode, an electrolyte and optionally a separator. The electrodes are current collectors with the active materials adhered to allow collection of electrons from the reacting materials. The active materials should be conducting and should readily be reduced or oxidized many times without changing form or deteriorating.

The electrolyte is a material with the purpose of conducting ions between the anode and the cathode. It is often a liquid, although alternatives like polymers are possible. In the case of liquid types the electrolyte is contained in the separator and electrodes. The separator is a passive part of the battery cell. Its role is to act as a container for the liquid electrolyte, give stability to the cell and remain stable throughout charging and aging. By separating the two electrodes, short circuiting is prevented [Daniel & Besenhard 2012].

The components of the cells are arranged and encased in a protective pouch or in an outer layer. There are a few different ways of doing this. The electrodes are always layered, but can then either be inserted directly into a flat pouch or casing; or they can be rolled and inserted into a round casing. For the purpose of this thesis, the flat pouch cells are used as models for cells. The use of this design is beneficial since the cells are easier to pack efficiently, easier to cool and are straightforward to model in two dimensions [Nelson et al. 2011]. The material of the pouches can vary, often a thinly rolled plastic-metal-plastic material is used. This material protects the cell and is only broken by the protrusion of current collector tabs, from which many cells and a load circuit can be connected.

Modularization

Modularization of the battery pack implies the subdivision of the total amount of cells contained in the pack into smaller sub units. The cells in the battery are contained in separated boxes, called modules, which interconnected build up the battery pack (figure 1.3,1.2). The modularization can be explained as the almost infinite number of options to group a large number of cells in different configurations. Modularization is a wide concept, and it impacts various aspects of the physical battery properties, and influences the use and the remanufacturing possibilities.

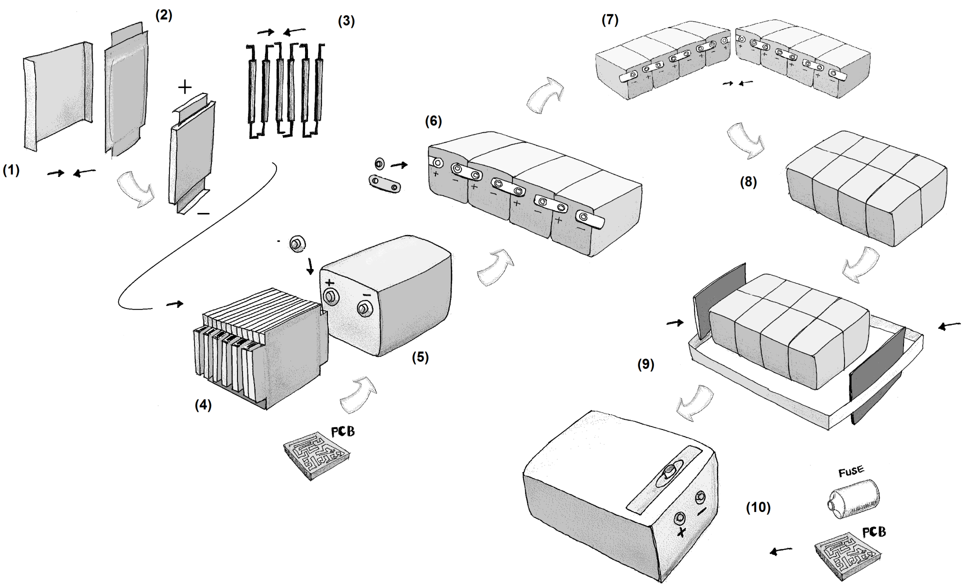

Figure 1.3: The composition and assembly of the battery pack. 1) cooling plates, 2) cell, 3) cell interconnection, 4) cell group, 5) cells contained in module housing with positive and negative terminals, 6) modules connected in row, 7) assembly of two module rows, 8) module group, 9) assembly of steel plates and steel straps to module group, 9) pack containing the modules with terminals and coolant inlet.

Pack design

The pack is a system component that contains all modules and all subcomponents needed in the complete system. It is typically viewed as the box containing interconnected modules with cells, some control units, measurement sensors, parts of the cooling system and safety installations such as fuses. All of the pack components can be seen in figure 1.3. Attention should, however, be paid not to confuse the battery pack with the ESS, since several packs may be used to achieve the full functionality needed for the vehicle. In other words, the ESS may consist of one or several battery packs.

One main function of the pack is to contain the different control units needed to ensure proper functioning of the whole system. For safety reasons, and for prolonging the life of the battery, the voltage and currents need to be controlled to avoid dispersion in load among the cells. It is important that no cells are overloaded and fail, since this would result in reduced functionality of the battery.

To secure good functioning of the ESS, an integrated control system is needed. The management of the whole system control is usually called battery monitoring system (BMS), consisting of printed circuit boards (PCB) and electronics. Additionally for safety reasons, fuses are integrated to hinder any electric dysfunction in the system to spread.

During the charge and discharge of the battery, heat is generated. The battery aging is dependent on the temperature, and so a thermal management system is also needed in the pack. The cooling system should be able to keep the battery at a stable temperature ideally about $35\,°C$, creating a need for cooling plates and pumps [Nelson et al. 2011]. If cooling plates are used the thickness of the plates is adapted to the rate of heat rejection. Thick cooling plates are especially important for fast charging of the battery when the temperatures may rise very fast [1].

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[1] Personal communication with Jens Groot, 2013.

Current limitations

In general, there are a few common factors that limit the performance of battery energy storage systems. For automotive applications the main issues are weight, volume and cost. These can be especially relevant when considering fully electrified vehicles, as heavy systems (250-700 kg) are needed to get a reasonable range. This is in turn coupled with high cost and environmental impact due to a larger energy consumption when driving, and a more costly production of the parts.

All batteries have life-length problems, degrading over time as a function of the number of cycles. Currently they are not able to perform up to the required standards during the whole life-time of the vehicle, leading to a need for replacement. This is caused both by charging and discharging, 'cycling' issues, but also by side reactions when the battery is passive for a longer period of time, 'calendar life'.

The battery system and its active materials need to compete when it comes to energy density, both volumetric and gravimetric. This gives rise to a general need for development towards lighter materials with good capacity and fast charge/discharge. A longer life-time is also a key factor as it reduces the overall impact of the processing step and the need for servicing.

1.7 Designing for a plug-in hybrid electric bus

For vehicle size systems there are a multitude of factors determining the choice of components on all levels of the system, from chemistry to casing. The vehicle use determines the required energy storage capacity, as well as the required voltage, charge capacity, and power. These factors do in turn impact the number of cells needed, what chemistries these can be and the configuration (series or parallel) of the cells. The vehicle use can vary greatly depending on drive cycles, range of driving and time of driving. The ESS might also have to conform to the requirements placed by existing infrastructure, and be suitable for different climates. The PHEV bus typically has a predefined route with predictable accelerations, driving speeds, number of stops, and charging places.

The electric range of the battery is dimensioned according to the driving cycle for the set route [Pesaran, Markel, Tataria & Howell 2009]. The goal is often to make a certain percentage totally electric in order to for example to keep the driving silent or to not emit in urban areas. A common electric distance for a PHEV bus is 5-10 km. For the rest of the driving distance the ICE engine is included and shares the load with the electric engine as efficiently as possible, using also the power from regenerative breaking [Pesaran et al. 2009]. For a city bus, a 5-10 km electric range is close to the distance between end stations, giving opportunity to recharge after this distance.

The battery is dimensioned so that the energy needed to achieve the electrical range is available, taking into consideration the SOC window available for the battery during its life [Pesaran et al. 2009]. Normally, the window is at most 40% in order to make the battery last longer. Common sizes of a battery system for a 10 km electric range in city driving are between 20-60 kWh depending on the driving cycle[2]. Moreover, the accelerating power is dimensioned as the maximum power that should be extracted from the battery, and the braking power is dimensioned as the power that should be absorbed in the regenerative braking. The power of the electric motor often ranges between 120-150 kW[Volvo Buses 2013*a*] depending on the size of the bus, at voltages of 500-730 V[2].

The type of cell used in the system can also influence the size and design. This since a bus is a heavy vehicle and thus requires more power compared to energy storage than for example

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[2] Estimate from personal communication with Jens Groot, 2013.

a car. This in turn has implication both for the supporting material in cell and pack, since they need to cope with large currents and corresponding heat generation. Also the need for fast charging in a city bus that spends most of its time on the road is of importance for the cooling system.

The weight of a battery system depends on what demands are placed on the desired electric range, and what energy storage capacity is needed. For a PHEV as described above a typical range is from 250-700 kg assuming a specific energy of $84\ {}^{\mathrm{Wh}}/_{\mathrm{kg\ battery\ pack}}$[3]. For the total battery system. The cells used in this system weigh around 500-600 g each.

The last stage of design is placing the battery somewhere on the vehicle body. The outer frames should fit in the available space, and be balanced against the weight of other equipment, both in layout and in total weight. An over dimensioned battery can have the implication of lowering the legally advised number of passengers on the bus, penalizing the functionality.

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[3] Estimate from BatPaC calculation

Life cycle assessment methodology

A life cycle assessment is often conducted in several typical steps [Baumann & Tillman 2004]. First the goal and scope are defined, then an inventory analysis is performed. In the inventory analysis a model of the life cycle is built based on the goal and scope, data is collected for all the stages included in the model, and the amounts of material, energy and emissions included in each step of the model are calculated. After the inventory analysis an impact assessment is performed to indicate the resulting impacts from the model created in the inventory analysis. In this thesis the inventory analysis and models are presented in chapter 4 and the impact assessment is presented in chapter 5.

2.1 Goal and scope definition

The LCA type in this thesis is a stand-alone LCA, meaning that only one product is evaluated and no comparison with other products are conducted [Baumann & Tillman 2004]. This aim is to identify hot spots in the complete life cycle, and the goal and scope are aimed at producing results that highlight these hot-spots.

Life cycle analysis goal statement

The goal of the LCA conducted in this thesis is to highlight the key steps in the development and design of an ESS, and their contribution to environmental impact of the system. The assessment can lead both to recommendation for improvement of certain life cycle steps, but also to guidance for future development plans. The assessment aims to answer the following questions

- What are the key components influencing the life cycle of a complete system?
- What are the key steps of cell production?
- What is the effect of modularization?
- What are the possible gains of different strategies of reuse, second life use and recycling?
- What would be the impact of changing the cell chemistry used in the system?
- What would be the impact of changing pack and module materials in the system?

To answer these questions the LCA was divided in both a full cradle-to-grave assessment, but also into several cradle-to-gate and gate-grave assessments for subprocesses and input materials.

Scope and functional unit

The scope of this LCA includes the study of a complete ESS with all its subcomponents. The ESS is sized for use in a PHEV city bus. The system is specified to provide appropriate energy and power for this application, regardless of the battery type. Other components of a PHEV bus, apart from the ESS, are only considered as a black box, albeit with some parameterization such as reacting to changes in weight by changing energy consumption for driving.

The functional unit of the LCA is one full ESS scaled for heavy vehicles, with a 3 year life length. All results will correspond to this functional unit as all the components are scaled accordingly. The cell size, number of cells, and pack size are all suited for the functional unit.

The motivation for this choice of functional unit is that the different design alternatives in this thesis lead to the need for different pack sizes, different relative weight between the components and different size of the total energy storage capacity. Therefore a per kg or per kWh functional unit would be misleading in light of these changes. The priority is to show the results in light of the function of the energy storage system that is to supply energy to a PHEV bus for 3 years.

System boundaries

The aim of the thesis was to assess and highlight the most important impact categories for the different life cycle steps of a vehicle battery in a very general manner. This means that no geographical boundaries were set, and global or European averages were used where possible. Due to this a choice was made to exclude the impact from transportation, and infrastructure like plants. This is acceptable, since transport has a gross energy demand in the order of 1% of the total demand during cell production [Rydh & Sandén 2005]. The timescale of the LCA was set to include present data only.

The technical boundaries include the cut-off of all components outside the boundary of the ESS and its case. Previous work concludes that the battery is a dominant factor both in global warming potential and acidification potential compared to other components in the drive line [Laudon & Inzunza Soriano 2012]. The ESS may be a key component, but the results will still be limited to indicate possible improvements and key impact factors connected to the battery materials, processing, assembly, reuse and recycling.

2.2 Impact categories and weighting methods

Material or system environmental impacts can be obtained by looking at different impact categories. Apart from looking at the energy consumption, this thesis uses seven impact categories:

- Global warming potential (GWP), CO_2-equiv.
- Abiotic Depletion Potential of elements (ADP elements), Sb-equiv.
- Abiotic Depletion Potential of fossils (ADP fossil), MJ.
- Acidification Potential (AP), SO_2-equiv.
- Eutrophication Potential (EP), phosphate-equiv.
- Human Toxicity Potential (HTP), DCB-equiv.
- Photochemical Ozone Creation Potential (POCP), ethene-quiv.

To further understand why these are of relevance, a short description of each category will follow:

Energy: Represents the total net calorific value of fuels related to transports and processes for the production of materials or services. This category is measured in MJ.

Abiotic depletion potential: Measures the depletion of non-renewable, non-biological resources that are not recreated by nature within a very long period. Examples are metals, minerals, and fossils. The category is based on determined existing resources, and may vary if new sources are discovered [Baumann & Tillman 2004], [en Waterstaat & Waterbouwkunde 2002]. The category is of interest due to the possible depletion of elements with high importance for the industrialized society, for example fossil fuels and rare metals used in electronics. The ADP of elements is measured in kg antimony-equivalents, and that of fossils in MJ energy contained.

Eutrophication potential: Measures the substances emitted to nature that can lead to an increase in biological productivity in terrestrial systems, lakes and waters (aquatic systems) leading to lack of oxygen, so called eutrophication. The increased biological activity is due to nutrients such as phosphates and nitrates being emitted [Baumann & Tillman 2004]. The biological organisms consumes the oxygen in the water for their metabolism until the water oxygen content is depleted, and fish and other aerobe beings go towards extinction, while anaerobe metabolisms take over[Hans De Keulenaer 2006*b*].

Acidification potential: Is impacted by the emissions of sulfur and other substances leading to acidification of ground and waters, and measured in kg SO_2-equivalents. The acidification leads to changes in pH in the environment changing the living conditions for the biosphere, often in a negative way[Baumann & Tillman 2004]. The acidification is a problem especially for grounds with low content of calcium and other minerals being natural pH stabilizer, such as those in the pine forests in Scandinavia [Krug, Frink et al. 1983]. The acidification may for example lead to leaching of heavy metals to the ground water due to chemical reactions favored by the acidity, the degradation of cultural monuments of marble, and difficulties with survival for some species[Hans De Keulenaer 2006*a*].

Global warming potential: Is enhanced by the green house gas emissions to the atmosphere and measured in CO_2-equivalents. Global warming is the origin to secondary effects such as climate change [Baumann & Tillman 2004], thereby giving unpredictable but severe impacts to the environment such as; melting of glaciers, raised sea level, increase in natural disasters due to unstable weather, and extinction of species due to drastically changed living conditions induced by the temperature increase [Azar 2008].

Human Toxicity potential: Accounts for emissions of chemical substances to the environment that can be harmful to humans by inhalation, dermal contact with water and soil, or ingestion by produce, fish and meat. The exposure, spreading and fade of the dose is modeled and interpreted in dichlorobenzene (DCB) equivalents [Hertwich, Mateles, Pease & McKone 2001].

Photochemical ozone creation potential: The creation of ozone at ground level is a reaction between uncombusted hydrocarbons and NO_x from traffic emissions, catalyzed by sun radiation. Ozone at ground level is harmful to vegetation and is toxic for humans in high concentrations. The concentration of ozone and the related toxicity depends on weather conditions such as humidity and wind [Baumann & Tillman 2004]. The index is ethylene-equivalents.

Weighting methods

Weighting methods can be used to value the impact in different categories and summarize all values into a single score. This can give fast and easy comparison between different alternatives and designs. Different weighting methods can be used, each valuing different impacts more or less heavily. Weighting methods are standardized so as to present a common base for comparison.

In this thesis two weighting methods are used. The first is the Environmental Priority Strategies (EPS) method, measured in Environmental Load Units (ELU). The units are based on the willingness to pay for a certain environmental impact. The method was developed to aid in product development [Baumann & Tillman 2004].

The second weighting method used is the Eco-indicator 99 (EI99). Also EI99 was developed as a tool for product development, using one single impact score. Here the LCA impacts are categorized as belonging to one of three categories; Damage to human health, damage to ecosystem quality, and damage to resources. The relative importance of each of these categories can vary. In this thesis we use the hierarchic perspective, including both a shorter and a longer time frame, and based both on facts and political and scientific bodies [Baumann & Tillman 2004].

2.3 Sensitivity analysis

A sensitivity analysis is an assessment of the effect of changing a certain parameter between the value used in the LCA, and possible maximum and minimum values for the same parameter. Sensitivity analysis is an important part of LCA [Baumann & Tillman 2004], especially when dealing with assessments of components for which not much data exists, were the data is incomplete or not very detailed. By systematically changing the uncertain parameters and analyzing the effect this has on the system, the impact of the uncertainty can be determined. If the change in the system is small when changing a parameter, then the uncertainty is not a great issue. On the other hand, if the impact on the system is large it should be noted that the uncertainty of the parameter in question could have large impact on the overall assessment.

In this thesis, sensitivity analysis was performed on parameters that showed a large impact on the total result for one or more impact categories. Also parameters where there were known discrepancies in the data were tested, so that the effect of having uncertain data could be analyzed.

Components and design alternatives for energy storage systems

A large variety of different battery system concepts exist. Everything from the shape of the pack, module and cell, to the incorporated material can change. This chapter is aimed at providing a base for understanding possible and common choices for the different materials and design alternatives, as well as production methods and end of life alternatives for these. The presentation in divided into sections where the design and materials of different components are presented. These components include the cells, modules and packs. Also cell production and recycling, as well as second use and reuse alternatives are presented.

3.1 Current and future cell chemistries

This section provides an overview of the battery chemistries that were evaluated in this thesis work. Common designs and constituents of each type are described, and their coupling to automotive battery evolution discussed. Several of the chemistries are based on the lithium-ion concept, and a general description of this important type of battery is therefore presented. A presentation of specific lithium-ion chemistries and material follows, as well as a comment on other alternative battery designs and their materials. This builds a base for the interpretation of the LCA results presented in Chapter 5.

3.1.1 Lithium-ion batteries

Lithium-ion (Li-ion) batteries as a group are of high interest both when talking about current and future battery technologies, since they have high cell potential and low weight, resulting in high gravimetric power and energy densities. Generally Li-ion batteries are valued for their long lifetime, both in available cycles and calendar-life, compared to older types of rechargeable batteries such as the nickel-metal hydride (NiMH) batteries or lead acid batteries (PbA).

The basis of Li-ion batteries is the rocking-chair mechanism, meaning the lithium ions rock between the anode and cathode during charge and discharge. The electrodes consist of a supporting and conducting foil to which the active material, and possibly some conductive additive, are adhered with a binder. Between and inside the electrodes, the electrolyte is contained. A schematic representation of the electrode setup is illustrated in figure 3.1.

Figure 3.2 illustrates the potential of several different energy storage alternatives. Li-ion is the only option at present that can be tuned to fit many different needs, and thus many different applications, as exemplified by their use in both portable electronics and vehicles. Therefore this thesis focuses on this technology, and several different Li-ion chemistries are evaluated. The

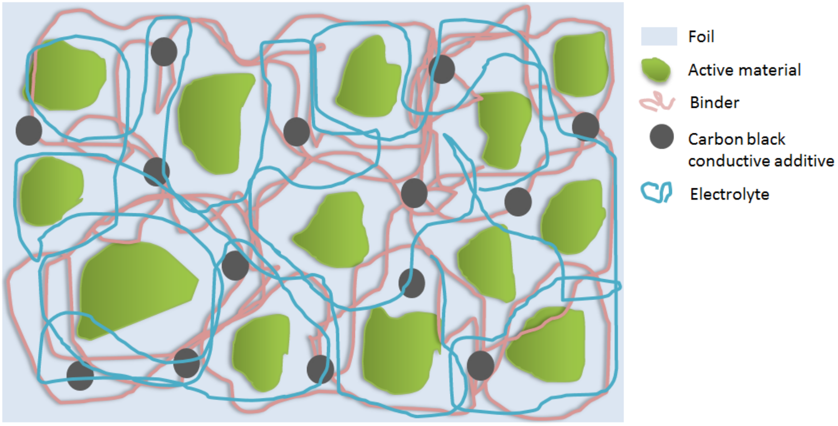

Figure 3.1: Schematic illustration of a lithium-ion electrode. The foil is a flat metallic surface, the active material particles and conductive additive are adhered to the foil with a binder (dried). The liquid electrolyte is contained between the active material particles.

choices of chemistries represent different power and energy properties as well as different states of development.

The different chemistries are often denoted by their cathode active material. The electrode active material consists of an intercalation or insertion material, capable of hosting lithium ions without deforming their structure. There are a wide variety of cathode active materials to choose from, and also some different anode active materials, although most current chemistries use graphite. Some commercially available alternatives are presented in table 3.1

Table 3.1: The table presents some of the commercially available and most common choices for lithium-ion battery cathodes and anodes. Some of the most promising and relevant options for heavy vehicles have been included in the life cycle assessment presented in this thesis.

	Active material	**Included in LCA**
Cathodes	Lithium iron phosphate	Yes
	Lithium nickel manganese cobalt oxide	Yes
	Lithium manganese oxide	No
	Lithium cobalt oxide	No
	Lithium nickel cobalt aluminium	No
Anodes	Graphite	Yes
	Lithium titanate	Yes

Many configurations choices, small modifications and indeed also mixes of these materials are possible. Additionally there is a constant development of new and promising electrode active materials for Li-ion batteries. The complete selection of included electrode active materials for the LCA consists of both the current alternatives mentioned in table 3.1, and future candidates including lithium manganese phosphate and lithium iron silicate.

There are also some general drawbacks associated with Li-ion batteries. For automotive purposes the issue of safety will always be important, all current Li-ion batteries need to be operated under controlled temperature and voltage conditions to avoid unwanted reactions in the cell. If they are punctured during an accident there is a risk that anode and cathode come in contact, causing high currents to run, and heat generation that leads to potential fire hazard.

The use of certain materials in the Li-ion cells might be an issue. Some chemistries contain cobalt and nickel, increasing the environmental burden, see section 3.1.5, whilst others lack the economic incentive for recycling, as will be discussed in section 3.5. For future light weight

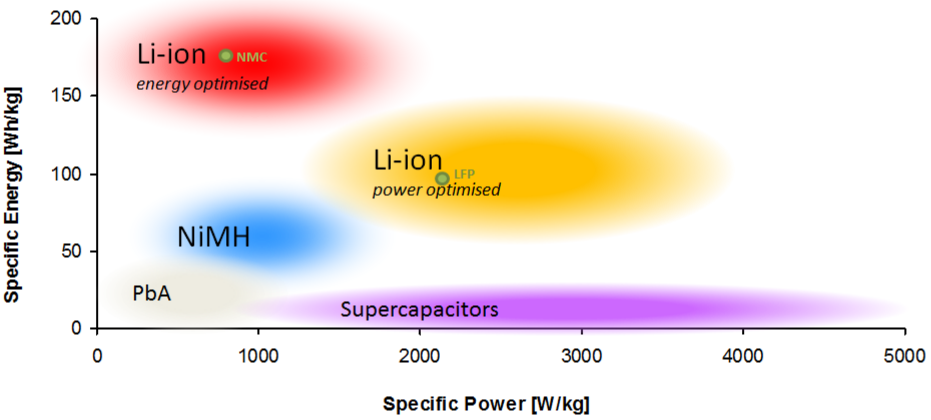

Figure 3.2: Gravimetric energy and power densities are shown for several different energy storage alternatives, including lithium-ion battery systems. Some examples of typical high energy and high power lithium-ion chemistries are indicated in the figure. The figure illustrates the great diversity and thus applicability of lithium-ion batteries, both as high-energy and high-power batteries.

battery alternatives, focus is also shifted from Li-ion cells to alternatives with higher capacities. This since their achievable capacities are reaching the theoretical maxima. At the moment, however, the lithium-ion batteries are both the most commercially viable and have the best performance.

Electrolyte, separator and supporting material for Li-ion batteries

To great extent, the different Li-ion chemistries use similar electrolytes and separators. These components are of course also under development, and a range of different alternatives are emerging. However, most applications use a common approach.

The electrolyte choice for Li-ion batteries is commonly different kinds of lithium salts dissolved in nonaqueous organic solutions. These solutions are liquid carbonate blends, providing a large liquid temperature range, large voltage windows, low viscosity and good solubility compared with alternative liquid electrolytes such aqueous electrolytes [Goodenough & Kim 2009]. The penalty compared to aqueous alternatives is higher cost, flammability and decreased conductivity. Compared to solid electrolytes they have better conductivity and again a larger voltage window [Daniel & Besenhard 2012].

The voltage window of an electrolyte is defined as the difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). The anode and cathode potentials need to lie within these limits or the electrolyte will react with the electrodes. In some cases, if the difference is small, a solid electrolyte interphase (SEI) layer can be formed to change the potential of the electrodes and make them stable together with the electrolyte. This layer passivates the electrode by hindering electronic conduction, but also decreases the wanted ionic conductivity. Carbonates generally have a HOMO at around 4.7 V and a LUMO around 1.0 V versus lithium [Goodenough & Kim 2009]. All potentials will henceforth be referenced versus lithium.

A common variant of nonaqueous electrolytes, that will serve as a good representative for the electrolyte, is lithium hexafluoride, $LiPF_6$, dissolved in a blend of ethylene carbonate (EC) and dimethyl carbonate (DMC). 1 M $LiPF_6$ in a solution of EC/DMC shows a conductivity of $10.7\,{}^{\mathrm{mS}}/_{\mathrm{cm}}$. It has limitations arising from its decomposition at high voltages into LiF and PF_5, however, where PF_5 reacts irreversibly with traces of water present. At temperatures above $50\,°C$ reactions with the carbonates in the electrolyte also occur [Goodenough & Kim 2009]. The electrolyte also presents a safety risk since it is flammable. Due to these factors the electrolyte type is not applicable to all possible chemistries, but it is currently used in most commercial cells. Common operating ranges are below 50 $°C$ and 4.5 V due to the decomposition temperature and HOMO. Despite its disadvantages for some chemistries, this electrolyte does of course fulfill many of the requirements put on an electrolyte, such as good ion conductivity, low electronic conductivity, and acceptable voltage window. This is the reason that 1 M $LiPF_6$ in EC/DEC/DMC is the most common variant of electrolyte in current commercial cells..

At the moment the most common separator, matching the above mentioned choice of electrolyte, is a micro-porous polyolefin membrane. These membranes often consist of polyethylene (PE) or polypropylene (PP), and most often a lamination of the two. This type of membrane is set between the two electrodes, and the electrolyte is contained within its pores, as well as in the electrodes.

The setup with a polyolefin membrane with $LiPF_6$ in EC/DEC/DMC provides a level of safety for the cells since the membrane will melt in the case of a thermal runaway, a situation where an increase in temperature promotes further increase. When the separator melts it hinders further increase in temperature due to high current. The choice of PE and PP also gives good mechanical and chemical stability, at an acceptable cost [Arora & Zhang 2004]. Having the separator melt is, however, a worst case scenario, since the battery then will be unusable. Development of new separator and electrolyte alternatives that inherently resist thermal runaway is therefore of interest for further development. Flammability and decomposition temperatures also need to be improved.

Other key supporting materials are the current collector foils, to which the active material is adhered, for mechanical support and conduction. The material of choice is aluminium due to its good conductive properties, low weight and reasonable price. However, the low potential of the active material might lead to corrosion of aluminium and unwanted alloying between the aluminium and lithium. The cathode active materials have high potential, so here aluminium foils can be used exclusively. The anode active materials have lower potentials, and due to this the aluminium foils might need to be changed to copper foils which corrodes at much higher potentials than aluminium.

The foils are also used to design high power cells. By using thicker foils, more current capacity is achieved and thus higher power. In addition, adhering a smaller amount of active material to each foil gives the need for more foils to carry the total amount for material needed, but it also decreases the diffusion lengths giving higher power. These factors are used in this thesis to scale the cells for high power applications.

3.1.2 Lithium-ion battery cathode active materials

Layered metal oxides

Layered metal oxides as cathodes for lithium-ion batteries were the first to be commercialized, starting with the use of the material $LiCoO_2$ by Sony in 1990, a variant mostly used for electronics [Daniel & Besenhard 2012]. The layered oxides have the general formula $LiMO_2$ where M stands for metal and can be Co, Ni, V or Cr. The lithium is intercalated in planes, allowing diffusion in two dimensions. The metal is located in the alternating planes in a structure called the O3 layered structure, shown in figure 3.3. Layered metal oxide materials have good electronic conductivity due to the structural contact between the metal atoms, and good diffusivity due to the two dimensional movement.

The potential intercalation is one lithium ion per unit cell, resulting in a theoretical capacity of approximately 274 $^{mAh}/_{g}$. However only around 50% of this capacity, 150 $^{mAh}/_{g}$ can be realized. This since the materials are not stable at deep cycling, and will start to loose oxygen and cobalt to the electrolyte. The materials do however have a high density, for example 5.1 $^{g}/_{cm^3}$

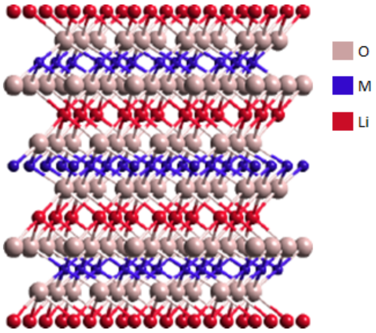

Figure 3.3: Basic structure of the layered oxides ($LiMO_2$). The metals and lithium are located in alternating planes between oxygen layers. The metal M can for example be Co, Ni or Mn or combinations of the three. Lithium is found in 2D layers in the material. Courtesy of D. Abraham, ANL.

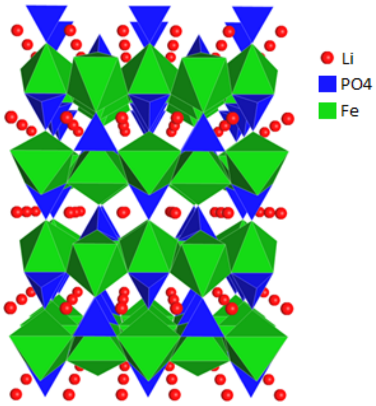

Figure 3.4: Basic olivine structure of the phopho-olivines. M can be Fe, Mn, Ni or Co. Lithium is present in 1D tunnels in the material. Courtesy of D. Abraham, ANL.

for $LiCoO_2$, making them compact and appropriate for low volume applications. One of the main limitations of these materials is not their performance, but rather their need for scarce constituents such as cobalt. In light of this, a continued use of layered oxides without very large recycling might lead to constraints on material availability.

For layered metal oxides, there is also the opportunity to mix the metals used, creating blends of for example Ni, Mn and Co oxides. The use of all three elements is often referred to as NMC, short for NickelManganeseCobalt oxides, and denoted with numbers to explain the relative amounts. NMC ($Li(Ni_{1/3}Mn_{1/3}Co_{1/3})O_2$) is a common variant with equal amounts of Ni, Mn and Co. The use of aluminium in the oxides gives materials like nickel cobalt aluminium oxides (NCA).

Layered metal oxides have not only been used in electronics. NMC is a good alternative for vehicle batteries, and there also exist mixes of layered oxides with for example spinel $LiMnO_2$. This type of oxide does not have the layered structure described above, but rather a stable spinel structure. This type has been discussed for automotive purposes, but will not be further assessed in this thesis. Layered oxides are high energy chemistries, and this must be taken into account when dimensioning for high power, heavy vehicle use.

Phospho-Olivines

Phospho-Olivines with the general formula $LiMPO_4$ (M is Fe, Mn, V Co or Ni) have received increasing attention the past decade. Due to the olivine structure and strong P-O bonds, these materials are structurally stable, and thus also a safer alternative than previous chemistries. The lithium is transported in 1D tunnels in the material, making it sensitive to impurities in these tunnels, see figure 3.4. This places demands on the processing, as high purity of the materials is required. However, acceptable purity can be obtained with current processing methods, as will be discussed in section 3.2.

Another key property of the material type is low conductivity, leading to a need for nano-sizing the material to minimize diffusion lengths for the lithium ions. Often it is also needed to add a conducting material to enhance the electronic conduction. The most common approach to improve electronic conductivity has traditionally been with some kind of carbon coating, added to the material during processing. Future possibilities include replacing this coating with a network of carbon nanotubes or with conducting polymers [Wang & Sun 2012].

In this thesis two types of phospho-olivine cathode active materials will be assessed, $LiFePO_4$ (LFP) and $LiMnPO_4$ (LMP). The other two alternatives involving Co and Ni present higher potentials, making them interesting, but adding the need for a new electrolyte with larger voltage window. Additionally, the use of Fe and Mn gives the opportunity to reduce the scarcity problems associated with Co and Ni, present in the layered metal oxides.

Compared to the layered oxides the olivine types have one further drawback in that they have a lower density. This impacts the volume of material needed in a battery, which may be a weakness, especially in smaller vehicles where space is scarce. LFP and LMP have densities of $3.6\,{}^{g}\!/_{cm^3}$ and $3.4\,{}^{g}\!/_{cm^3}$ respectively [Nelson et al. 2011].

LFP has emerged as an interesting candidate for larger energy storage systems for automotive applications. Its main attribute of interest is the improved safety compared to layered oxides, an important factor in vehicles. LFP batteries can also provide a rather high gravimetric power density and are thus applicable to heavy vehicles. However, the electronic conductivity of LFP is only $10^{-9}\,\mathrm{S/cm}$, and this will lead to a need for nano-sizing. LFP has a potential of 3.2-3.3 V versus lithium and theoretical capacity of $166\,\mathrm{mAh/g}$, where $150\,\mathrm{mAh/g}$ is commonly realized in commercial cells [Daniel & Besenhard 2012].

As a contrast to LFP, which is already in production, LMP is under development, and is interesting due to its higher potential of 4.1-4.2 V versus lithium. This gives the opportunity for higher specific power and energy, but also for coupling to new higher voltage anodes. As with LFP the materials involved are non-toxic and reasonably priced. The potential is also acceptable while using common electrolytes as it is below the 4.7 V HOMO of $LiPF_6$ in EC/DMC.

However, LMP shows even worse electronic conductivity than LFP due to a larger band gap, the conductivity only reaches $10^{-14}S/cm$. This may place even higher demands on the production, and may require demanding nano-scaling processes [Martha, Markovsky, Grinblat, Gofer, Haik, Zinigrad, Aurbach, Drezen, Wang, Deghenghi et al. 2009].

LMP has a theoretical capacity of $170\,\mathrm{mAh/g}$, and a capacity of $140\,\mathrm{mAh/g}$ has been achieved during several cycles [Martha et al. 2009]. This indicated that there is potential for these materials, and the possibility of achieving the same stable capacity as LFP. At the moment, this capacity has not been realized for longer cycling, but will serve as an assumed reference for the material during evaluation. If the low intrinsic conductivity of LMP turns out to be too limiting, it is still interesting to evaluate, since a mix of LFP and LMP could be possible to enhance the voltage.

Due to its higher potential compared to LFP, LMP could be a future candidate for automotive purposes. It has the same potential benefits, but could deliver longer life (coupled with a high potential anode) or better power and energy.

Silicates

Silicates are a group of cathode active material for Li-ion batteries that present an interesting evolution to the phospho-olivines. Using Li_2MSiO_4 (M= Fe, Co and Mn) gives similar structural stability due to strong Si-O bonds, but with an additional lithium ion available in the structure. This doubles the theoretical capacity to around $333\,\mathrm{mAh/g}$ [Daniel & Besenhard 2012]. In addition, the material also does not incorporate any of the previously questionable materials in lithium ion batteries, such as cobalt or nickel. Instead it uses the very abundant Si, and if matched with a common metal such as Fe or Mn it is appealing option from a materials sustainability point of view.

One example of this group of materials is Li_2FeSiO_4 (LFS). This is an especially interesting material alternative, as both iron and silicon are such abundant materials. This could decrease the problems associated with using scarce materials while maintaining good stability and performance. Intrinsically LFS does however have low conductivity, around $6 \cdot 10^{-14}\,{}^{S}/_{cm}$, which might put even higher demands on the particle size and need for conductive additives compared to for example LFP. The density is also low, around $1.3\,{}^{g}/_{cm^3}$ when calculated from the unit cell size [Nytén, Abouimrane, Armand, Gustafsson & Thomas 2005], resulting in low volumetric energy and power densities.

Using this new cathode active material might lead to the need for another electrolyte salt, such as LiTFSI [Nytén et al. 2005]. This is due to the risk of reaction between the $LiPF_6$ salt and the fluorophilic Si. However, since the main attributes of this electrolyte is close to that of our previously presented electrolyte this factor will not be taken into further consideration in this thesis.

Although it is possible to extract two lithium ions from LFS, the material has only been proven to provide capacities around $140\,{}^{mAh}/_{g}$, closer to the theoretical capacity when only one lithium ion is free for transport. The reason for this is that currently only the $Fe^{2+/3+}$ redox reaction has been shown to take place at room temperature. However, it still holds the future possibility that a well-developed LFS cell could perform around $300\,{}^{mAh}/_{g}$ if all the lithium is used, based on the theoretical capacity.

It has been shown that the capacity of the first cycle is close to 160mAh/g, but that it decreases after a few cycles. A similar change can be seen in the potential which changes from initial 3.1 V to 2.85 V in following cycles. This indicates that a structure change might be occurring during the first cycles [Islam, Dominko, Masquelier, Sirisopanaporn, Armstrong & Bruce 2011]. Practically, a capacity of only around $85\,{}^{mAh}/_{g}$ can be assumed at present [Chen 2013]. Further investigation of the changes occurring in the material during cycling, and the parameters influencing the redox reactions will be necessary to fully evaluate the potential of LFS.

It is clear that LFS faces many obstacles before it can be realized as a viable electrode active material. However, since it potentially presents an intrinsic improvement compared to LFP, it is an interesting material to evaluate. The low density is, however, a problem for some small scale applications. In large scale vehicles the chemistry might be more interesting, especially if the volume constraints are not too severe.

3.1.3 Lithium-ion battery anode active materials

The first alternative for anodes in Li-ion batteries was lithium metal. The difficulties arising from using this material are, however, quite large and other anodes were developed to solve these issues. Although lithium has a high specific capacity of $3860\,{}^{mAh}/_{g}$, it is plagued by dendrite formation when cycling and by its inherent reactivity [Daniel & Besenhard 2012]. Today, the most common anode in Li-ion batteries is graphite. A viable alternative for high potential cathodes is the use of $Li_4Ti_5O_{12}$ (LTO), which will be discussed below.

Graphite anodes

Different kinds of carbon materials are possible as anodes for Li-ion batteries. Graphite has a unique structure with separate sheets of carbon in a hexagonal lattice. The bond between the carbon atoms in the lattice are covalent bonds involving three of the four valance atoms, but the interplanar bonds are weak van der Waals bonds. This results in good possibilities for storing Li-ions as they are intercalated between the planes of the graphite. The fourth valence atom is free, and gives graphite its conductive properties, thus making it appropriate as electrode active material. Lithiated graphite is stable up to LiC$_6$, giving it a theoretical capacity of 372 mAh/g, where 330 mAh/g is readily realized after initial cycling [Daniel & Besenhard 2012]. The density is around 2.24 g/cm^3 if battery grade graphite is used [Nelson et al. 2011].

One drawback of the graphite as anode for Li-ion batteries is that it has a slightly too low potential (0.1-0.2 V potential versus lithium) compared to common electrolytes LUMO, resulting in a reaction between the electrolyte and the anode. This is mitigated by the solid electrolyte interphase layer, the SEI layer, produced during the first cycle. Having a stable SEI is necessary when using a carbon anode, and is thus an inherent limitation. Having EC in the electrolyte mix helps the creation of a passivating SEI and hinders further reaction [Goodenough & Kim 2009].

LTO anodes

LTO is an anode match for high potential cathodes and it has been explored during several years. One of its main advantages is a prolonged life-time. This is due to LTO having almost no expansion upon lithiation. An LFP cathode coupled with LTO can last up to 10000 deep cycles, compared to 3000 deep cycles when coupled to graphite [Kushnir & Sandén 2011].

Another improvement compared to graphite is that there is no formation of a SEI, and no need for one, since LTO has a higher potential and does not react with the electrolyte. This gives the opportunity for faster charge/discharge, since one limiting step is removed. The potential is 1.5 V versus lithium [Nelson et al. 2011].

In general LTO itself provides faster charge/discharge times compared to graphite, at least if the diffusion lengths in the material are not too long. That means that the material needs to be of nano-size for optimal performance. As a last benefit LTO can also function in a larger temperature range than graphite, allowing comparably fast and safe use at -50 $^{\circ}C$ to 75 $^{\circ}C$. However, LTO has lower capacity than graphite, 170 mAh/g is a reasonable result for this material [Nelson et al. 2011].

Of course there is also a price to pay for the benefits of LTO. Due to the higher potential, the material puts limits on what cathodes are reasonable. The anode needs to be coupled with high potential cathodes in order not to decrease the open circuit voltage (OCV) too much. LTO also has worse electronic conductivity than carbon based anodes, and thus needs nano-sizing for optimal performance. The weight of the material may also be a limitation, especially for automotive purposes. However, the density of LTO is 3.4 g/cm^3 compared to graphite's 2.24 g/cm^3, making LTO volumetrically more beneficial [Nelson et al. 2011].

A common choice of cathode to couple with LTO is the spinel lithium manganese oxide (LMO), but in light of some of the future cathode active materials investigated in this thesis LMP is also a viable candidate due to its high potential.

Future anodes

The main goal when looking for future anode active materials is to find a material with better energy and power gravimetric densities. The best current anode is graphite with 372mAh/g as theoretical maximum capacity. Silicon and tin based materials could be one opportunity to improve the capacity. Transition metal oxides are a possible alternative, although they suffer from a problematic voltage hysteresis during charge and discharge [Chen 2013]. Silicon based materials will be discussed in some greater detail below, and will act as representative of future anodes with greatly improved capacity, but currently with stability issues.

Pure silicon has a theoretical capacity of 4200 mAh/g, but the volume expansion during charge is up to 400% [Chen 2013]. Due to this, the initially high capacity is quickly reduced when the materials is cycled. The expansion does not only damage the material, but also breaks the SEI causing reactions between the electrolyte and anode that can be both dangerous and deteriorating. There are, however, possible solutions to volume expansions of this magnitude in electrode active materials.

One alternative is to nano-structure or nano-size the material. The volume expansion for each particle can then be fit into the increased amount of free space present between the particles [Chen 2013]. Another alternative is to have the silicon in a porous structure of some more stable materials like carbon, thus dividing the roles of the electrode active material between two materials, one for reaction and one for stability. Porous carbon silicon composites leave space for the expansion of the silicon, but the added material does of course penalize the weight. Silicon is only one interesting candidate, but it highlights the problems of large expansion that need to be overcome for the materials to work in applications.

3.1.4 Novel cell types

Lithium-ion batteries with intercalation electrodes may be a dominating player on the rechargeable battery market at the moment, however, other alternatives exist. This section discusses the concept of lithium-sulfur batteries, sodium-ion batteries and also organic batteries, representing new approaches.

Lithium-Sulfur

Lithium sulfur (Li-S) batteries are a modified approach to Li-ion batteries as they do not contain any metals besides lithium and uses a cathode of only sulfur. Li-S uses no excess materials to create a stable crystal structure, like for example Fe, Ni, Co and Mn in LFP or NMC. This makes it cheap, light and environmentally sustainable. Due to its weight the capacity can be very high, up to 1675 $^{\mathrm{mAh}}/_{\mathrm{g}}$ [Ji & Nazar 2010], and this could compensate the low potential of 2.15 V. The anode is often metallic lithium, which causes problems due to reactivity. Other anode types have not been proven to give good performance [Daniel & Besenhard 2012].

Li-S batteries have not, to date, been realized in a way that would make them applicable for automotive purposes in the near future. However, since they present such an appealing environmental alternative, work continues to reach a viable Li-S battery in the future. The main issue is the poor cyclability. When running a Li-S cell soluble polysulfides are generated during the reduction steps. These compounds diffuse trough the electrolyte due to the concentration gradient. At the anode they react to form lower order polysulfides, creating a new concentration gradient and diffusion back to the cathode were they oxidize back to their original form. This phenomena is called a shuttle mechanism and decreases the capacity of the cell as well as causes high self-discharge [Ji & Nazar 2010]. If at some point the sulfides are fully reduced (Li_2S), they act as an insulator, possibly passivating both the anode and cathode [Barchasz, Leprêtre, Alloin & Patoux 2012].

Li-S batteries are also limited by the insulating nature of sulfur and lithium sulfide. To increase rate capability and electrical properties the cathode active material needs to be placed in a structure of conducting carbon or possibly even metals.

Na-ion batteries

One issue with the Li-ion batteries is the cost, and possible scarcity issues of lithium. Sodium-ion batteries (Na-ion) are a possible solution to this problem, since sodium is abundant, and has similar properties to lithium. Sodium also comes at a lower cost than lithium, an important factor in the search for a cost effective energy storage system. It also has a reasonable potential around 2.5-3 V [Ellis & Nazar 2012], and good theoretical capacity around 150 $^{\mathrm{mAh}}/_{\mathrm{g}}$.

Focusing on the automotive industry Na-ion, however, has one large drawback, its weight. Due to it being a heavier element, and with its lower potential, the Na-ion battery has lower gravimetric density than a comparable Li-ion chemistry. However, sodium is becoming a viable candidate in light of the increasing need for cheap battery material [Ellis & Nazar 2012]. This is especially true for large volume applications where the weight of Na can be compensated by its price.

Different types of Na-ion batteries exist, much like for Li-ion. Examples of cathode active materials are sodium manganese oxides and sodium iron phosphates, reminiscent to their Li-ion counterparts. The basics of the structures are similar, but due to the larger size of sodium the most effective structure may differ. As an example of performance, olivine $NaFePO_4$ (comparable to the $LiFePO_4$) has a theoretical capacity of $154\,\mathrm{mAh}/\mathrm{g}$ [Palomares, Serras, Villaluenga, Hueso, Carretero-González & Rojo 2012].

Organic batteries

The term 'organic battery' covers a wide range of different battery types, from batteries where each component is organic, to Li-ion batteries with organic electrode active materials. Generally the point is to reduce the impact of materials processing, simplify and improve recycling and reduce the amount of toxic components in the batteries.

Fully organic batteries rely on a redox-active organic compound to constitute both electrodes. The materials also need to be active when paired together as anode and cathode, a demand that has limited the amount of possible materials [Zhu, Lei, Cao, Ai & Yang 2013]. The idea has however been realized with, for example, n- and p-doped radical polymers. The huge drawback with these batteries at the moment is that they have a very low specific energy due to low potentials and limited energy storage. The concept is interesting, but work on finding and developing materials that will be stable as electrodes and produce high enough voltages is still in an early stage. Both the gravimetric and volumetric energy density needs to undergo much development before these materials are considerable for any purpose, let alone automotive.

A way of incorporating organic materials that is closer to realization is to use organic electrodes for a Li-ion battery. Organic electrodes for lithium ion batteries is not a new idea, but due the fast development and success of inorganic cathodes such as layered oxides and phospho-olivines they received less attention during the 90-ies and in the beginning of this century. However, since these inorganic materials are reaching the limit of performance progress, organic electrode active materials are again more interesting. Organic based electrodes do not only present a possibly well performing material with capacities usually over $400\,\mathrm{mAh}/\mathrm{g}$ [Liang, Tao & Chen 2012], they are also interesting due to their potential environmental friendliness; they do not incorporate scarce metals, do not require high temperatures or milling to achieve good crystal properties, and their energy and materials impacts are low. In addition, these factors make them potentially less expensive and non-toxic.

There are a variety of organic electrode alternatives for Li-ion batteries such as; organosulfur compounds, organic free radical compounds or carbonyl compound to mention a few groups. The main challenge for all types is to achieve good specific energy and power while maintaining cycling stability, but a universal answer is hard to find since many different materials are being tested. Therefor organic electrodes will become possible candidates first when more work has been conducted to find fewer and more effective candidates, and these candidates have been evaluated and improved. The structure and ion transport in the materials needs to be further understood [Liang et al. 2012]. For automotive purposes it is also important that the new electrodes have sufficient stability to ensure safety.

3.1.5 Environmental impact of battery constituents

Any kind of switch from fossil based fuels to other technologies should be accompanied with a discussion about the potential for material scarcity and environmental impacts of the new technology, due to the large scale of the transportation sector. It is important to be aware of how long the resources needed for a new technology may last, and how much environmental impact the use of these materials will have, both now and in the future. Achieving good insight into the possible limitation of new technologies is, however, easier said than done.

Assessing all possible scenarios for future improvements, market sizes and material choices is impossible. None the less, no matter how many uncertainties exist concerning the future supply and impact of using different materials, it is still important to prepare and evaluate as many scenarios as possible. Having evaluated different effects that might come from changes in supply and price helps guard against unwanted backlashes that may come when the technology becomes more widely used. This thesis will not evaluate different scenarios, but a short summary of some current assessments of the material resources available for vehicle batteries is presented. This information will provide a base for discussion of the advantages and disadvantages that might arise in the future from using different chemistries.

Lithium

The impact and scarcity of using lithium is an important factor to consider if Li-ion batteries are to be used as ESS in an expanding market of electric vehicles, because lithium is ultimately the only material that cannot be substituted. Opinions vary concerning if and when (and for which actors) a lithium shortage may occur. The critical factor will most likely be the rate at which lithium can be extracted, and if this rate can keep up with the rate with which electrified vehicles increase [Andersson & Råde 2001]. If not, the extraction rate will be the factor that limits the spread of electrified vehicles.

It is interesting to notice that all assessments of lithium resources assume that used batteries will be recycled for lithium, yet this assumption may prove to be difficult to fulfill [Kushnir & Sanden 2012]. At the moment, the lithium stock available in used batteries is small compared to the potential future demand. The future need for recycling is, however, an interesting point, since recycling today is not well developed for lithium. The state of recycling will be discussed in section 3.5.

Geographical location of the lithium resources is another potential problem for large scale use of lithium based batteries. At present, Chile is the dominating producer of lithium. In the same region Bolivia has smaller production, but large reserves. China and the USA also have opportunities for rather large production, however, their reserves come nowhere near those of Chile [Gaines, Nelson et al. 2009]. However, the lithium production in the world is not limited to the above mentioned countries. The U.S. import is a good example; their prime suppliers are in order Russia, Norway, China, Canada, Finland, Zambia, Belgium, Australia, Brazil and Morocco [Gaines et al. 2009].

Nevertheless, the fact that such a large portion of the world's lithium reserves lies in such a small geographical area as Chile and Bolivia could become a problem if the use of electrified vehicles expands greatly. In this case the need for lithium will be very large and all reserves will need to be accessible. The limitation of having few and localized producers may lead to many other political consequences. Assessing these are of great interest, but will not be further covered here. The use of lithium as a key component in future propulsion technologies will however imply a need to evaluate these questions further, and partly motivates the discussion on recycling in this thesis.

Cobalt, nickel and manganese

Cobalt, nickel and manganese represent the possible metal components in layered metal oxide cathodes. Cobalt, and to a lesser degree nickel are scarce and valuable, and thus represent a potential limitation for chemistries based on oxides with these elements. Manganese is less scarce than the other two elements. Gaines et al. [2009] estimates a reserve availability of 5200 million tons, compared to cobalt's 13 million and nickel's 150 million tons. One electric car would roughly need 30 kg of cobalt or nickel, and for a $LiCoO_2$ battery this would mean the supply would sustain 450 million vehicles [Andersson & Råde 2001]. This should be viewed in light of the total worldwide sales of 81.7 million vehicles during 2012 [OICA - International Organization of Motor Vehicle Manufacturers 2013]. With ever increasing sales, and a larger and larger part of these vehicles being electric, this would mean a fast depletion of the reserves. Using NMC with only a third of the amount of cobalt would imply an increased amount of vehicles, but no long term viability. Larger batteries with more active material could also increase the material consumption.

Cobalt and nickel are limiting factors if chemistries with large amounts of these elements are used [Andersson & Råde 2001]. However, these elements are also the only ones that are successfully being recycled at the moment, due to their high value. With the factors of value and recovery in mind, the use of these more scarce materials can be possible, at least for a prolonged period of time. It is safe to say that the risks of using cobalt and nickel have sparked the search for more sustainable materials choices.

Other common battery materials

The remaining battery components can be made of a wide range of different materials. However, some materials are more common than others. Aluminum and copper are the most common current collectors. Titanium and graphite are present in common anodes and iron and phosphorous in the common LFP chemistry. None of these have the scarcity issues of the above mentioned metals. Copper can be expensive, but has a good recycling chain, and more than 40% of total world copper demand is met by using recycled copper [BIR - Bureau of International Recycling 2013]. For aluminium this number is more than 33%, and for both metals it is less energy intense to recycle than to extract virgin material.

It can be concluded that recycling is of great importance, if a large fleet of electrified vehicles is the target. Lithium is a key resource, and the supply needs to be ensured for a future case with a much larger stock present in used batteries. Nickel and cobalt based alternatives will never be viable on a long time scale, but much less so without recycling.

3.2 Materials manufacturing

The processing and production of different materials is an important factor to consider when choosing chemistry and evaluating the environmental impact. The processes chosen can be tweaked and modified in almost every step to suit the material being processed. Several process methods that are inherently different also exist for most materials. 'Dry' processes involve high temperatures to synthesize the material, relying of simple mixing and heating of the precursors. 'Wet' methods instead use low temperatures, but have a need for chemicals or solvents. These methods will be presented in more detail in this section.

The methods place different burdens on the life cycle and are appropriate for different materials and precursors. They also provide different opportunities when it comes to nano-sizing the materials. With dry production methods there is a need for energy intense milling if small sizes are desired. Wet methods on the other hand, can produce nano-sized materials directly during synthesis.

Dry synthesis active material production

As mentioned, dry synthesis methods are synthesis routes where the precursors are heated to high temperatures in order to obtain reaction and good material properties. Solid state synthesis is one of the most commonly used synthesis methods to date and simply uses different heating and mixing steps. Microwave heating is an interesting alternative dry synthesis route. Here the precursors are heated with microwaves to achieve a uniform heating in short time [Jugović & Uskoković 2009].

The solid state synthesis will be the dry synthesis route of choice for the purpose of this thesis, since it is rather straight forward. The precursors are simply mixed and then sintered for a varying number of hours until the desired crystallinity is reached. The temperatures and sintering times can vary with the active material being produced.

Solid-state synthesis of phospho-olivines and silicates is possible. Besides the sintering, a milling step is however required to achieve the nm size needed for these materials. The precursors for producing LFP and LMP via sold-state synthesis are stoichiometric amount of iron or manganese salts like iron-oxalate, lithium in the form of for example LiOH and a phosphorous source, most commonly ammonium phosphate [Jugović & Uskoković 2009]. For LFS the precursors can be similar as for LFP, but silica is used instead of ammonium phosphate [Huang, Li, Wang, Pan, Qu & Yu 2010].

Solid-state synthesis is commonly used for layered metal oxide cathodes like NMC. Since there is no need for nano-sizing, the process provides sufficiently performing material without having to include the energy intense milling step. Possible precursors for this synthesis route are LiOH with metal sources from Ni, Mn and Co oxides [Wang, Sun, Chen & Huang 2004].

Wet synthesis active material production

Wet synthesis methods are a group of methods based on treating precursors in water solution. By dissolving the precursors, opportunity to achieve better homogeneity and control of particle size is achieved. Examples of wet processes are hydrothermal, sol-gel and co-precipitation synthesis. Hydrothermal will be the wet process assessed in this thesis, since it is cheap, possibly low-energy and has been shown to provide Li-ion cathode active material with good properties. The main approach for hydrothermal synthesis is to dissolve the precursors in water. The solution is then heated for a varying number of hours, depending in the material being produced. Next, the reacted material is filtered from the solution and dried. Finally the material is heat treated in order to obtain the desired crystallinity.

A few factors have been shown to contribute to material performance if using hydrothermal synthesis for the phospho-olivines and silicates. It has been shown that the temperature cannot be too low if good results are to be achieved with the processed material. Below $175\,°C$ the metal disorder can reach 8% [Chen, Wang & Whittingham 2007], meaning that 8% of the iron in LFP is located in the lithium diffusion channels which strongly hinders the performance of the material. Apart from this demand there is also a need to stop the unwanted oxidation of ferrous to ferric iron, which readily occurs in water if no reductive agent is added. An example of such an additive to hinder oxidation is sugar.

The precursors for hydrothermal synthesis of LFP and LMP are LiOH, H_3PO_4 and $FeSO_4$ or $MnSO_4$, and these will be used in this thesis, although others are possible. For LFS precursors for wet synthesis such as LiOH, SiO_2 and $H_8Cl_2FeO_4$ have been explored [Dominko, Bele, Gaberscek, Meden, Remskar & Jamnik 2006].

Hydrothermal synthesis of NMC is perhaps not as beneficial as for LFP and other materials needing nano-sizing. However, hydrothermal synthesis is possible and may be beneficial if the total energy-use can be reduced. Generally the process starts from LiOH and $Ni_{1/3}Mn_{1/3}Co_{1/3}(OH)_2$. The metal hydroxide is prepared from $NiSO_4$, $CoSO_4$, $MnSO_4$ and NaOH. In this stage a chelating agent is needed as well, since this prevent the formation of unwanted single metal hydrides like $Co(OH)_2$ [Lee, Kang, Myung & Sun 2004].

Anode active material production

Graphite anode production methods are not similar to the cathode methods, since the material is so different in nature. Battery grade graphite has higher requirements placed on it than normal graphite. Therefore the graphite is usually baked, so as to remove any oxygen impurities [Majeau-Bettez, Hawkins & Strømman 2011].

LTO on the other hand can be produced in similar ways to the cathode active materials. However, there mainly exists one method, used by the company Altair [Verhulst, Sabacky, Spitler & Prochazka 2003*a*]. They make use of a hydrolysis step followed by calcining, wet milling and drying. As opposed to the nano-cathode active materials, the size of the LTO achieved with hydrothermal synthesis is not adequate, since LTO requires a particle size of down to 20 nm. This makes production of LTO very energy intense since it requires both milling and hydrothermal synthesis.

Carbon coating

Some of the materials of interest need conductive coating to perform well. In these cases a carbon coating step needs to be incorporated into the process, and this can be done in several ways. In general the coating can be added ex situ, after the active material is produced, or in situ by mixing the carbon additive with the precursors before reacting. Examples of additives are sugars, pure carbon like acetylene black or conductive carbons like carbon nanotubes [Chen et al. 2007].

If the carbon is added after the material is produced the coating can be formed by a milling and sintering step[Konarova & Taniguchi 2009], or other mixing and heating alternative. This is often the alternative chosen for solid-state synthesis routes. A risk is that the heating step needed to achieve conductive carbon negatively affects the particle size [Li & Zhou 2012]. For hydrothermal synthesis the in situ addition of carbon additive to the precursor solution can provide a way to incorporate the additive on a smaller scale, thus giving a better distribution of the coating over the particles and less risk for particle growth due to heating.

3.3 ESS design

The technical design of the ESS have many criteria to satisfy, as discussed briefly in section 1.6. Firstly there are the most fundamental ones of voltage, pack energy capacity, power output and allowance of different discharge rates. Then follows constraints on the safety, controllability, volume, dimension, weight, physical robustness, opportunity to diagnose, cost and life length. From a manufacturing point of view, the ESS should be easy to mount and to disassembly. Adding to this the possible environmental constrains makes the task to find an optimum design quite complex. However, the environmental aspects enter in only a few on the design criteria. These are the construction- competing with robustness, safety, and costs - the weight, and the choice of materials - competing with costs. Further on the design of the ESS can be made compatible with a number of organizational options of use. Depending on the economics, the use of the same ESS could be promoted in different applications, some components could be dismantled and used again, and the ESS could be sold to another organization with other uses than the automotive. These aspects are secondary, but equally important in the choice of ESS design, adding extra requirements to the original set up of limits and constraints.

Interoperability

Since the battery prices are important for the growth of the xEV fleet it is of high interest to see what solutions there are for cost reductions and what could be the environmental impacts related to those measures. The standardization of components will be an important step towards cheaper battery packs and for this a large production volume is needed. To achieve this many different applications could go together in using the same product, in a so called interoperability.

The system level of future interoperability has many question marks. It could be that either pack, modules, cells or specific components of the pack such as the housings and electronics are designed in common to suit various different applications. With the highly varying requirements for different types of battery applications [Eyer & Corey 2010] it may be difficult to perform interoperability on a cell level or of a complete module unit due to the varying chemistry related properties. If instead different cell types could be fit in the same standard module and pack housings and electronics, some reduction in manufacturing costs could be possible. The component dimensions and volumes will then be parameters related to environmental impacts. Even in case the cell chemistry could be kept the same, the connections between the cells could need to be different to suit different voltage requirements from the applications. For interoperability of complete packs, there may be a need for using a multiple of one common pack size to satisfy different applications. To make an example of interoperability the choice is made to use a PHEV car as an additional application that the PHEV bus module unit should be designed according to. In this thesis the changes in materials and components when design measures are taken to perform interoperability on a battery pack or module will be accounted for in the environmental impact assessment.

3.3.1 Pack manufacturing

The manufacturing of the pack is made in two distinct steps; the first consisting of the module assembly, in which cells are connected and inserted into the module, and the second similarly consisting of the insertion and interconnection of the modules into the pack housing. These two steps are the last in a chain of processes from extraction of materials to the shaping of the pack components and assembly leading to the final product. Different designs can be better or worse from an environmental and economic point of view. To find out if and how economic and environmental aspects can be joined, a comparison between the most costly processes and the most environmentally demanding processes needs to be done. In the same way the most cost efficient and environmentally efficient pack design options may be compared.

An environmentally beneficial pack design contains materials of low process energy and of high availability in the earth crust. From an economical point of view the pack should also contain cost efficient components and materials. These materials could potentially conflict with the need to minimize time, and the complexity of the actions needed to include these cost reducing materials in the manufacturing stage. All these three materials factors - environmental, cost and simply manufacturing - have to be balanced in the quest for an environmentally efficient pack design, since one of the big barriers for a larger introduction of lithium ion batteries is the high costs.

For some components in the pack - copper and electronics - both the environmental and the economic costs are high. For other components such as housings as steel, plastics and aluminium, the environmental aspects and the costs may promote different optimal solutions [Ashby 2012]. The common and secure factor of both cost and environmental load is at present the energy in terms of fueling different processes and the energy needed for transport and use phase. The costs related to the pack production can be allocated to purchased items and materials, and to the man hours needed for the assembly.

From an environmental point of view, the most energy intense processes are found in the materials extraction and production of metals. In contrast, the energy need for assembly of different components into a product is smaller in comparison. The comparison between cost and environmental impact is, however, only valid in an instantaneous perspective. As it is derived from the intrinsic value of nature resources, the environmental impact has the property

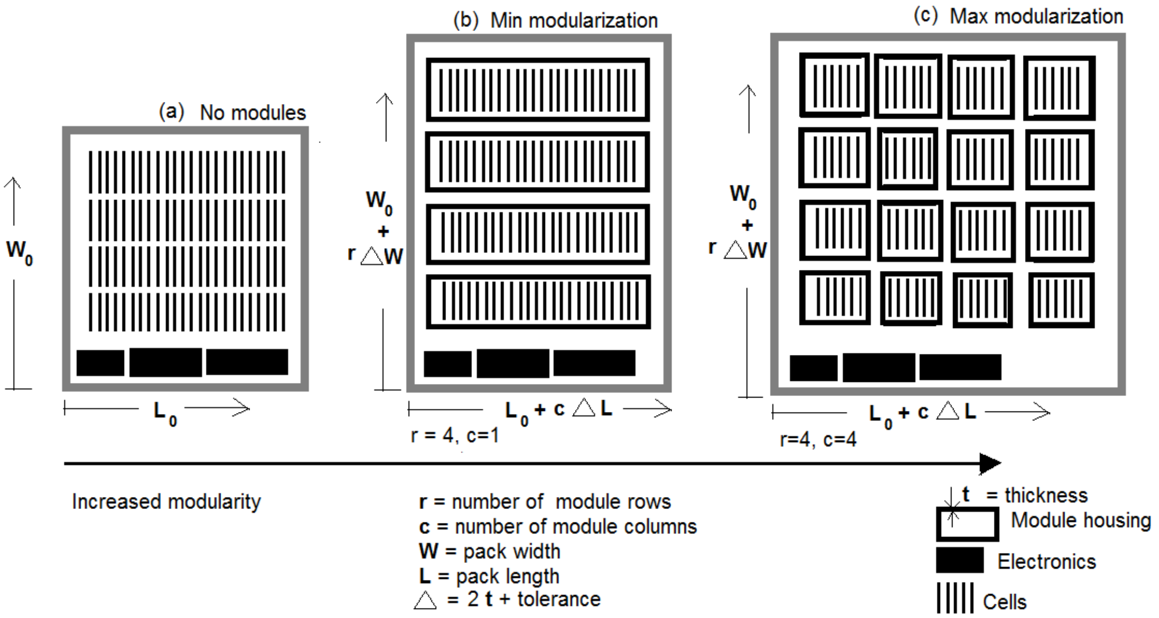

Figure 3.5: The battery pack modularization, a) no containing module walls, b) minimum modularization, cell string row included in module, c) maximum modularization, 1-4 cells contained in module.

of independence from the world market forces, and will thus be the same no matter fluctuating material prices.

3.3.2 Modular design

A topic investigated more closely in the battery pack design is the modularity and its implications on the ESS design parameters. The choice of using modularity in the pack is due some different reasons, all depending mainly on controllability and safety, but secondary effects on other parameters are many. Modularity as a design approach is illustrated in figure 3.5 where the impacts of added interfaces are made visible.

The economic reasons for modularity can be derived from the concepts of production volume, reuse and remanufacturing. Ultimately, the benefits of modularization are that defect units can be detected and exchanged without need to change the whole system. Second life applications may be favored since the remanufacture is facilitated, (suitable units may be extracted and used again), and standardization of modules and packs may reduce the long term manufacturing costs.

Modularization advantages and drawbacks

The disadvantage of modularization is that it requires more passive material and thus increased weight and cost both at module and pack level. The increased amount of material is needed for connecting and protecting the cells. A scaled up modularization leads, in particular, to increased total module surface with a corresponding increase in number of electric interconnections and container walls. To conclude, the simple rule is; the smaller the modules, the higher the proportion of passive materials will be, and the lower the gravimetric energy density.

If smaller modules are the key to higher production volumes and cost reduction, the positive impact from electrified vehicles will be damped from the higher rates of materials used. The significance of the impact of increased passive materials should be analyzed. To do so, the passive materials must be defined in detail, and the possible amounts used for different types of modularization assessed.

The following list will describe the driving forces for increased subdivision in modules (modular scale-down):

- Standardization (smaller units suit a wide range of applications when assembled).
- Decreased module unit costs from increased production volume.
- Increased control possibilities and diagnose precision.
- Lower voltage per module, more safety.
- Facilitating remanufacturing and second use (switching modules).
- Standardization leading to cost reduction and increasing xEV use.

In contrast to there are also driving forces for decreased subdivision in modules (modular scale-up):

- Decreased weight from module interface walls and interconnects.
- Decreased energy consumption during driving due to battery pack weight.
- Decreased embodied energy from module and pack housing materials.
- Less parts to assembly in battery pack meaning decreased assembly cost.
- Marginally less battery pack housing materials needed.
- Minimize losses from resistances in module interconnects (Voltage drop).
- Less complicated cooling circuitry needed.

Module dimensioning coupled to voltage constraints

The best size of the module depends on various constraints that should be respected. The maximum voltage, for example, limits the number of cells in series contained within one module in order to guarantee safe handling. Additionally, other voltage limits to respect are those of the vehicle. For the bus, 500-730 V is the nominal pack voltage range [1], [Volvo Buses 2013*b*]. For the PHEV car, lower voltages are required, for this thesis assumed to be 200-430 V [1], an example is Volvo V60 plug in hybrid of 400 V [Volvo Cars 2013].

In figure 3.6, the options of pack capacity are visualized together with the required connection types and the number of cells for the PHEV bus, given the voltage limits. If interoperability between a bus and a car is wanted for reasons previously described in section 3.3, the module will most likely need to have flexible connection types. Making an example of interoperability between a bus and a car with a NMC pack of30-60 kWh, respectively 5-15 kWh, the smaller car pack would require cells in series connection or two cells in parallel connection in order to respect the voltage constrains, while the larger bus pack would require and 3-4 parallel connections to satisfy the voltage criteria. The method for determining possible interoperability can be seen in figure 3.7. It should be noted that the capacities in this figure are indicative, assuming no losses in the system, and that the focus is set on the voltages. The real cases have losses of 4-10% [2] in capacity depending on the amount of connections etc., and for each case a more profound modeling should be done in BatPaC to obtain realistic numbers.

The possibility of interoperability is higher for two packs of similar size, for example 24 kWh and 40 kWh, if they can meet at a an adjusted voltage of for example 480 V, since they could use the same connections, even if the solution is rather unpractical for both applications. The

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[1] Estimate from personal communication with Jens Groot, 2013.

[2] Estimates from calculations in BatPaC

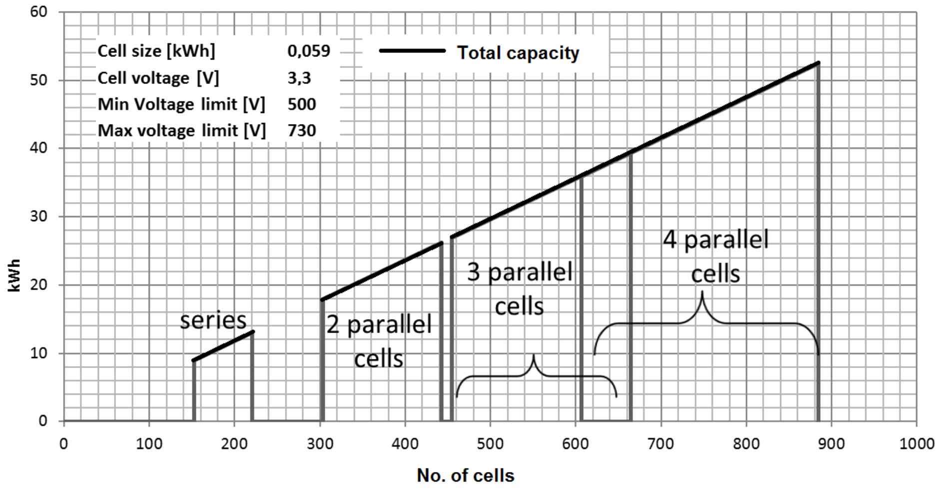

Figure 3.6: The available options of LFP pack capacity in relation to number of cells and parallel connections respecting voltage limits for a bus are illustrated. The method illustrated in the scheme may be used as a guide to determine the possible pack capacities when dimensioning a pack based on a certain cell type, and the connection types needed.

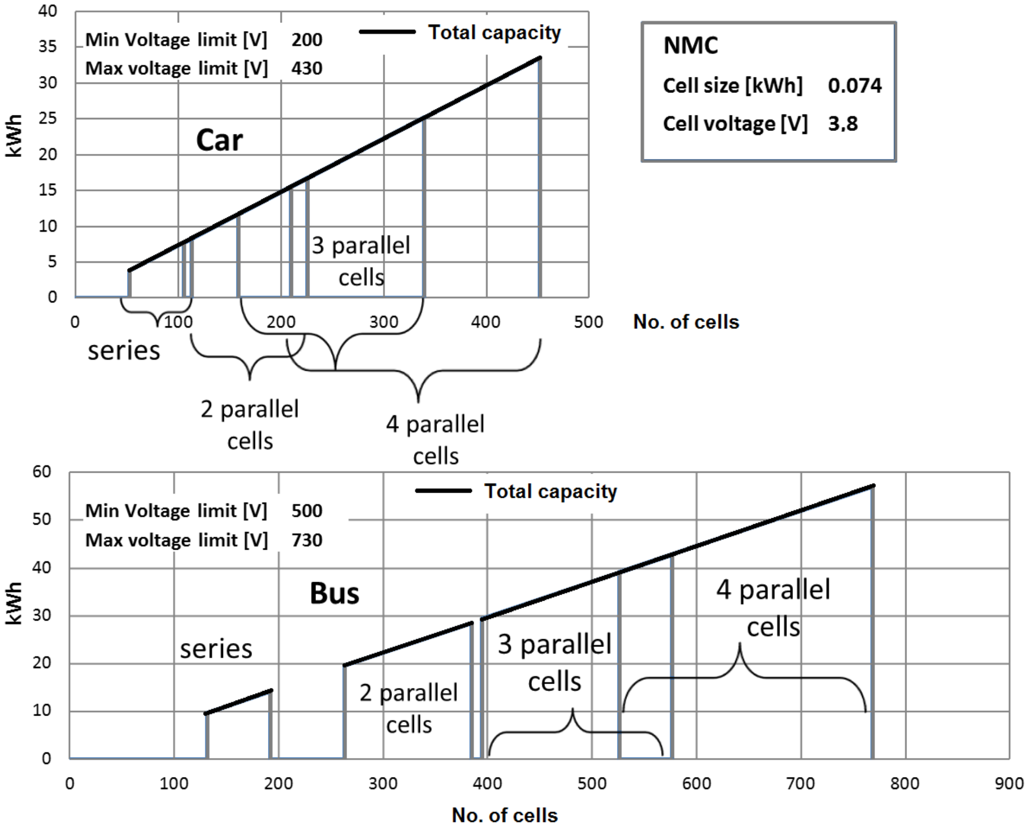

Figure 3.7: The figure shows the NMC pack capacity in relation to number of cells and parallel connections for the voltage constraints of a car and a bus. The scheme can be used for a preliminary overview of possible options of interoperability for module units between bus and car, telling if the same type of connections can be used.

best would be to have interoperability only between units of the same voltage requirements. As a last solution for applications of different voltage criteria, the parallel connection of modules, or module strings could be an option especially when the difference in pack size is high. In this case, the low voltage solution for the small pack can be series connected to a module string which stays within the ranges of the larger pack maximum voltage limits. For example a car pack of 12 kWh, 180 cells and 3 parallel connections could build up a bus pack of 41 kWh and 540 cells, by series connecting three of the car packs. To reach larger capacities this module string can then be multiplied and parallel connected to reach the wanted capacity. An important comment is, however, that the parallel connection on the module string level is expensive and difficult to manage in terms of control and regulation systems. The implications of parallel connections on different system levels are shown in table 3.2.

Table 3.2: The drawbacks and advantages related to different options of system level for parallel connection, see system definitions shown in figure 3.8. * The higher level of parallel connection makes the control units treat higher amount of data, measuring the voltage of each cell comprised within the parallel connected system part.

Parallel Connection Type	**Advantages**	**Drawbacks**
Cell A-A	Less monitoring info for Bus. No constraint on number of modules per string.	Low voltage for car. Difficult to exchange single cells. Complicated welding if 3 cells in parallel. Requires that No. of cells per module is dividable with No. of cells in parallel.
Module B-B	Flexible choice of parallel connection. No constraint on cells per module	More monitoring data for bus*. Requires that No. of modules is dividable with No. of strings in parallel.
Pack C-C	Flexible choice of parallel connection. No constraint on No. of cells per module or No. of modules/string.	More monitoring data for bus. Difficult to respect max voltage constraint and lowest voltage constraint, capacity constraint.

After having defined the voltage ranges, and the capacity of the pack, the same should be done for the module. The modularization has the consequence of adding extra material to the battery pack. One approach is to take the total cells fulfilling the capacity and power criteria of the vehicle and divide them into a certain number of modules in a top down approach. Unfortunately this method sets rather fixed limits on the possibilities of modularization. The exact number of cells will most likely not be kept if both pack dimensional requests and voltage requirements should be satisfied. If instead a bottom up approach is used, the available ranges of defined module sizes, can be built up to the wanted pack. This way of designing the pack, makes sure that the voltage, connection type, and safety properties of the modules are always respected, which further implies that the pack voltage and safety parameters will be fulfilled no matter of the geometry of the pack.

Module dimensioning coupled to control circuitry

The number of cells that can be mounted by a single printed circuit board (PCB) used for BMS and SOC controllers is normally 6 or 12 [Conte 2006]. The control units can be strategically placed in the ESS system. Two possibilities are present, the first, to position the SOC controllers independently from the modular configuration, or the second, to integrate them in the module unit. In the largest module, with an internally placed control unit, the cells per module (CPM) should not exceed 12. However for externally placed control units, the number of CPM is more flexible, but attention should be paid to make efficient use of the PCB since the it is expensive and has high environmental impact.

The choice of independently positioned PCB optimizes the rate of used inputs for all modular designs with a number of CPM different from 12 or 6. In this design, all cells of the pack are monitored by a group of PCB units. For a PCB of 12 connected cells an example of the efficiency of use of the control units is estimated for some different number of CPM (table 3.3). The conclusion is that an independent external control unit gives more efficient use of PCB and gives more freedom in the module dimensioning. The disadvantage of the independent PCB group is that the diagnosis of the single modules is lost at module reuse.

Table 3.3: Example of use rates of PCB depending on cells per module and internal and external placement of the control unit: The externally placed unit is less sensitive to the number of cells per modules for an efficient use, compared to the internally placed PCB.

Cells per module	13	12	11	10	9
Rate of external unused PCB %	3	0	1.8	1.8	0.9
Rate of internal unused PCB %	-	8.3	0	16.7	25
Number of modules	50	54	60	66	74
Total cells	650	648	660	660	666

Table 3.4: Example of modularization effects on module housing: The module housing surface decreases with increasing number of cells per module for the same amount of total cells in a battery pack.

Cells per module	4	6	12	54	216
Module surface (m^2)	16	12	8	4.9	4.3
Number of modules	162	108	54	12	3
Total cells	648	648	648	648	648

Controlling cells in terms of voltage and temperature when divided into smaller subunits is an easier task than to regulate the whole amount of cells in one large chunk [3]. Modularization is consequently a way to reduce the amount of information to treat by each control unit, making the regulation more efficient. Finally, for the simple reason of controlling the cells position some walls are needed around the cells, and from a manufacturing point of view the module unit makes the positioning of the cells in the pack easier.

Modularity impacts on the total material needs

Different module sizes imply different number of interfaces in the pack, and the total surface for the housings will vary according to the module size, considering design choices in which the number of cells is constant within the pack. As a first approach to quantify the modularization impact on the battery, the minimum and maximum cases of modularity should be identified.

As an example, if the minimum module is set to contain a cell group of 4 cells, and the largest to reach a maximum of 60 V (the legal safety limit) with maximum 3 cells in parallel, using LFP cells at 3.3 V per cell would produce a module with $3 \cdot 60/3.3 = 54$ cells. From 4-54 cells could thus be included in one module with internal parallel connection. In case of only a series connection, the number of cells per module should be 18 to stay within the 60 V

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[3] Personal communication with Jens Groot, 2013.

safety limit. Assuming pack dimensions of 0.3 m x 0.5 m x 2 m, and cell dimensions of 160 mm x 230 mm and 8 mm thickness (consistent with cells modeled in this thesis, see section 4.1.1), the surface of the minimum module of 4 cells has a surface of 0.099 m^2 and the maximum of 54 cells has a surface of 0.41 m^2. For a total pack of 648 cells, the smallest module unit results in 16 m^2 surface (162 modules) and the largest module results in 5 m^2 surface. The material needed for the smallest module size of the pack is thus about three times larger than the largest module option. See table 3.4. Assuming copper connects of 40 g each between modules, the total amount copper would differ between 0.5-7.6 kg from the largest to the smallest modules.

For a steel module housing, the difference between the highest and the lowest rate of modularity would equal about 43 kg steel, and between 45 and 360 USD depending on if stainless steel or low alloy steel is used. Counting embodied energy cradle to gate, the difference is of 1400 MJ (low alloy) to 3600 MJ (stainless) [Ashby 2012]. For aluminium the difference would be 15 kg housing, 41 USD and 3700 MJ embodied energy cradle to gate [Ashby 2012]. The aluminium is lighter, cheaper, has a similar energy impact of chromium steel, is stable to corrosion, but has a lower Young's modulus (gives less strength to the construction). Generally, increased Young's modulus implies higher embodied energy [Ashby 2012]. Due to the battery weight related fuel consumption, the aluminium housing is preferable from the environmental aspects.

Pack geometries and material

The battery pack can be built up according to different geometries, to achieve a long pack, prismatic compact pack (cuboid), or cubic final shape. The long pack is suitable in cases when the modules can be series connected in a single row and stay within limits, otherwise the pack will be difficult to connect. The cuboid pack is suitable for relatively large amount of modules, which can be organized in one single layer for easy access. The cubic pack is the least material consuming solution but has the disadvantage of complicated access to certain module units, a problem for assembly and disassembly. The influence of using different layouts can be seen in some examples of a 40 kWh pack in table 3.5.

Table 3.5: Example of module layout configurations effects on pack housing surface. The same number of modules build up a 40 kWh LFP pack of different geometries.

Pack type	**Long pack**	**Cuboid Pack**	**Cuboid Pack**	**Cubic Pack**
Module layout	1x54	2x27	3x18	3x3x6
Pack height [m]	0.23	0.23	0.23	0.69
Pack length [m]	5.18	2.59	1.73	0.58
Pack width [m]	0.16	0.32	0.48	0.48
Pack surface [m^2]	4	3	2.7	2
Module surface [m^2]	8	8	8	8

The pack casing surface can be related to the geometries. For the module size of 12 cells, the dimensions are assumed to be 230 mm height, 160 mm width, 100 mm thick. For 54 modules the different geometries results in a pack surface of between 4 m^2 for the long pack and 2 m^2 for the cubic pack, see table 3.5. The pack surface is in the worst case 50% of the module surface and in the best case 25% of the module surface. The pack volume is 0.191 m^3, and the minimum surface is for the cubic pack geometry 2.01 m^2, quite close to the theoretical surface of a perfect cube 1.99 m^2. This means that even with a prismatic module unit, a quite optimized pack geometry could be achieved from a material point of view.

Safety aspects of modularity

As seen previously the environmental load, and the material costs are high for small modules. None the less, the commercially available Nissan LEAF [U.S. Department of Energy, Energy Efficiency & Renewable Energy, Vehicle Technologies Program 2013] with a 24 kWh pack of 192 total cells, has only 4 cells per module with resulting 0.5 $^{\text{kWh}}/_{\text{module}}$. The reason may not be that small modules increase the ability to build a pack with a precise energy capacity, since there is no evident advantage in comparison to a slightly larger module of for example 8 cells per module and for example 1 $^{\text{kWh}}/_{\text{module}}$. The question is than what other criteria has the priority, and what the driving force to make a small module of 4 cells is.

Since material is both costly and heavy, the reason for this high rate modularity must be safety. To start with, safety is increased through subdivision in modules since any accidental dysfunction or accident leading to leakage, swelling, fire and gaseous emissions is contained within one module and does therefore not spread easily within the whole ESS. The subdivision in modules also helps to regulate the functioning of the system. Smaller cells have less problems with swelling and gas production from the chemical reactions[4]. Another benefit from small cells is that the cooling plates can be integrated at a higher rate in the module, and make the thermal management more efficient. Presumably these gains in safety can outweigh the losses in material mass and energy density for small battery packs.

Organizational implications of modularity

The organizational driving force for modularization is cost reduction, and the organizational requirement is design collaboration so that several applications can be served with the same module unit. This means in practice that other equipment in the drive line may need to be dimensioned to keep the battery module fixed. A critical question is whether the module and drive line should be designed separately or not. This is the cheapest solution and requires standardized interfaces from both vehicle manufacturer and battery manufacturer. It means that a black box approach is used during design by both the battery manufacturer and vehicle manufacturer. The second step of getting a more optimized battery drive line system, is to adapt either the drive line to the battery or the battery to the drive line. The adaptation of the battery pack to the existing drive line, is the present way of doing it. On the other hand if a battery manufacturer can provide low price modules in a few standardized sizes, perhaps the drive line will need to be designed according to the battery. This design choice has implications for the overall efficiency of electric transport and thus for its competitiveness and environmental impact. An additional benefit from an administrative point of view is that cell testing becomes more practical using the modules as smallest units. During module assembly, each cell should be validated; the grouping in modules makes cell testing easier to follow and less time consuming. The administration of the manufacturing is simplified since one module fits in many products, meaning that there are less diversity in the items to account and organize.

3.4 Reuse and second use of energy storage system components

At the end of its ‘first’ lifetime in a vehicle, the ESS can meet different destinies, such as landfill, combustion, reuse, or reengineering/remanufacturing for a ‘second life’ [Ashby 2012]. Ideally, the channel used for each of these treatments should be of similar rate as the end of life flow, and be cost efficient. To use several of these channels in parallel in the end of life of the product,

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[4] Personal communication with Jens Groot, 2013.

may be difficult to accomplish, in order to efficiently match the rate of rejection [Ashby 2012]. The end of a first life can occur for various reasons:

- Physical life - the product breaks down and it is no longer economical to repair or refurbish.
- Functional life - the customer does not any longer need the product.
- Technical life - the competition from other more advanced technology makes the product less attractive on the market.
- Economic life - other products are both more technologically advanced providing the same function at a lower price.
- Legal life - legislation, new standards or directives make the product illegal, and not viable.

In general, the physical life determines the when a battery is rejected; in the future, the economic life and possibly the functional life might be relevant. The physical life is determined by the degrading and ageing of the cyclable cells. There is still no method to reengineer a cell that has been passivated on a material level; the end of the chemical reactions is definitive. The cycle life length of the cells depends on the charging conditions; fast charging degrades the battery at a higher rate per cycle, and the SOC state of charge should be kept within a small window, max 40% of total SOC window, to make the battery degrade as little as possible for every cycle. The EOL for a vehicle battery is met when the battery cannot supply the requested amount of power, which generally is the moment in which the capacity of the battery is 75% of the original capacity neubauer2012techno. Depending on the driving cycle and use pattern of the vehicle, in relation to the initial power and capacity of the battery, the ESS lifetime will vary.

The economic life becomes significant for the case of second life of car batteries since they usually lasts 10-12 years in the vehicle. The possibility of reuse within the same product or a second use in another application, even if technically feasible, may then be dependent on future advances in technology and design leading to cost reduction for the alternative of simply buying a new battery. This becomes a difficult business case if the battery prices decrease as predicted [Neubauer & Pesaran 2011]. The bus battery examined in this thesis, with an expected lifetime of 3 years [5] , depending on driving cycles, will reach end of life at a rate in which the technology advancement is less ahead. New batteries would therefore be relatively less competitive and second life therefore more interesting. However the first barrier for reuse and second use is the capacity degrading of the battery pack. The 75% of remaining capacity means that 33% more used battery is required to achieve the same function as a new battery in a second life application.

3.4.1 Reuse

The reuse criteria are based on the fact that the functionality of the whole system may differ at different points, which motivates a construction based on many subsystems that can be interchanged and refurbished separately. This can optimize the function of the battery pack during use and avoid the waste of fully functional units. Such a goal is only achievable if the system design allows precision in the detection and disconnection of components. The increased division in subsystems can be obtained through an increased number of cell modules, however this has the downside of an increase in material needed for cell module containers related to the increased total module system area. As mentioned before the number of interconnects between modules are increased, and fixing points to fasten modules to the pack, having the consequence of more parts to assembly/disassembly, and slightly higher weight. The battery pack components, such as cables, housings, BMS, electronics and the battery cells, can be assumed to be reused

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[5] Estimate from personal communication with Jens Groot, 2013.

to different extents, assuming that the degradation of cells varies within the battery packs and that this degradation can be diagnosed. The weakest cell unit will set the limit for the whole pack performance; this means that even though the total battery capacity at EOL may be below the cutoff criteria, module units or even cells could be reutilized depending on their individual health. Testing and remanufacturing costs are important to determine whether this scenario is feasible. However the environmental impact from different scenarios is interesting to motivate reuse at different system levels. The single cells can have variations in degradation; depending on internal manufacturing errors/variations, or to the circumstances during use, such as variation in temperature within the pack, or use that goes over the recommended limits for charging procedures and parking duration and temperature conditions [Groot 2012]. The most 'efficient' use of the battery would require frequent service and exchange of single cells, and thus a complicated sensor system including every cell in the diagnosis. Such system is however likely to be quite impractical and costly.

In conclusion, reuse in itself has contradictions between the driving force of increased division in subsystems, and the driving force to facilitate the assembly/disassembly of parts. A trade-off between optimized precision in interchange and in simplicity of assembly is needed. The optimal trade-off is determined by identifying the most frequent issue of failure and the most valuable items of longest life length in the battery pack. The assembly should permit to easily extract and interchange those items. The optimum scenario from a cost perspective may look different from the best scenario of the environmental perspective.

Battery exchange to improve performance

Exchanging a vehicle battery for a new one makes the electric driving performance more equal during the vehicle life. In some cases the vehicle construction and the integration of the ESS limits the possibility of such an exchange. In cars, where space is limited, the ESS is often placed to maximize the inner space in the vehicle cabin. This means preferably under seats and in mass equilibrium with other drive line systems. The design priority is not given to battery interchange, for the primary reason that the range of the EV battery is designed to have adequate performance all the vehicle life, and so there is no explicit need for exchange. In the case of most electric cars, the battery is released only when the vehicle is sent to end of life management. If the construction and design of the ESS-Vehicle interface is not adapted for easy extraction of the battery, it may be difficult to upgrade a battery during the vehicle life. However if the waste management facility can extract the ESS and redeliver it to the car manufacturer, reuse could be applied at end of life. For the PHEV bus, battery reuse is a more natural choice, since the ESS needs to be exchanged a couple of times during the vehicle lifetime, and at every interchange, supplementary actions such as repurposing testing and diagnosis may be taken.

Theoretically the battery could be interchanged at every full discharge by an automated system instead of in-vehicle charging [MacCarley 2000]. This concept allows short stop times, and reduce the wear of the battery due to fast charging, giving the allowance for slow charging outside the vehicle. From a repurpose and reuse point of view, this could be an ideal way to refurbish the ESS, since an instant detection and action can be taken to substitute failing or degraded components. A frequent upgrading of the ESS can keep the vehicle electric performance at the highest possible level. Until present the method has shown few actual applications since some huge challenges in installing the infrastructure and machinery for such a service have to be overcome. As some ideas show, [MacCarley 2000] the automatized battery exchange machinery could be placed underground, which means large investments. Even though the solution is clever, the volume of the xEV is yet too small to create incentive for such an investment.

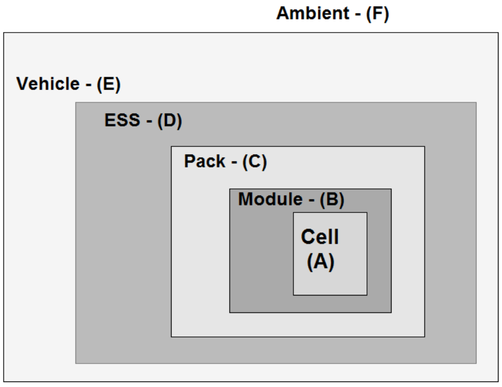

Figure 3.8: Interfaces of systems from cell to vehicle. The boundaries of the systems A to D give an idea about the need for protecting casings and housings materials, and from a maintenance point of view the several layers that must be removed in order to reach the cells and modules.

Mechanics needed for remanufacturing and reuse

The actual mechanics of replacing a battery are critical to the possibility of reuse. There are two principal questions for reuse and refurbishment: whether the service of refurbishment can be made fast- on the fly failed unit replacement [MacCarley 2000], and if it can be made at low costs.

To investigate these questions, it is necessary to know:

- At what system level the cell can be reached- at module, pack or vehicle level.
- At what system level the module can be reached- at pack or vehicle level.

The less interfaces (figure 3.8) between cell and vehicle and the easier it is to remove these interfaces, the total time and cost can be reduced for the replacement.

The difficulty of accessing single module units depends on the plane on which the electrodes and interconnections are positioned and how many module layers in this plane there are. A single layer of modules makes the inserting, disconnection, or testing of a certain unit easier, facilitating selective module reuse, refurbishment, second use and disassembly. The definition of an accessible module is one that has direct contact with the outermost system boundary, see the system boundary definitions in figure 3.8; opening one side of the pack casing, the module would be accessible without need to remove other system units. The highest level of access is given when the entire module unit has an interface with the same plane of the pack.

The weight and size of the battery pack determines if machinery for lifting and displacing is needed. A relatively light pack could be handled by a person while a large pack could require investment of extra equipment. To reduce the time and costs of refurbishment the initial number of actions needed to dismantle the case should be reduced. This means less connects, screws, etc. At the same time the refurbishment should not be simplified for unauthorized people. This can be solved by using seals with need for special instruments.

The optimum for second use, reuse, and switching of modules is a pack that does not need to be removed from the vehicle to access the modules. The requirement for switching modules of an integrated pack is that the access plane is freed from external covering equipment enabling to open the pack easily. The definition of an accessible module is one that has direct contact with the outermost system boundary, see the system boundary definitions in figure 3.8; opening one side of the pack casing, the module would be accessible without need to remove other system units. The highest level of access is given when the entire module unit has an interface with the same plane of the pack.

In addition to the mentioned criteria the definition of accessible connection in a free pack (important for second use, refurbishment, reuse, module unit switching) is the orientation of the module terminal sides towards the outermost system boundary. Thanks to this configuration, the connections are easy to reach and the single modules can be disconnected individually without an explicit need to disassembly the whole pack. For a fast upgrading of a few module units, this is an important criteria.

3.4.2 Battery systems in grid applications

Regarding the electricity consumption in the society, solutions are being investigated of how to save electricity and gain more independence from fossil fuels. Many measures are possible for the future. Two important concepts are the management of the power production units comprising integration of renewable energy sources (RES), and the demand side management which is the responsibility of the electricity end user to control and consume electricity at preferred hours in accordance with high RES supply and low electricity prices [Steen, Le & Bertling 2012].

Until precise predictions exist for how the electricity demand and supply curves look at a consumer level, and the price predictions are available to end-users and power market actors, we may need an energy storage solution to succeed with the flexible demand and supply, and the demand side management. The ideal system in which the power supply of RES is directly balanced by for example hydro power, and the demand side could react instantly to the oscillations in the power supply, but the market, infrastructure and technology are not there yet. Until the moment in which market strategies are changed – towards possibly more predictable supply and demand curves we may need the storage capacity at the decentralized level. The role of the battery is possibly transient but still important[Eyer & Corey 2010], [Greenpeace International and European Renewable Energy Council 2009].

It can be discussed how the price oscillation will flatten at high implementation of energy storage and demand control and what technology and energy use this would give incentive to. However the physical transmission grid and the renewable energy sources will always be remaining constraints for the market development, in whatever direction the monitoring and regulations around it are created [Viljanen, Makkonen, Annala & Kuleshov 2011].

The reinforcement of the European electricity grid is on the planning stage with some large projects aiming to free the electricity trade over national borders [Buchan 2011]. The need for eliminating bottlenecks, smoothing load curves and proposing security of supply is the first step to achieve the free trade. The introduction of high amounts of RES supply as a mean to decrease fossil fuel dependence increases the intermittency and need for peak shaving and electric energy storage [Greenpeace International and European Renewable Energy Council 2009]. It is possible that there is an increase of the stationary applications in the future to balance the RES, it may be the result of new market strategies but it may also be induced be legislation [Viljanen et al. 2011].

Second life

The possibility to give the automotive batteries a longer life by letting them serve in stationary applications after the automotive end of life (EOL) is called second use or second life. This may be a way to decrease PHEV costs and to decrease the environmental load from the battery. As mentioned earlier, given that the battery has to satisfy high requests on energy capacity, power output and efficiency to function properly for vehicle applications, the end of life enters at 75-70% remaining capacity. With this capacity and lower energy density, the battery is more than adequate for the performance needs of many stationary applications such as on or off-grid decentralized storage. A few different examples of applications that are of interest for the second use of automotive batteries are uninterruptible power supply (UPS), electric power quality and reliability services, transmission support, wind power generation support etc [Neubauer, Pesaran, Williams, Ferry & Eyer 2012].

The current state of the art is that used batteries are being tested in some applications. One example is Chevrolet Volt batteries in off grid applications for electricity supply to apartments [ABB 2012], but this is not done at a large scale and commercialized techniques are still in the future. The barriers for a wider use are related to the difficulty of predicting the actual end of life of the battery depending on the previous use patterns. Models and diagnosis systems have to be developed in order to secure, and possibly certify, the functioning of the used battery to be sufficient for the second use application. There is lots of R&D needed to enable second life in practice.

Market based introduction of second life batteries

The second use consideration, is that repurposed vehicle batteries replace the supply of new batteries requested by the stationary service. The amount of old batteries needed to replace one new can be determined according to different methods; allocation by energy storage capacity, power, allocation by willingness to pay, allocation by customer perception, or a combination of these aspects through weighting factors [Neubauer & Pesaran 2011]. The choice can be made to consider the second life market as a share of the existing stationary markets. The alternative would be to consider the second use market as a new market created on the incentive from the upcoming fleet of used batteries. Taking into account the immatureness of the second use technique, a limited share of the existing market should be willing to use second life batteries.

At the current state of testing and validation of the concept, it is reasonable to assume a low number of applications in the next years, and if positively received an increased acceptance and growing market share can be expected. The lower limit of the available fleet of second life batteries is determined by the development and sales of the PHEV and EV sector. The upper limit of batteries applied in second use is determined by the market demand for electrical energy storage to stationary applications. The existing amount of electrical energy storage in current stationary applications can be retrieved, given the geographical area of interest and the type of application [Neubauer & Pesaran 2011]. The infrastructure changes in the electricity grid are slow, due to the related high investment costs [Buchan 2011], and so the power supply capacity demand can for simplicity be assumed to be constant.

As follows the determinant for the second use application possibility in the coming years is the prediction of the EV market development. In conclusion, the relation between the used battery fleet and the size of electrical energy stationary storage is important for the scale of second use[Neubauer et al. 2012].

Modularity and pack size impact for second life

The modularization of the battery will have an impact mostly on the remanufacturing possibility seen from the point of view of the second life application actor. The size of the energy storage for second life is often much larger than the vehicle batteries, especially when it comes to on grid applications for example Siemens provides modular ESS systems from 16 kWh up to 500 kWh [Siemens AG 2013]. This means that the priority would be to send whole battery packs to second use. Apartments instead could make use of smaller batteries, with an average daily consumption of 50 kWh, and an average yearly consumption of about 18600 $^{\text{kWh}}/_{\text{household}}$ in Sweden [Zimmermann 2009] which promotes second life of single modules.

Either the second life could enter for modules, packs or both, the diagnosis and life cycle registration are important parameters, as is the remanufacturing moment of exchanging the critically degraded cells and adapting the ESS unit to suit the new function. A clever modularization will facilitate the remanufacturing and service of the batteries for any other actor taking on this task. The role of battery life management is significant for the handover of the battery between one user phase and another. The state of health (SOH) of the battery at end of the vehicle use phase depends on the battery monitoring and control [Conte 2006], and on the strategy of battery service.

In the case of frequent service the battery will have overall the same SOH in all modules during all the vehicle lifetime. In case of less frequent service or none, the moment of battery EOL and vehicle EOL may occur at different times. In the case of battery EOL at vehicle EOL the value of the battery will be low, and the need for remanufacturing is major. If the vehicle EOL occurs in the beginning of the battery life the opportunity of second life actors is greater. The issue is to define who is responsible for the remanufacturing and at what moment the battery is exchanged, and if maintenance will be given to the battery.

3.5 Recycling

If the application of rechargeable batteries for vehicles will continue to expand, recycling will be a factor of great importance for the sustainability of the technology. The advantages of recycling can be both to reduce the need for raw material extraction, and to limit the amount of residual waste. It is of course also desirable that this can be achieved at competitive prices. To reach this goal, the process of recycling must be both more energy efficient and less costly than the use of virgin materials. The recycling can occur in all levels of the system, from pack casing materials, to modules, cells and electronics.

3.5.1 Pack recycling

Recycling the pack is rather straight forward since many of the materials like steel, aluminium and plastics are common to many other applications and thus have well developed recycling methods. However, before any components can be removed, the pack needs to be discharged for safety reasons. The housing, module housing, electronics, connects and cells can then be separated.

The pack components are sorted depending on material. Steel and aluminium in the casings are sent to metal recycling. If there are plastics, and these are pure, then recycling is possible also for these materials. Recycling aluminium is very efficient, and uses 95% less energy compared to production from virgin materials [BIR - Bureau of International Recycling 2013]. Also the recycling of steel is performed on a large scale, in average 60% of steel is from recycled material.

Metal connects, often of copper, are economically valuable and are separated and recycled with common copper scrap recycling methods. The recycled copper can be used in wires, and could thus possible be included in new battery packs [BIR - Bureau of International Recycling 2013]. No specific methods for recycling metals or other materials will be discussed in this thesis.

3.5.2 Cell recycling

Cells are separated from other scrap and sent to specialized facilities. Today the main reason for recycling cells, besides possible legislations, is the monetary value of the noble metals (cobalt, nickel, copper, etc.) contained in some Li-ion chemistries. Due to this, the recycling initiative for chemistries with less expensive constituent is limited. Among such chemistries with low recycling initiative are options such as LFP. Since the need for recycling is evident, it is important to also assess how the recycling of these batteries can become viable.

Currently, no process is being applied that extracts lithium compounds from the waste lithium-ion battery material, mainly due to the low economic value of lithium. As mentioned in section 3.1.5, the sustainability of an expanding electric vehicle market is questionable without lithium recycling.

Another limitation and difficulty with recycling cells is the very wide variety of chemistries that are on the market. This leads to uncertainty of value and the need to use methods that can be applied to any type of battery. Recycling is simplified by using a smaller diversity of materials. Hopefully the industry will develop a more standardized approach as the battery technology evolves. This may open for processes that are very specialized on specific chemistries, but still receive large quantities, making them more efficient and economically viable.

Due to the low degree of recycling today this thesis will not aim at only looking at current models for recycling Li-ion batteries, but also try to model future methods capable of extracting a larger part of the constituent materials. This is based on the EU target for 2016, of extracting a minimum of 50% by weight [European Parliament 2008], but also due to the interest of looking at way to extract lithium and other materials not targeted today. Assessing future recycling possibilities and gains is an important step in motivating the sustainability of a battery powered automotive sector. It can also help to show at what price recycling of currently uneconomical materials becomes viable.

Three groups of recycling methods will be presented; pyrometallurgical, hydrometallurgical and physical recycling. These represent different approaches to extract materials, as well as different opportunities to extract other materials that may be important, for example lithium.

Pyrometallurgical methods

Pyrometallurgy is a commercialized approach to extract valuable materials from the discarded batteries. This is a high energy approach that can accept almost any kind of battery and that extracts valuable metals like copper, cobalt, nickel and possibly some iron. In the general process, all organics in the cell are incinerated for process energy, and valuable metals are extracted through different purification steps. Waste materials that are not possible to extract are released as slag and used as for example additives in concrete.

Some corporations are already applying this type of process to battery material streams, both smaller consumer product batteries, and larger vehicle batteries. Umicore's Val'Eas Process has been chosen as a good model for a representative and currently available process. The company claims to recycle 69% of the metal, however, this is not equal to the percentage that is recycled into reusable material. An example of why these numbers differ is due to the fact that the lithium and aluminium slag is counted as recycled, although it is down cycled or lost [Dunn, Gaines, Barnes, Wang & Sullivan 2012].

The Umicore process has been investigated for previous LCAs by Dunn, Gaines, Barnes, Wang & Sullivan [2012]. Here the process is described in several steps. First two preparation steps are performed; pre-heating and plastics pyrolizing. The first step is to evaporate the electrolyte to ensure that there is no explosion risk. The second is to start burning the plastic, helping the system reach higher temperatures.

After these preparation steps, the material is put through a smelting step where the organic material is continuously incinerated for heat, and additional materials divided into a slag fraction containing Li, Mn and Al, and into a valuable alloy containing for example Co, Ni and Cu. This alloy is then separated into its constituent metals with leaching, oxidizing and solvent extraction steps. The method also contains a last firing step to produce the wanted $LiCoO_2$ from the recycled Co.

Using this process allows for the extraction of the valuable metals like Co, Ni and Cu present in some Li-ion batteries. For batteries with less of these materials, the process is not viable from a cost perspective, since most of the content then is incinerated or ends up in slag. However, the process is viable for NMC batteries, and is performed today.

Hydrometallurgical methods

The goal of future recycling process will have to be to recycle lithium as well as other scarce materials used in the batteries. In order to obtain lithium from the battery, the use of a solely pyrometallurgical approach is not enough; instead a combination of pyro- and hydrometallurgy could be used [Georgi-Maschler, Friedrich, Weyhe, Heegn & Rutz 2012].

The general idea of a hydrometallurgical approach is to use several leaching and solvent extraction steps, increasing the need for chemicals, but reducing the need for heating. This leaves the materials in more or less pure states when they have been extracted. Large parts of the constituent materials can in this way be salvaged.

One possible recycling route would be to first leach the electrodes, thus dissolving the active material in an aqueous solution. In this way, the foils and separator can be removed, and the metals in the foils can be recycled. To obtain the active material constituent, solvent extraction could be used. An organic solvent would then be added to the aqueous solution from the leaching step, and some metals would be extracted into this phase, giving opportunity for recovery. In this way lithium, iron and other metals can be recovered [Kosaraju 2012].

Physical recycling

Physical recycling includes methods where the parts are crushed and then mechanically separated by different means. Firstly plastics could be removed on a shaker table. After that different filters and processes can be added to the materials to separate them in different ways, depending on properties. This method places very high demands on the inputs, since the materials cannot be successfully separated if their properties are not known. Even when the inputs are known, some materials might be difficult to separate. However, if the materials are successfully separated the method provides greater opportunity for recycling the components back to battery grade materials because they are not intrinsically transformed.

Data collection, modeling and inventory analysis

The life cycle in this thesis is modeled in different parts. The cells, the modules and packs, the use phase and the end of life scenarios are all modeled independently. The models and data used for the different parts are presented in this chapter. They can be view as stand-alone, but they are also correlated with the functional unit. That is, they are designed to provide the function of powering a PHEV bus. The division of the total model life cycle model into steps, and the sections in which each step is described can be seen in table 4.1.

Table 4.1: The stand-alone parts of the data collection. All sections are independent, but coupled by the design to function in a battery system capable of powering a PHEV bus.

Production		**Use**	**End of Life**	
Cell, sec 4.2	Module/Pack, sec 4.3	sec 4.4	Second use, sec 4.5	Recycling, sec 4.6

4.1 Cell materials models and data

A life cycle cradle to gate assessment was performed on different lithium-ion cells. A variety of different chemistries were chosen with the aim of modeling both present high-performing systems as well as possibilities realizable in the future. In compliance with the functional unit, all the cells where designed to function in a PHEV bus, and all of the chemistries where scaled to suit high-power applications. The chemistries were

- Lithium iron phosphate (LFP) cathode - Graphite anode.
- Lithium nickel manganese cobalt oxide (NMC) cathode - Graphite anode.
- Lithium iron silicate (LFS) cathode - Graphite anode.
- Lithium manganese phosphate (LMP) cathode - Lithium titanate (LTO) anode.

The assessed chemistries represent different properties and stages of development, see figure 4.1. Only Li-ion battery materials were chosen for the LCA. The motivation for this is the current relevance of this group of batteries, giving the opportunity for reliable inputs to LCA due to the large amount of confirmed data available for many component materials. The basic data for cell composition and weight percent was taken from BatPaC. The composition varies with chemistry, and the modeled weight percentages of different subcomponents of the cell and electrodes can be seen in full in table A.1 in Appendix A.

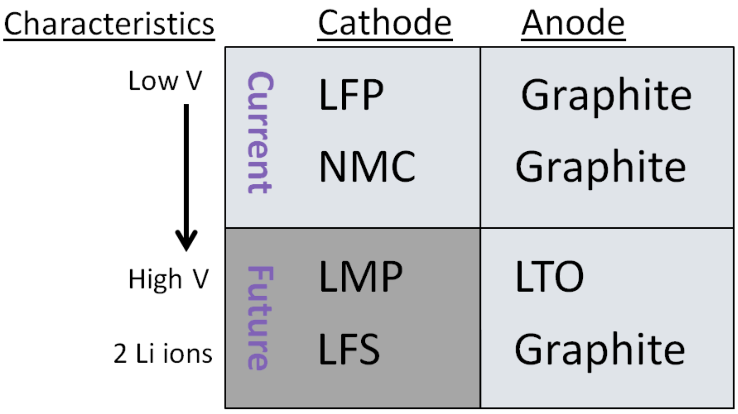

Figure 4.1: Schematics of the chosen chemistries and their key properties. Also the choice of corresponding anode active material for each cathode active material is given. Dark gray areas mark future alternatives for lithium-ion cathode materials. The characteristics are high and lower voltages, as well as the amount of lithium ions available. The metals involved also vary.

Outside the LCA Na-ion, Li-S and organic cathodes, as well as Si-based anodes were evaluated based on the Li-ion LCA results. Their opportunity to improve certain life cycle steps or impact categories was analyzed.

Since not all materials being evaluated are actually produced today, the scale and production inputs of the material extraction and cell fabrication were modeled as systems that are viable for production today, or systems that would be viable for production if the technology had been developed thus far. This means that possible future systems were scaled up in a way as to represent a realistic future scenario of full scale production. Capacities were chosen close to the theoretical values, and issues that are not inherent to the material were assumed to have been solved. Inherent limitations such as low conductivity were assumed to be solved in similar ways as for materials used today, for example by nano-scaling.

4.1.1 BatPaC chemistry and cell parameters

BatPaC was used to model the four combinations of cathode and anode materials chosen. LFP, NMC, LTO and graphite models were pre-existing in BatPaC, and used with only slight modification. LMP and LFS were modeled as modifications of LFP. LMP was modeled as having the same capacity as LFP, and LFS was modeled as having 300 $^{\mathrm{mAh}}/_{\mathrm{g}}$, close to its theoretical capacity

To assess the property changes associated with changing the active material a few parameters were targeted as most important for modeling different materials. These were changed in BatPaC's chemistry sheet, with effect on the performance and size of the pack. The three parameters in question, defining the key properties of the materials were; density of active material, capacity of active material and the anode–cathode voltage. The amounts, densities and basic structure for all cell components apart from the electrodes were taken directly from BatPaC. This includes the electrolyte, cell casing, current collectors and separator.

Apart from the three parameters, some alterations were made to make the battery more suited for high power use. This was done by changing the coating thickness of active material. The value was changed from the original 100 μm to 35 μm; resulting in higher specific power because of the shorter diffusion lengths, but lower specific energy, since more passive material such as current collectors and electrolyte is obtained per amount of active material. This makes both LFP and NMC more power optimized, but due to the fact that NMC is a high-energy chemistry, rather than high-power, a system using NMC still needs to be treated differently than one using LFP. This impact the capacity of the cells, and the energy storage capacity of the total system. Both thicknesses are, however, reasonable, depending on if an energy or power optimized system is desired. Therefore a sensitivity analysis on this component is performed.

The amount of cell material needed to construct one cell was based on a battery pack calculation in BatPaC. The aim was 20 Ah cells for LFP, LMP and LFS and 26 Ah cells for NMC, suitable scaling of each cell when optimized for the high power needs of heavy vehicles. These parameters were fulfilled with a cell size, 160 mm x 160x230 mm, comparable to current commercial cells like C020 from EiG[EiG - Energy innovation group 2013] and AMP20 from A123 [A123 Systems 2013]. To comply with these requirements the thickness of the cell was slightly changed between chemistries, ranging from 8-9 mm. The resulting weight, power density and energy density for the cells are shown in table 4.2:

Table 4.2: The table shows the resulting weights, energy densities and power densities from the BatPaC models on different cell chemistries.

	LFP	**NMC**	**LMP**	**LFS**
Weight [g]	670	650	600	660
Power density [W/kg$_{cell}$]	2145	1587	4373	2318
Energy density [WH/kg$_{cell}$]	97	143	90	93

The resulting material weights for one cell based on this model were used for modeling cells in GaBi.

Supporting component models:

The supporting components, kept constant between chemistries, were discussed in section 3.1.1, and illustrated in figure 3.1.

Electrolyte: The modeled electrolyte for all Li-ion battery chemistries was lithium hexafluorophosphate ($LiPF_6$) in a blend of ethylene carbonate (EC) and dimethyl carbonate (DMC). The choice of the specific salt and composition of solvent was done based on the BatPaC model of the electrolyte and the fact that this electrolyte is used in many production-phase batteries. From BatPaC the electrolyte is assumed to have a salt concentration of 1 M and a density of $1.2\, g/cm^3$.

Separator: The choice of separator was motivated in much the same way as the choice of electrolyte. The match for this choice of electrolyte is a micro-porous membrane of polyethylene between polypropylene. The choice of this laminate is based on the data available in BatPaC and is modeled as 20% PE and 80% PP. The thickness of the separator was set to $20\, \mu m$ and the density is $0.46\, {}^{\mathrm{g}}/_{cm^{-3}}$ based on the assumptions in BatPaC.

Cell casing: The cell casing was modeled as a pouch type, with a PP coated aluminium material. The thickness of the aluminium layer was set to $100\, \mu m$ as in BatPaC, and the thickness of the plastic coating was set to $50\, \mu m$, where $20\, \mu m$ is PP and $30\, \mu m$ is PET (Polyethylene terephthalate).

Current collector foils: For graphite as anode the negative current collector foils were copper and the positive aluminium. For the LTO anode the copper was replaced by the cheaper aluminium as the higher voltage of this material allows for this change. The thickness of the aluminium and copper collectors tabs protruding from the cells were set to 1 mm. The current collector foils used to support the active material were set to have the thicknesses 12 μm for the copper ones and 20 μm for aluminium, all according to BatPaC.

Binder and solvent: For the production of the electrodes a binder is needed to adhere the active material paste to the current collector and possibly to some added conductive material. For this purpose it was assumed that a Polyvinylidene fluoride (PVdF) binder is used, and that this needs to be dissolved in a N-methyl-2-pyrrolidone (NMP) solvent. These assumptions are in line with those made in BatPaC.

Conductive additive: For all of the active materials, apart from graphite, a carbon black additive was modeled as conductive additive when manufacturing the electrodes.

4.2 Modeling of cell production

The production of the cell and its component was modeled to obtain LCA data for these steps, the different components and processes included can be seen in figure 4.2. For all processes it was assumed that stoichiometric ratios of the different precursors were used, and that the processes have a 100% yield. The assumption is in line with the 95-98% assumed in previous LCAs [Majeau-Bettez et al. 2011], and the effects of decreasing the yield was determined by a sensitivity analysis. The complete account of materials needed, and corresponding energy consumption for the different processes and different materials can be found in Appendix A. Also different modeling choices for less common materials are presented there, see table A.2. It is assumed that all heat is wasted and that all chemicals are collected after the process, with exception of emissions stated, since these in industrial processes are highly limited and controlled.

Two production paths were modeled, representing one dry and one wet processes. These two paths were assumed to have similar steps independent of what active material is being produced. Only variations due to the need of nano-sizing and coating are added. For the active materials needing nano-size particles a maximum of 200 nm is assumed as a reasonable limit for the particles. Zhang [2011] concluded that particles with sizes in the range of 150-300 nm have best capacity, when using conductive carbon additives.

When no production site information was available, or when the results were to be kept general, one electricity and one heat source were used. Electricity was modeled as the EU-27: Electricity grid mix from the PE International database. This mix has its main contributions from uranium, natural gas, hard coal and lignite resources. As a generic process heat source RER: heat, natural gas, at industrial furnace >100 kW was used, taken from the Ecoinvent database where RER indicates European values. These choices are important to have in mind when considering the results.

Transportation of materials and components are not included in this thesis. This is partly due to the broad and general nature of the thesis, giving little or no specific production sites. Another factor contributing to the this choice is the aim to highlight the effects of different processes due to the inherent properties of the method, and no other impacts. The need for specific infrastructure to process the materials for the batteries has also been excluded. In reality transport does have an impact in the order of 1% of the total gross energy demand[Rydh & Sandén 2005] or 3% of the manufacturing CO_2 emissions [Zackrisson, Avellán & Orlenius 2010]. However, the fact that this impact is highly dependent on very site specific data remains, making the assumption of no impact reasonable for the purpose of this thesis.

4.2.1 Cathode active material synthesis

There are a wide variety of different synthesis paths for cathode active materials. Depending on the material they put different requirements on the need for energy and additives. Two different production paths were modeled in this thesis, representing proxies for one wet and one dry synthesis.

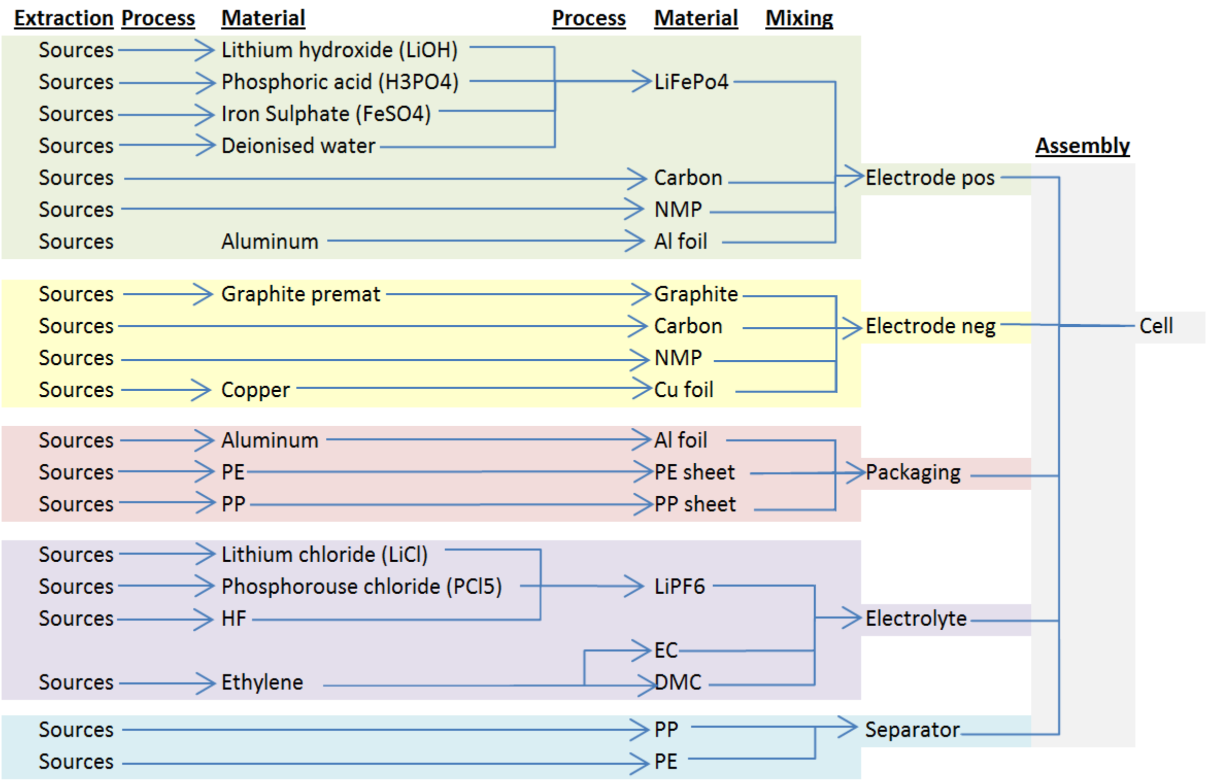

Figure 4.2: The figure illustrates the flow from extraction, through production to assembly of a complete LFP cell. All active and passive components are included. The components included in the LCA are presented in this flow.

Dry synthesis

The dry process is modeled as a sintering process. The process energy was estimated based on the Indium tin oxide sintering process in GaBi, assuming that the sintering required $1.5\,{}^{\mathrm{MJ}_{heat}}/_{\mathrm{kg}}$.

For NMC production via dry synthesis it was a assumed that a simple grinding step was the only post processing needed after sintering. The energy consumption for this step was taken from Dunn, Gaines, Barnes, Wang & Sullivan [2012] who collected a number of different grinding processes and took an average of these to estimate the energy consumption probable for a grinding step. This value, which was used in this thesis for grinding steps, was $1.28\,{}^{\mathrm{MJ}_{electricity}}/_{\mathrm{kg}}$.

For the materials needing nano-sized particles it was assumed that the material would need to be milled to the desired 200 nm after the sintering had occurred. This milling was assumed to be a wet type milling, and the energy needs for this process were taken from the work by Cho, Lee & Lee [2006]. Since the milling is done under wet conditions a drying step was also added. The energy consumption for this step was taken from Dunn, Gaines, Barnes, Wang & Sullivan [2012] where they have estimated a drying step for Li_2CO_3 to need $2.43\,{}^{\mathrm{MJ}_{electricity}}/_{\mathrm{kg}}$ product. A number also used for our different cathode active materials, when they needed drying.

It was assumed that LFP, LMP and LFS need carbon coating in order to perform well. In the dry process this was modeled as an ex situ addition of acetylene black in the milling process. The only further process needed was to heat the coated active materials, which is done in the final drying/calcining step [Konarova & Taniguchi 2009].

Wet synthesis

As a wet synthesis method a hydrothermal approach was modeled. The general approach of a hydrothermal synthesis route is to treat the precursors in solution, and heat them for a number of hours. After this step is done the material is calcined and dried. The first of these steps is modeled by heating the solution, water, in what is assumed to by a no-loss environment. This is acceptable since it has been shown that the heat losses, when taken into account, only contribute energy use about two orders of magnitude less than the heating itself [Majeau-Bettez et al. 2011]. The second step in the hydrothermal proxy is a combined calcining an drying step. Dunn, Gaines, Barnes, Wang & Sullivan [2012] collected data of available calcining process to find an approximation for a calcining step at around $1300\,^{\circ}C$. This data is used for the calcining and drying step in the wet process proxy, using $0.08\,{}^{\mathrm{MJ}_{electricity}}/_{\mathrm{kg}}$ and $2.1\,{}^{\mathrm{MJ}_{heat}}/_{\mathrm{kg}}$.

As the hydrothermal route gives the opportunity to directly achieve nano-sizes in the range of the wanted 200nm, no additional milling is required for this process. The only difference in the model between the different materials is in the temperature the solvent is heated to. For LFP and LMP this temperature is $200\,^{\circ}C$, a temperature chosen to be above the $175\,^{\circ}C$ necessary for good performance [Chen et al. 2007]. For the LFS and NMC chemistries the chosen temperatures were $150\,^{\circ}C$ [Nytén et al. 2005] and $170\,^{\circ}C$ [Myung, Lee, Komaba, Kumagai & Sun 2005], respectively. The hydroxide precursors for NMC production was assumed to be produced by a simple mixing step followed by drying. The drying was modeled as described in the dry synthesis case.

The amount of water used for the reaction influences the energy consumption to a high degree, since it is that amount that needs to be heated. It was assumed that 100 kg of water was needed for every kg of LiOH precursor, based on the wet synthesis process presented for LFP by Majeau-Bettez et al. [2011]. Since this had a great impact on energy consumption, the impact of changing the amount of water was analyzed with the sensitivity analysis.

For good performance of LFP, LMP and LFS a carbon coating proxy was added to the model. This was assumed to be achieved in situ by a carbon additive in the precursor mix. The additive chosen was glucose as described by Murugan, Muraliganth & Manthiram [2009].

4.2.2 Anode active material synthesis

The battery grade graphite was taken from the Ecoinvent database. This battery grade graphite is a modification of graphite production, with an additional 40 MJ hard coal coke. This to provide the extra baking needed to achieve battery grade graphite.

The approximations for the LTO processes were based on the production processes presented by the company Altair [Verhulst, Sabacky, Spitler & Prochazka 2003*b*]. The first step included in the LCA was a hydrolysis step consuming $31\,{}^{\mathrm{MJ}_{heat}}/_{\mathrm{kg}}$. This data was based on the data given by Altair for the production of TiO_2. For LTO the same process can be assumed, with the addition of a LiCl precursor for the chloride production method [Verhulst et al. 2003*b*]. The second step is to calcine the material to obtain the desired crystal structure.

The third step included is a milling step due to the need for nano-sizing. This is modeled in the same way as mentioned above for the cathode active materials, that is, with data from Cho et al. [2006]. Since the milling was performed in a wet environment a drying step after is assumed to be needed. The drying process was assumed to be similar to the drying and calcining step of the cathode production.

4.2.3 Production of electrolyte, separator, electrodes and casing

The production of the sub components was held constant for each cell type. The electrolyte was modeled as a no energy mixing process from $LiPF_6$ salt and 50% each mix of EC and DMC as solvent [Dunn, Gaines, Barnes, Wang & Sullivan 2012]. The salt production was assumed to require no energy, simply mixing the precursors LiCl, PCl_5 and HF. The solvents were modeled as ethylene glycol for EC and DMC was modeled as produced from phosgene and methanol.

The separator was assumed to be produced by a process similar to that applied when producing plastic films, but with a mix of PP and PE as inputs.

The electrode assembly required a coating and drying process which was modeled according to the graphite anode production data available in the Ecoinvent database. The binder and solvent used were NMP in PVdF, and the conductive additive was carbon black. Lastly, the cell casing was modeled as sheet rolling for the aluminium part and extrusion of the plastic part.

4.2.4 Cell assembly

The assembly of the entire cell was modeled according to Dunn, Gaines, Barnes, Wang & Sullivan [2012], who modeled each component in the assembly chain from the bottom-up, approximating each step in the assembly with known industrial processes and equipment. These steps included assembly in a dry room and cycling as the most important processes, representing around 60% of the total $1.11\,\mathrm{MJ}_{electricity}$ and $1.16\,\mathrm{MJ}_{heat}$ required to assemble the cell.

However, it should be noted the assembly process has been assigned much higher impact in other studies. Majeau-Bettez et al. [2011] take a top-down approach to credit a set total energy to different steps. They assume that around 20 MJ each of electricity and heat are required to assembly the electrodes and the entire cell. For the purpose of this thesis, the bottom-up approach of Dunn, Gaines, Barnes, Wang & Sullivan [2012] is better suited since most of the other processes are modeled based on the processes and not the total energy. Dunn, Gaines, Sullivan & Wang [2012] conducted a sensitivity analysis confirming that a change in the dry room energy need from 60% to only 20% still keeps the energy required for assembly well below the top-down assumption of Majeau-Bettez et al. [2011]. $10\,{}^{\mathrm{MJ}}/_{\mathrm{kg}}$ should be an upper limit to the assembly step, and this limit will be used in a sensitivity analysis to assess the maximum impact of the assembly.

4.3 Battery pack design and implications for environmental parameters

The battery design is related to environmental effects in many areas. For example the amount of passive material added in the ESS has consequences on the environmental impact both in terms of energy consumption during the driving phase and of the embodied energy in the pack components. Certain pack designs may be more material efficient than others, keeping in mind the material strengths, densities and energy needed for material extraction and production. A few key issues are illustrated in the LCA scenarios; the implications of housing material choices, impact of having the parallel connections on different system levels, the impact from using two small packs instead of one large, and the effect of oversizing the housings in order to create flexibility in the cell choice.

Selection of battery pack capacities

Before the pack design can be considered, the pack energy storage capacity needs to be determined, to determine the size. The selection of the optimum battery size is a complex process that is simplified in this thesis to keep a general approach. To determine the needed battery capacity an approximation was done from the required driving range and the necessary SOC window for the battery use. The PHEV bus electricity consumption of an assumed 8 km driving route requires an available battery capacity of about 12 kWh ($1.5\,{}^{\mathrm{kWh}}/_{\mathrm{km}} \cdot 8\,\mathrm{km}$). To keep a SOC window of 40%, implies that the total battery capacity should be 30 kWh. The total capacity of the battery will degrade during its service life to about 75% of the original capacity.

In order to make the electric driving range no less than 8 km during the total service life 33% extra capacity is added. With this extra margin the final pack capacity becomes 40 kWh. In this thesis, we further on consider the LFP chemistry battery to be 40 kWh, and the NMC battery to be 60 kWh - 50% larger to compensate for the fact that the NMC chemistry is better for energy than for power and both packs should last 3 years to be comparable.

Modularization and pack design assumptions

To determine the impact of modularization, the aspects of battery pack weight, volume, voltage and cost were investigated, given specifications for the needed power and range of the battery. The increased modularization on pack level and module level influences the volume, weight and the cost of the battery and, most importantly, the specific energy (Wh/kg) and the energy density (Wh/l).

The modularization question has been treated on a generic basis. The 40 kWh LFP pack was modeled with different material choices and thicknesses, and cooling configurations. Also the size up in kWh from 40 kWh to 60 kWh in the case of NMC was considered. The purpose was to give a range of different pack configurations and compare the related impacts and added weight. This since the function of the battery was set to a hypothetical ESS able to provide the amount of energy storage capacity and power needed for the city driving cycle and the right voltage (500-730 V nominal). Dimensioning and use criteria on what rates of electric and hybrid mode to be used can result in an LFP pack of 20-40 kWh, or an NMC pack of 40-60 kWh[1]. In the following paragraphs, different scenarios of design choices are illustrated.

Battery pack design in BatPaC

The battery pack was modeled by varying the following parameters in BatPaC:

- The numbers of cells included in each module.
- The number of modules per battery pack.
- The number of packs per vehicle.
- The energy storage capacity (kWh).
- The power (kW).
- The number of cells or modules in parallel.
- The number of modules in row.
- The number of module rows.
- The type of cooling system (liquid or air).

In addition to these primary parameters, the following criteria have been used in this thesis to dimension the cells and pack models by iteration:

- The final pack dimensions of 0.3 m height, 0.5 m width, 2 m length.
- The voltage of 500-730 V for the PHEV bus.
- The voltage of 220- 480 V for PHEV car (taken into consideration for interoperability of module units).

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[1] Estimate from personal communication with Jens Groot, 2013.

Some issues are not treated as inputs in the BatPaC model such as orientation of modules in a pack, the layout of the pack, materials of the housings and casing and the cell dimensions. Some of the fixed parameters in BatPaC were changed as follows:

- The cell height to width dimension ratio.
- The material of the housing- stainless steel, plastic, (PP).
- The material thickness of the housing and casing.
- The material contents in BMS and SOC controllers.
- The material contents in insulation, here assumed to be polyurethane (PU) foam.

Requirements for battery pack design

The modularization and the pack design should take into account certain requirements and concepts previously described in section 3.3. For the modeling of the modularization the constraints in table 4.3 and 4.4 have been used. In addition to this an assumption of the maximum module weight of 10 kg is made to make the extraction of module units easier for an assumed reuse.

Table 4.3: The table shows the constraint for the number of cells, cells per module, cells in series and aligned cells for both LFP and NMC chemistries. Upper and lower limits for these parameters are also shown. The values are dimensioned after the 20 Ah of LFP and 26 Ah of NMC. A maximum of 3 cells in parallel is assumed.

	Min LFP	**Max LFP**	**Min NMC**	**Max NMC**	**Limiting constraints**
Number of cells	624	648	624	648	Capacity
Cells per module	10	54	10	47	Control unit input, voltage
Cells in series	-	220	-	195	Maximum voltage
Cells aligned	7	243	7	216	Space

Table 4.4: The pack design parameters set by the vehicle interface. Important to note are the different energy storage capacities related to different chemistries, and maximum and minimum resulting voltages.

	Min LFP	**Max LFP**	**Min NMC**	**Max NMC**	**Limiting constraints**
Capacity kWh	39	41	58	62	Driving range
Power kW	150	170	150	170	Braking power/EM power
Voltage V	500	730	500	730	Maximum voltage

4.3.1 Using BatPaC as reference model for pack design

The objective when modeling the battery pack was to create a realistic, well performing pack corresponding to the given constraints. To achieve this, the BatPaC model was used with only minor changes in the data set to suit the assumed reference cells and pack geometry. The validation of the models was done on a theoretical basis. Here follows a description of the scenarios created for the LCA with the help of BatPaC.

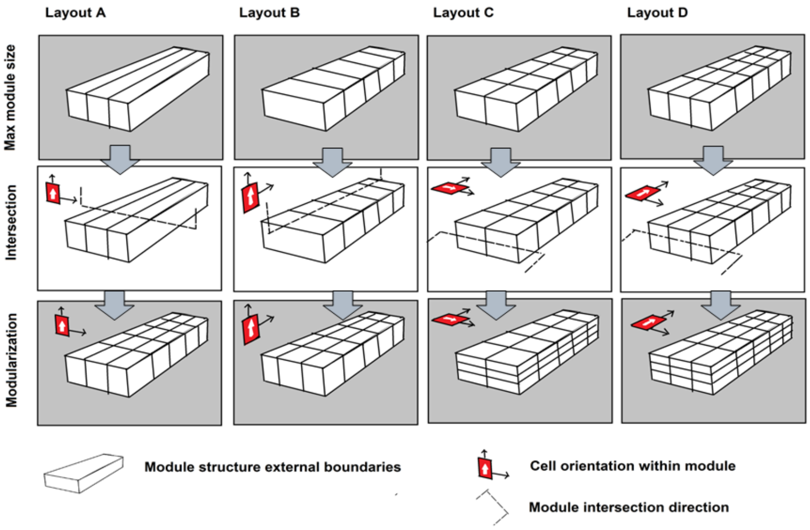

Figure 4.3: Examples of possible module layouts depending on cell orientation in relation to the pack geometry, in the case of cuboid pack. Layout A is the most convenient from an assembly point of view and gives the highest modularization flexibility for the cuboid pack allowing the highest number of cells per module.

Scope and limitations of modularity selection

The inputs given to the BatPaC model include how many cells and modules are desired in the total system and how these are configured to produce the total power and energy. For simplicity the modules are all considered to have the same number of cells and size although in reality some different module sizes can be joined in one pack. The diversity in module size is a design approach which is good for a very specific use but the drawbacks of diversity in module size are that the manufacturing may become more complicated, that a more complex control system is needed and the pack risks to be less efficiently packed.

The choice of singular module size is made to keep the general approach of the thesis. To further give a focus to the modularization the approach has been to select module sizes so that the modules should be a suitable subunit to both a bus pack of 39-41 kWh and a car pack of 10-12 kWh. The total number of cells of the pack has from the beginning been selected to be dividable with sets of two and three to allow many different symmetric configurations and layouts. The prime numbers of priority has been set to 2 and 3 for highest possible flexibility in the modularization.

Method of modularity calculation

Focusing on using the control units as efficiently as possible, the minimum CPM was set to 6 and the maximum to 19 to keep the module weight under 10 kg. The pack was build up iteratively to capacities of 38-40 kWh and 10-12 kWh, having set a minimum and maximum of module rows, layers and columns to fit the pack within the dimensional constraints. Alternating the number of cells per module from minimum to maximum, going from a high to low number of modules per pack, all possible symmetric pack configurations for this data set up were retrieved.

A sensitivity analysis was made to see the difference in pack housing materials depending on the six different cell orientations within the module assuming a cuboid cell. The investigated cell dimensions showed little sensitivity and finally the direction of cells was kept as shown in the layout A in figure 4.3, based on practical reasons explained in section 3.4.1. The materials for housings and connects were calculated for each of the retrieved configurations to show the impact of modularization, see figure 4.4.

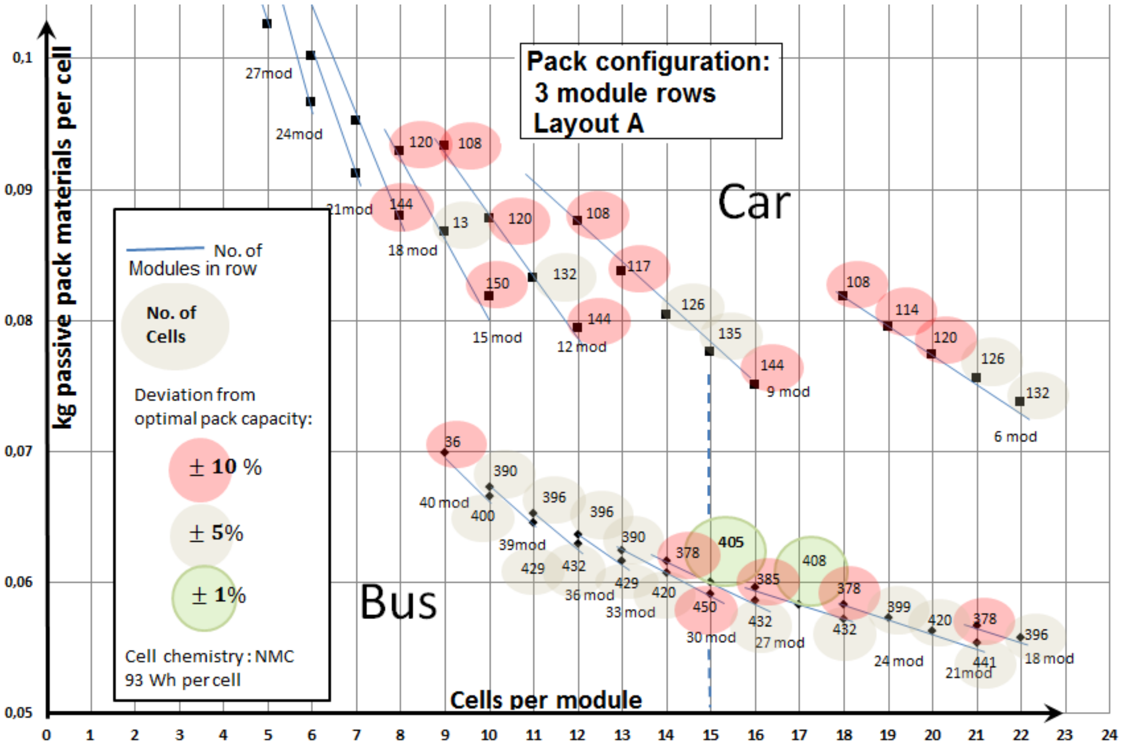

Figure 4.4: Modularization method examle with the number of cells per modules shown for interoperability between a car and a bus for an example of a 12 kWh and a 40 kWh NMC pack, related to the number of modules per pack, the total number of cells per pack and the amount of passive pack materials weight per cell. In the figure can be seen, what modular solutions are possible in terms of capacity for both the car and the bus and what rate of modularization gives the lowest rate of added passive pack materials. Typically, the higher number of cells per module means the less weight of passive pack materials. The optimal pack capacity needs to be approximated to accept a certain module layout, which means that depending on the certain number of cells per module, the pack capacity will deviate more or less from this optimum. In the example the number of cells per module allowing the most optimal capacity for the bus pack is 15. Assuming the same pack layout for the car, this modularity will on the contrary not be optimal. The conclusion from this example is that another pack layout for the car is needed to possibly achieve a good modularity for interoperability for both the car and the bus. Most likely a compromise needs to be done for one or both applications to succeed with interoperability of module units.

4.3.2 Selection of modularization in BatPaC

The pack selected for the LCA has 54 modules of 12 cells per modules, which is a pack of 648 cells since this set up works for different types of parallel connections on cell level and module level, respects the number of inputs for the control unit. Additionally the module can be used to build up the car battery pack, and is of medium size requiring not too much surface materials as shown in table 3.4. To make the different cell chemistries comparable, the same configuration of cells, modules and connections have been used for both the NMC and the LFP pack (table 4.5).

Three cells in parallel were used, and three rows of 18 modules in each to make a cuboid pack geometry, suitable for the positioning in the bus. This modularization is realistic in terms of voltage, weight and dimension, and has been used for the material calculations done in BatPaC for the different scenarios. The pack voltage is then about 700 V, suitable for the PHEV bus applications. The difference between the NMC pack and the LFP pack is the dimensions. Slightly larger for the NMC pack than the LFP pack due to a difference in volume between the cells. The NMC cell is considered 20 volume% larger than the LFP cells. See bill of materials in table A.4 and A.5 in Appendix A.

Table 4.5: Summary of the configurations and modularization of the packs modeled in the LCA. NMC and LFP have the same set up with different total pack capacities depending on the difference in cell capacity.

Parameter	**NMC**	**LFP**
Pack [kWh]	60	40
Modules	54	54
CPM	12	12
Total cells	648	648
Cell strings in parallel	3	3
Rows of modules	3	3

4.3.3 Components and materials

The following components were collected among the ones treated in the BatPaC program for battery pack design, and from realistic assumptions of components in existing packs. Some components are fundamental for the function of the pack; in this group are the items in figure 4.5, such as cells, BMS, thermal management and electronics, etc. Those components cannot be excluded from the system.

At the same time, some secondary components are present in the ESS that are there to mechanically keep the structure together. Those are module housing and linking elements, such as connects etc. The extra interfaces needed for modularization implies that separating elements are inserted, which creates the need for more interconnections. The connecting and separating elements are presented in figure 4.6. The modularity and extra interfaces are not directly related to the battery function of delivering electricity, so from a battery functional point of view, these interfaces should be minimized.

The assembly of the pack components has been allocated 2.7 $^{\mathrm{MJ}}/_{\mathrm{kg}}$ battery pack according to [Dunn, Gaines, Sullivan & Wang 2012]. The shaping and production techniques of pack components from original materials have been omitted.

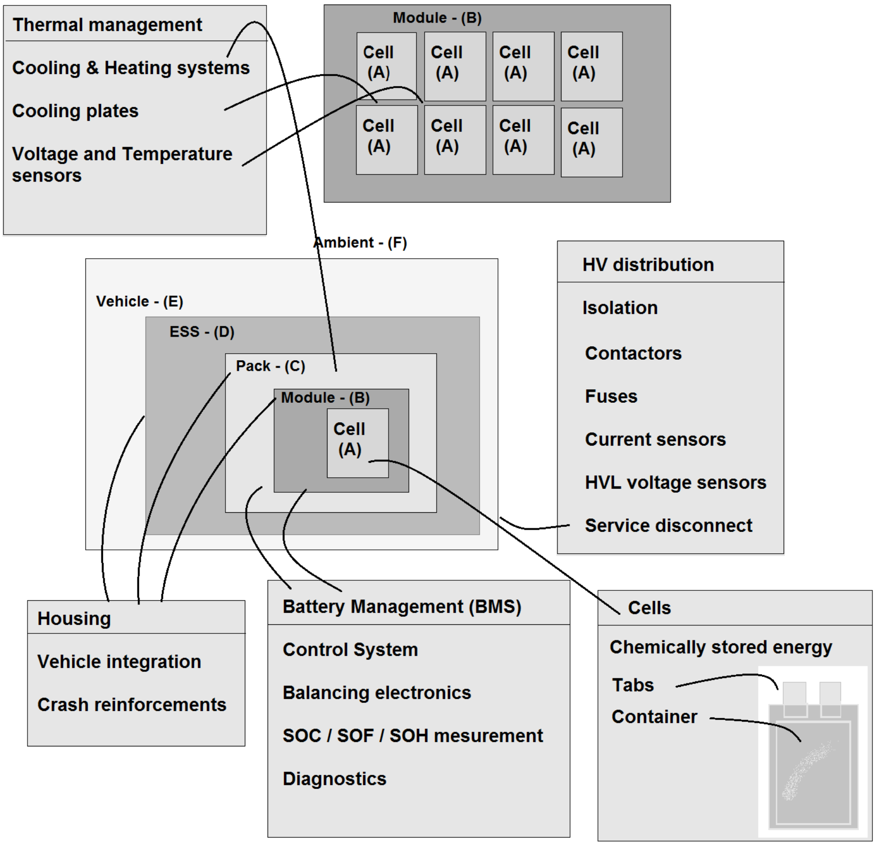

Figure 4.5: The different components present in the battery pack with their function and grouping.

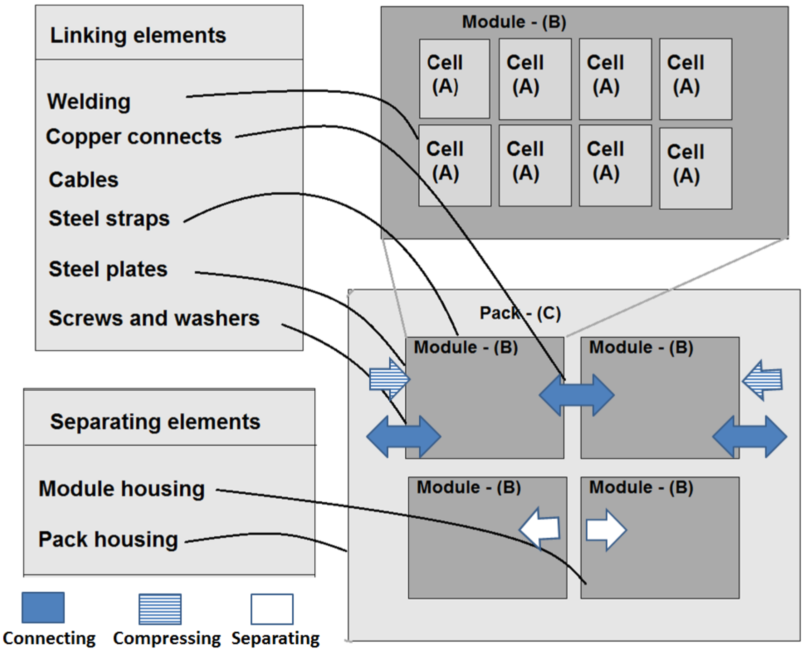

Figure 4.6: The different components present in the battery pack with their function and grouping. The connects act between modules, the steel straps and pressure plates compress modules, while module walls separate the cell groups.

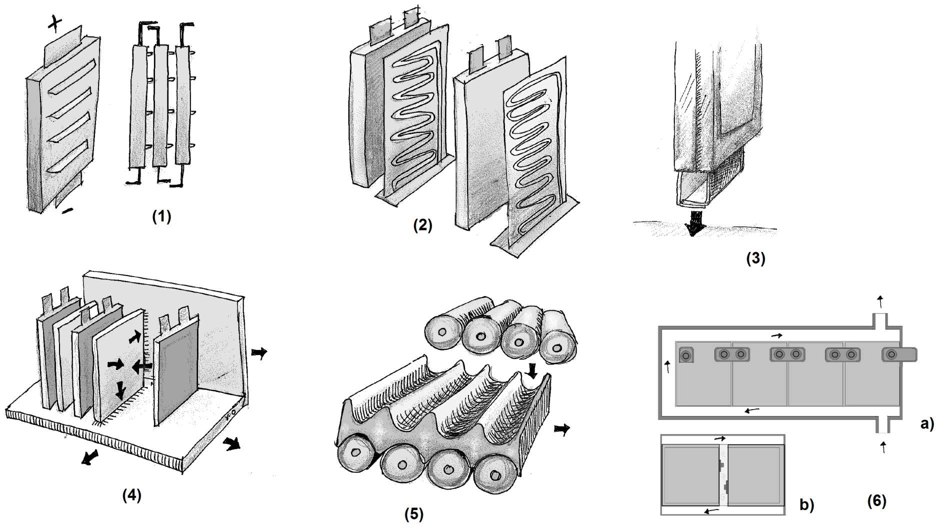

Figure 4.7: Cooling system structure options. 1) Air cooling: Cells equipped with distance fins for air flow. 2) Liquid cooling: Aluminium fins with integrated cooling channels. 3) Heat rejection directly from cell tabs to cooling plate made of electrical isolating material. 4) solid cooling plates integrated between cells, to cooled walls and bottom plate. 5) Liquid cooling: cylindrical cells, with wave shaped cooling channel. 6) BatPaC coolant flows, 6a) Pack cut open between positive and negative terminal, 6b) pack cut open in parallel plane to the pack terminal side.

The implications of cell modeling on the pack

BatPaC generates a model of a stiff pouch cell with stacked plates, and states that the model represents most other types of cells of the same chemical and physical properties. This means that little differences are seen in comparison to other shapes of cells such as cylindrical with wounded windings and cells with flat wound, in terms of terminal material, current collectors and cost [Nelson et al. 2011].

An advantage is given for the flat cells in the heat rejection, which is more efficient than the cylindrical cells. This is, however, to only main difference between the cell types in BatPaC, implying that the results from the BatPaC modeling can be considered indicative for generic batteries. However, the dimensions of the ESS are specific for the flat cells, since cylindrical cells would occupy more space due to their geometry.

Cooling plates of prismatic soft cells

The thermal management of the battery pack attempts to guarantee that all the cells keep the same temperature during use, and also that the temperatures are kept close to the optimum $35\,^{\circ}C$[2], since deviation from this optimal temperature can speed up the aging of the cells. The cooling is needed in between the cells, requiring a medium to reject the heat produced. A 50% ethylene glycol in water solution is used, in BatPaC assumed to have a density of $1070\,\mathrm{kg/m_3}$, heat capacity, $3.26\,\mathrm{J/g^{\circ}}C$, with a fluid flow velocity of $2.5\,\mathrm{cm/s}$. A power of 87 W is required for the pump and motor to circulate the fluid.

The coolant should not be in direct contact with the cells for safety reasons, so aluminium cooling plates are inserted between the cells, figure 1.3 (1) and 4.7. The positioning of the aluminium plates can be made in different ways, either with internal integrated channels for the coolant, figure 4.7 (2), or solid metal in connection to the module walls/module base, figure 4.7 (4). The solid cooling plate can at the same time serve as supporting wall. In this solution no additional module walls are needed.

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[2] Estimate from personal communication with Jens Groot, 2013.

The pressure is given by steel bars connecting and tying the cooling plates together, figure 1.3 (9). In case extruded solid aluminum plates are used, the base can be given the shape of snap fit, reducing the time of assembly, disassembly, and need for additional screws and connects. The alternative is solid cast profiles. This type of module construction is clever from a flexibility point of view; the cell width and size can vary and still fit the in the aluminum profile construction.

A last option for the cooling is to directly use the tabs of the cells. The tabs have both the properties of electrical conductors and of heat conductors and so they can lead heat to a cooling plate or the module house, that in turn must be of an isolating material, figure 4.7 (3).

The cooling structure of the pouch cells is quite small in comparison to the cylindrical cells. From a volume perspective the cells of cylindrical shape fill up the pack space less efficiently and a lot of material for the wave shaped cooling structure is needed to guarantee the heat transfer between the cells and the coolant, figure 4.7 (5). The pouch cells can be packed very efficiently thanks to their prismatic shape, this means that the cooling structure is limiting the most efficient packing of the cells, and thus the volumetric energy density, and in some extent the specific energy of the pack.

The cooling plates can vary in thickness; producing a tradeoff between added weight and cost, and the rate of heat rejection. The heat transport is increased with a thicker plate of up to 3 mm [3]. For a thin thermal conductor, the mass flow rate of the coolant must be higher, requiring more electricity for fans and pumping in the cooling system. The BatPaC cooling plates (called thermal enclosures or aluminium conductors) are thin, 0.4 mm, folding each cell, figure 1.3 (1). They are in connection to the module wall, which is cooled by circulation liquid flowing between the pack wall and the module walls, figure 4.7 (6).

The BatPaC construction implies that the module terminals are isolated from the cooling fluid by a plastic foam. From a reuse, or remanufacturing perspective this is not an optimal construction, since the plastic isolator must be removed to access the modules. A general difficulty is that the cell side and the cooling plate must be in direct contact for efficient heat rejection. The soft pouch cell can vary in thickness during its life because of swelling. In this case, thin sheets of plastic foam can be added to guarantee good contact between cooling plate and cell.

In the models, a cooling plate of 0.73 g is added to each cell according to the BatPaC design as the best case, making a total of less than 26 kg. This design of cooling system is good for slow charging when the heat flow is within the normal ranges, as in BatPaC [Nelson et al. 2011]. Instead in the case of fast charging of the pack, heat is created at high rate. A more efficient cooling system is thus needed and often thicker cooling plates needs to be used. A sensitivity analysis is used to see the impact of a cooling plate of 3 mm, and the weight of 300 g added to half the cells or to every cell about 113-220 kg. These scenarios are outlined in the results. In the last design, some of the module housing is directly substituted by the cooling plates.

Interconnections

For cells: The pouch cells are either welded or connected by screws. The first option is simple, but does not allow remanufacturing or reuse on the cell level. The screws and joining connection plates/cables makes the interchange of cells possible but increase the number of parts of the system, making the assembly more demanding. In the BatPaC model, the cells are welded. For parallel connection, a cell group interconnect of 13 g (LFP) and 7 g (NMC) is added for each module. The interconnects are dimensioned according to the voltage and the current. In the selected models, the cells are connected in 3 parallel strings. The pouch cells interconnects are less complex than the cylindrical cells interconnects/bus bars and so higher part costs and slightly more materials needed due to the less efficient packing should be allocated for the

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[3] Estimate from personal communication with Tomas Thelin, 2013.

connection of cylindrical cells. The BatPaC model is not representative for cylindrical cells in this aspect [Nelson et al. 2011].

For modules: The interconnects consist of a copper connect part, conducting the current between modules, figure 1.3 (6). In BatPaC these interconnects are 30-42 g each and are dimensioned according to the voltage and the current. If the modules are supposed to be placed in parallel, an additional bus bar is needed to interconnect the rows.

Stabilizing pack components

Stabilizing pack components consist of all pack and module housing materials that are present to increase the mechanical stability and safety of the system. The function of each component is presented in section 3.3.

Plastic module frames: The pouch cell group can be stabilized with plastic frames, in some different configurations. In a row, these frames constitute the module wall. In the beginning and end of each module, a steel plate can be added to keep the cell group compressed. Steel rods keep the cell grouping together. Suitable plastic materials according to yield strength and Young's modulus are polypropylene (PP), Polyvinyl chloride (PVC), polycarbonate (PC) and polyamide (PA) [Klason, Rigdahl, Boldizar & Kubát 2008]. The materials used in the modeling are polypropylene (PP) with a thickness of 2 mm. Extra steel plates are added on each module for increased stability. The recyclability of the different plastics may vary, but is not of further focus in the modeling.

Steel pressure plates and steel straps: In addition to the steel rods, pressure plates can be adapted to add force in the compression of the modules, figure 1.3 (9). The cells may swell slightly towards the end of life from gas formation wherefore it is needed to force them into shape by pressure. The pressure plates can be added on both sides of one module, or in the beginning and the end of the pack in the cell alignment direction. The thickness of the plates is assumed to be 1.5 mm, weight minimum 590 g/plate in all models. According to the BatPaC construction, the steel straps keep the modules in shape, surrounding the whole pack, figure 1.3 (9). The steel plates and the steel straps weight are summed in the models. Chromium steel 304 is assumed since the coolant flows directly between module housings and pack housings, and must not oxidize the materials it is in direct contact with, figure 4.7.

Module housing: The walls around the cell group make the housing of the module, figure 1.3 (5). The housing has the mechanical function of stabilizing the cell group, and making the part easy to handle, move, lift, store, limit spreading of fire etc. The housing is modeled by either plastic, aluminum or steel. Some of the module housing can be excluded, to reduce weight of the unit, if the base of the module gives enough support. In the model, plastic, stainless steel and aluminium have been used for the module housing. Stainless steel and aluminium cold rolled sheets of the thickness 0.5 mm are assumed in the models, and molded plastic (PP) of 2 mm thickness. The increased thickness of the plastic sheet compared to the original thickness of 0.5 mm, has been set to compensate for the lower strength of the plastic material per m^3 [Ashby 2012]. Even though the increased housing thickness would have an impact on the total pack housing dimensions, this effect has been omitted for simplicity. In fact the impact of the pack housing surface change is small in comparison to the module housing surface as seen in chapter 3.

Pack housing: The housing of the pack has the function of covering the row of modules, figure 1.3 (10). The pack housing can be excluded if the surrounding vehicle construction can take that function which is the case for example in cars. The material recommended for the pack housing is aluminum or plastic for light weight construction.

Pack housing insulation: The insulation is sandwiched between two sheets of aluminium in the ESS casing. It contributes to a more stable thermal climate in the pack. In the model is assumed a 1 cm thick layer of polyurethane (PU). The thermal conductivity of the pack jacket insulation is described 0.00027 W/cm°C in BatPaC.

ESS: The bus ESS has a prismatic shape, normally with one layer of module rows. Common materials for the ESS casing are steel and aluminum. It can be equipped with isolation plastic to reduce impacts from temperature changes. In the models, chromium steel sheet of 3 mm, and aluminium sheet of 2 mm are assumed. Welding and connects such as screws and washers are neglected. In the models, the ESS casing is equivalent to the pack casing.

Electronic components

For the control of the pack, grid to vehicle charging, and safety, a number of electronic components are present in the pack. The fuses, disconnect unit, Battery Management System (BMS) add expensive materials and parts to the system. The components are dimensioned according to voltage levels and current magnitudes. BatPaC uses a fixed set up of those components- 4 kg of BMS. The variable components are the SOC controllers. Those components are purchased and the material compositions are not known in detail.

The amount of printed circuit board (PCB) is partly dependent on the number of modules in the pack. The SOC controller, disconnect unit and BMS are accounted for as BMS in the modeling, with a material content of 10% PCB, 50% copper, 40% steel [Majeau-Bettez et al. 2011]. Two different PCB of high and low gold content are tested in the models. The one of high gold content has about 100 times more gold than the low gold content PCB, and both make part of the PCB options of low to medium gold content. The impact of control units and PCB can highly influence the results according to previous studies [Majeau-Bettez et al. 2011]. Since there is no exact data available for the PCB, these two possible assumptions are tested in the sensitivity analysis.

Weight collocation of battery components and design choices

In order to make a realistic assumption of the possible battery weight increase due to different design choices a maximum weight scenario was calculated. This scenarios was used as a worst case weight increase in the LCA

Assuming a minimum pack energy storage capacity of 20 kWh, 324 LFP cells of 670 g/cell, 217 kg cells, and on the other hand a 60 kWh pack of 648 NMC cells, 421 kg, then the weight difference depending on the choice of chemistry and design is 204 kg.

The difference between the light case of aluminium and the more robust steel case is 78 kg. Dimensioning the cooling plates for fast charging can add between 113-220 kg kg aluminium compared to the minimum 27 kg aluminium for the thin cooling plates of the slow charging design, which makes a difference of 193 kg.

Increasing the modularization rate, keeping a low rate of cells per module, the result can be 27 kg extra aluminium.

The total possible difference between the lightest battery pack fulfilling the function and the heaviest pack responding to the technical requests is at least 502 kg.

The drive lines of the hybrid bus, and the PHEV bus are often of the same design, with a battery pack that is seen as a black box during the equipment design. The drive line will not be drastically changed for the conversion from HEV to PHEV, and so an unexpected weight increase of the battery pack design can result in a higher energy consumption. In addition the battery integration may also imply voltage mismatches in the drive line interfaces leading to the need for extra converters which also means extra weight.

Alternative component materials and uses

The modeling of the pack considers a few scenarios and set ups for the LCA from a variety of pack design possibilities. Some alternatives that would have been interesting to evaluate but could not be included in the LCA in this thesis are hereby described.

The steel chosen to represent all steel used in the ESS is stainless steel, due of the need for corrosion resistance when in contact the cooling liquid. For another choice of cooling system integration, the steel housings could be of another steel type with less chromium. The ESS will be completely integrated within the vehicle body and should thus not be exposed to possible corrosive ambient conditions, wherefore a less resistant material could be used, with a possible lower environmental impact.

Some plastic materials that are often present in commercial packs have been excluded by choosing the BatPaC design. The relative impact related to these other plastics are generally high in comparison to the plastics such as PP and PE used in this thesis, but since these other plastics are related to cables, isolation etc. their quantity is minimal and presumably their impacts will not change the overall results. This choice could, however, be further assessed.

The exchange of copper to aluminium in the connects and power system can be made to decrease the costs of the structure. It is likely that such a design change may have some impact in losses of heat from the electricity transmission, it is, however, recommended to check the efficiency loss of such a design.

To make the pack of aluminium less heavy and less complicated to recycle, the PU insulation could be eliminated. For the steel and plastics case- the extra stabilizing steel compression plates could be eliminated. Additionally for all the designs, the ESS housings could be reduced in weight by making use of the bus frames for some stabilizing and protecting function for the pack.

The efficiency and actual losses from parallel connections on module level, pack level and cell level should be studied in order to account for the costs of a shared modularization between car and bus.

With liquid cooling, conducted in between cells through channels in the aluminium plates, the rate of heat transfer could be higher, but the safety sets constraints on the type of cooling liquid. It should not be glycol and water which would act like an electrolyte if it comes in direct contact with the cell terminals. For liquid cooling between cells a non-electrically conductive coolant may be needed. The environmental impact of such a coolant needs to be investigated.

4.3.4 Pack scenarios included in the LCA

Apart from the standard pack design using one pack, a few other scenarios were evaluated in the LCA. Different materials for the pack and modules are assessed for the standard model, creating four different standard scenarios. Other scenarios include having an oversized pack, having two small packs instead of one large, and changing where in the system the parallel connections are placed. These are based on the first standard design, corresponding to BatPaC's original design. The effect of increased the amount of cooling plates, and the effect of having a larger gold content in the PCB are also assessed in the LCA, and also these are based on the first standard model scenario.

BatPaC standard model scenarios

The base case for the evaluation of the housing material choice of the pack is made in the same way for both NMC, and LFP, with some differences in size depending on the assumption of a NMC cell slightly larger than the LFP cell. Four standard cases were created; The first one, given the index design 1 is the original BatPaC design with aluminium housing in both pack case and module case and a thick layer of insulating plastic to withstand temperature oscillations. Design 2 has a steel housing for both pack and module, to represent a very robust pack. Design 3 was given a steel pack case and aluminium module housing, for robustness but at the same time with less weight from the module housings. Finally design 4 was made with a pack case of steel and a module housing in plastic (PP), to illustrate pack of a low weight, with cheaper material for the housing. The total bill of materials for the standard cases is found in tables A.5 and A.4 in Appendix A.

Oversized pack scenario in BatPaC

The choice of using the same module and pack casing size for both LFP cells and NMC cells illustrates a scenario in which the pack design is standardized to suit different applications. The winning is that the same manufacturing unit can be used for all the housings and the production costs may be lowered by reducing the diversity in specifications. The advantage could be seen by a xEV car manufacturer and a xEV bus manufacturer that could make use of the same standardized battery module unit even though the requests on type of cells are different. Additionally there may be consequences depending on different capacity (Ah) and voltage of the two different cells within the module. The number of cells is assumed to be kept the same for both cell types and some filling material or stabilizing structure needs to be added to the module housing to keep the cells in position. This extra material is omitted in the models due to lack or information. The indata can be seen in table A.4 in Appendix A.

Double pack scenario in BatPaC

The use of two small packs of 20 kWh to substitute a big one of 40 kWh has some implications in duplicated control units. The driving force is to make a small pack an independent element that is autonomous in terms of control and cooling system. The pack could be used alone or in multiples to suit different applications and reducing the production costs. The case is evaluated in terms of added materials for the original BatPaC design with aluminium and PU. The module housings stays the same and the ESS housing is a little increased. The important change is found in the control system. The indata used for the two packs can be seen in table A.4 in Appendix A.

Module parallel connection scenario in BatPaC

The influence of changing the system level of parallel connection is investigated. The connection of three module strings in parallel instead of three cells in parallel is modeled in BatPaC for the same modular configuration as in the NMC standard case. When parallel connecting three module rows some extra SOC control units are needed to treat the greater amount of information and less total amount of copper connects are required, see indata in table A.5 in Appendix A. The efficiency and actual losses from parallel connections on module level, pack level and cell level should be studied in order to account for the costs of a shared modularization between PHEV car and PHEV bus.

4.4 Use phase

The use phase is known to have a great impact of the vehicle life cycle. The aim to reduce emissions and fuel consumption has led to the PHEV solution which allows combining electric driving with ICE driving. For an appropriate evaluation of the battery environmental impact it is important to take both the electricity consumption into account and the fuel consumption which both can be related to the load carried on the vehicle at the medium speeds common in city driving. Fundamental for a bus in city service is to carry a high number of passengers, a need that may become limited by a weight increase of the bus due to the electrification. The scenarios for the use phase have been selected to illustrate city driving of a common bus size with average passenger load, comparing PHEV bus to a standard reference bus and a hybrid bus. The per passenger impact of the battery weight added is also made to give an illustrative example for the later battery life cycle impact assessment.

Vehicle and driving parameters

The use phase scenario is modeled after the intended use of a bus. A city driving cycle chosen similar to the European standard 'Braunshweig' cycle [Barlow, Latham, McCrae, Boulter et al. 2009]. The assumed average annual driving distance was assumed to be 120000 $^{\mathrm{km}}/_{\mathrm{year}}$. The electric range which is important for the possible fuel savings was kept high, at 80%[4] of the total driving range. Since the driving conditions are quite intense, the vehicle life length was assumed to be 9 years, for which three batteries were assumed to be consumed[5]. The battery life length is theoretical and should be validated once measured use data are available. For a summary of all data used in the modeling of the driving see table A.6 in Appendix A and table 4.6 for emissions accounted for.

Table 4.6: Emissions from driving, with 0.211 $^{\mathrm{kg\ diesel}}/_{\mathrm{kWh}}$, 40% efficiency. Ammonia emissions from urea are neglected. *Emission limits for the Euro VI legislation.

Emission	**g/kWh**
CO	0.0305 (1.5*)
HC	0.000026 (0.13*)
NO_x	0.107 (0.4*)
PM	0.0023 (0.01*)
CO_2	681
SO_2	0.0013

Energy consumption related to vehicle weight

The vehicle weight for truck or bus with two axes is 18000 kg, according to the Swedish transport authority [Transportstyrelsen 2013]. In reality the bus weight is measured from the front axis and the rear axis of the vehicle according to a set of rules implying that the total weight of the vehicle may be higher. The placement of the engine and battery has importance for the measured total bus weight and thus the number of passengers that are allowed. The distribution of the maximum passenger load together with the curb weight amounts to 19 tonnes for the hybrid bus 7900 [Volvo Buses 2013*a*] the same assumption was set for the PHEV bus.

A heavier vehicle will use more fuel. The fuel consumption increase was assumed to be linear, at least 2% increase for every added 1000 kg load on the vehicle [4]. In these speed ranges the air resistance force can be neglected, while the rolling resistance and the acceleration force ($m_{vehicle} \cdot a$) may be considered. On a vehicle of 12000 kg with 1000 kg added, the weight increase is 8% making the minimum energy consumption increase by the same percentage for a standard bus. In the hybrid bus the regenerative braking reduces the losses and the assumption of a max increase of 7% is reasonable [6]. The electric motor was assumed to have a proportional increase of electricity consumption in relation to the weight added [4]. The power of the battery was assumed to be 170 kW to suit the given vehicle weight and for absorbing the braking power and furnish the electric motor with the sufficient power in full electric mode with some margins for degradation of the power output during the battery service time. The reference electric motor is of 150 kW [Volvo Buses 2013*a*].

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[4] Estimate from personal communication with Edward Jobson, 2013.

[5] Estimate from personal communication with Jens Groot, 2013.

[6] Estimate from personal communication with Johan Johansson, 2013.

The fuel consumption for the average loaded standard bus was supposed to be 0.45 l/km, for the hybrid and PHEV bus, 0.31 l/km full hybrid mode, and 1.5 kWh per km full electric mode. To reduce the NO_x emissions according the Euro VI limits urea solution is injected with the diesel [Johnson 2008]. See table 4.7 for detailed data.

Table 4.7: Number of passengers and energy consumption related to normalization of the use phase per passenger and kWh charged electricity for PHEV bus scenario.

PHEV bus Parameter	**Value**	**Personal communication**
Average weight 1 passenger	75 kg	Martin Åslund
Linearized diesel consumption increase	7 %/tonne	Johan Johansson
Electricity consumption increase	Proportional to weight increase	Edward Jobson
Max All-diesel consumption full bus	0.40 l/km	[Calculation]
Max All-electricity consumption full bus	1.94 kWh/km	[Calculation]
Max passengers with 500 kg added battery weight	83	[Calculation]

The impact of weight increase on the bus due to the battery can be seen in different ways depending on the scenario used. The battery added on the maximally loaded bus will not change the fuel consumption but reduces the number of passengers [7], the battery added on a half loaded buss will only increase the energy consumption. In the case of lost passengers the allocation of an extra bus could be done to the marginal increase of battery weight [8]. The two first assumptions will be further considered in the modeling, and the last case will be discussed in the results.

As an example, to compare the per passenger and per km energy consumption of a full PHEV bus of 90 passengers and a similar bus with a 500 kg heavier battery, 7 less passengers would be transported in the heavier bus. If 1000 kg extra components and battery is added, and the total passengers are reduced by 13. The difference in fuel consumption per passenger and km depending on the added weight on the vehicle can be seen in table 4.8.

Table 4.8: Normalized energy consumption per passenger and km for PHEV bus. The actual energy consumption from the use phase is normalized per passenger in the case of full loaded bus, with 500 kg extra battery, and average loaded bus with 300 kg extra battery. Fuel and energy consumptions are taken from table 4.7 and A.6

Consumption	**Full load (ref) (90 people)**	**Full load 500 kg extra (83 people)**	**Average load (33 people)**	**Average load 300 kg extra (33 people)**
Electricity Wh/passenger km	8.8	9.5	18.4	18.8
Diesel Wh/passenger km	17.2	18.7	36.4	37.1
Energy Wh/passenger km	26	28.2	54.8	55.9
% of reference energy	100	108	211	215

Modeling of use phase and driving

The modeling of the use phase in the battery life has been done by adding 300 kg battery together with the average load of 33 passengers assuming that the drive line is similar to the hybrid bus 7900 and that extra battery weight has been added on top of existing components. The increase in energy consumption related to this increase in battery weight is accounted for.

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[7] Estimate from personal communication with Pontus Enhager, 2013.

[8] Personal communication with Lisbeth Dahllöf, 2013.

The original fuel consumption with 33 passengers on the bus is given in table A.6 in Appendix A, the increase is 0.0719 $^{\mathrm{kWh}}/_{\mathrm{km}}$ for the diesel consumption full ICE mode, and 0.0374 $^{\mathrm{kWh}}/_{\mathrm{km}}$ for the full electric mode. The results are normalized by kWh electricity charged and passenger. The relations between the energy consumption on a per passenger basis and the degree of completion of the number of passengers on the bus when the battery is added are shown in table 4.8.

4.4.1 Normalization and functional unit for LCA comparisons of the use phase

The normalization of the use phase of the battery is a difficult topic. The most uncertain parameter is the life length of the battery and it is quite difficult to determine and to predict since it depends on the driving style, about the slow or fast charging of the battery, on the dimensioning of the battery to suit these applications, on the BMS and management of cooling systems and voltage regulation. The only actual measurable parameter is how much electricity that has been charged to the battery and discharged from the battery.

It is tempting to calculate the impacts according to the number of cycles of the battery. The great disadvantage of this normalization is that one cycle of the battery can have different depth, different rates of power and to make it a unit means that a fictional average cycle depth should be created, in relation to the maximum SOC window. There is no standard method to translate the driving related battery cycles of different depths to an average cycle unit, with a clear relation to the battery life length. It is a lot different to cycle the battery cells in a laboratory under controllable conditions and to cycle the battery in the vehicle.

Still, a lot has to be done in research and development in this topic. A standardized method to determine the average cycle depth of the battery should be determined before it can be used in normalizations for the use phase of a vehicle. Two batteries used in the same type of vehicles in the same type of driving cycle and with equal control strategies could be compared over the same time. Since no such standardized control strategy of BMS is used in all vehicles this is the limiting factor.

To conclude, the battery is still a consumable product that can last for a long time or short time, serving the vehicle with more or less energy depending on how cleverly it has been used. It is up to the ESS manufacturer to furbish a battery with control strategies to withstand certain driving conditions, and up to the user to execute this precise driving in order to make the battery serve in its application as long as possible.

Per passenger and kWh electricity consumed by the battery

For the functional unit the choice has been done to look at the energy that passes through the battery during its service time in the vehicle. The efficiency of the battery is high around 95-98% [9] and decreases only marginally, less than 5% during service in the vehicle[9], thus the total electricity that is charged to the battery will be a measure of the function of the battery- to supply electricity. The measuring of the electricity upstream of the battery is feasible, the charged electricity from the grid to the battery is always counted. The amount of electricity will be large for a battery that lasts for many years and is used frequently, for a battery that fails during service the electricity consumed will be low. This means dividing the impacts with the consumed electricity for a highly functional battery will give a lower per unit impact than a less functional battery, which means that the functional unit serves its purpose. This functional unit avoids the issue of electric range, SOC, cycles, energy density and specific energy. The last two are drawbacks for this functional unit since the weight and volume of the pack are important parameters for the automotive service. However, the weight related to fuel consumption, and

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[9] Estimate from personal communication with Jens Groot, 2013.

volume indirectly determining the amount of battery capacity that can be fit into the vehicle are in this thesis considered as secondary from an environmental perspective. Instead the priority has been made to look at the life length of the battery. It should be taken into account when using this functional unit that a heavier battery will lead to a higher electricity consumption than a lighter one with the same performance.

To further include the purpose of the bus (which is to transport passengers), the functional unit for this thesis has been set to 'per passenger and kWh charged electricity', which means that the total life cycle impact results will be normalized with this unit.

4.5 Second use and reuse

Second use of the battery pack means prolonging the life of a product that otherwise would be scrapped, if it still is valid as energy storage. Hopefully second life will come to reduce costs for the PHEV user, and possibly reduce the environmental impacts of the battery life cycle. Previous LCA studies have shown that a 25% decrease of the environmental load is possible for a LFP 20 Ah lithium-ion battery life cycle when including second use [Cicconi, Landi, Morbidoni & Germani 2012]. Second use is, however, not in practice yet and some questions have to be answered in order to evaluate the viability: How does the battery design affect the possibility to use the battery in a second life application? Will then the use in the vehicle be reduced and the second life be longer?

As stated in section 3, the rationale for the battery retirement from automotive use can be both economical or performance based. One question is whether the battery should be retired earlier from the automotive service in order to continue in the second use sector. It has been shown that with a decreasing battery price it will always be more economically viable for the vehicle owner to keep the battery in the vehicle as long as the performance criteria are satisfied [Neubauer & Pesaran 2011]. It then is assumed that the investment cost of the battery is levelized per driven distance, the refurbishment cost is more than zero, and the repurposed battery will have a lower value (because of the consumer willingness to pay) than an equally performing new battery [Neubauer & Pesaran 2011].

The used automotive battery in second use application, will have a smaller amount of available cycles and a faster energy storage capacity fade than a new battery of the same initial capacity. Therefore, more second life batteries must be used to fill the same service life as of a new battery. In addition to the capacity fade the internal resistance of the battery will also increase, resulting in a high efficiency loss during the second life [Cicconi et al. 2012]. To account for this in LCA, the allocation of the replacement of batteries can be made by dividing the used battery, by a term of $N + 1$, where N is the number of battery replacements required by the second use, and adding the impact from the electricity loss due to efficiency decrease [Cicconi et al. 2012].

The second use and reuse rate depending on failure rates

The prediction of the cell failure rates in the second use, is important for making realistic assumptions about need for remanufacturing and exchange of cells. Such prediction requires tests of the cell failure rates at a certain number of cycles, for use patterns similar to the ones of the second use scenario. In a general approach it can be assumed that the probability of the need for a cell replacement should to be determined at the automotive EOL. Depending on the cell performance at the first EOL, it can be passed over to the second use or scrapped [Neubauer et al. 2012]. The amount of packs in a fleet of 1000 vehicles that can continue to second use with minor refurbishment at a cell fault rate of 0.0001 are 940 packs, counting the

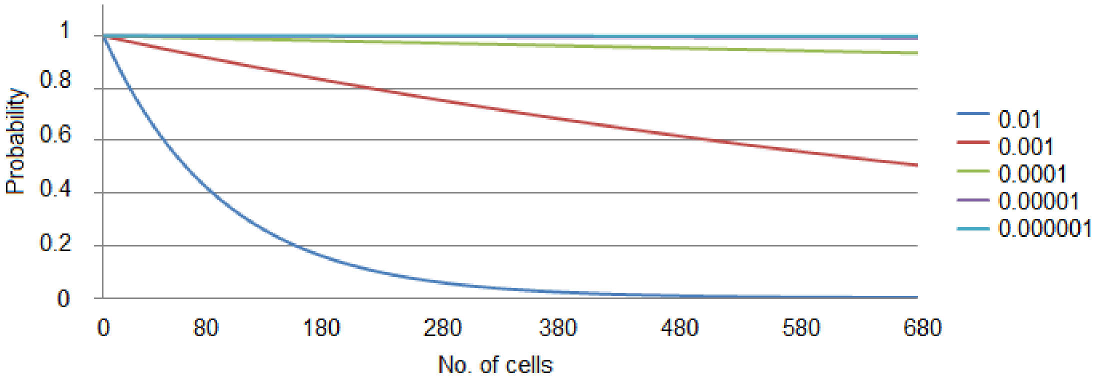


Figure 4.8: Theoretical module and pack yield in relation to different cell fault rates and numbers of cells, showing the probability of a functioning module or pack at a certain content of cells, after first use.

probability for the functioning of altogether 648 cells, $(1 - 1/10000)^{648}$. In the same way, a fault rate of 0.001, reduces the packs sent to second use to 520, and with 0.01 cell fault rate only 1.5 packs could be sent to second use. Thus second life could be possible only if the cell fault rate is less than 0.01 the second life could be possible, see figure 4.8.

If refurbishment is considered on a module level, the worst case of a cell fault rate of 0.1, for 12 cells per module, and 54 modules per pack would generate 15 functioning modules in one pack (28%), and if the fault rate is 0.001, the yield of functioning modules would be 53 (99%). For a smaller module of 4 cells the fault rate of 0.1, generates 66% module yield, and for a larger module of 24 cells, the yield would be only 8%. As stated in the article by Neubauer et al. [2012], the higher the fault rate, the smaller the module that would be required to make the second use scenario viable.

The refurbishment of the modules exchanging single cells, is a possible choice if high fault rates are unavoidable, and the refurbishment of complete packs, is an option in case of very low fault rates. Different options of remanufacturing of the system are showed in table A.7 in Appendix A. Either the battery packs are kept intact and are changed whenever the requirements of power and energy storage capacity no longer are met or the modules are exchanged when their internal capacity is below requirements.

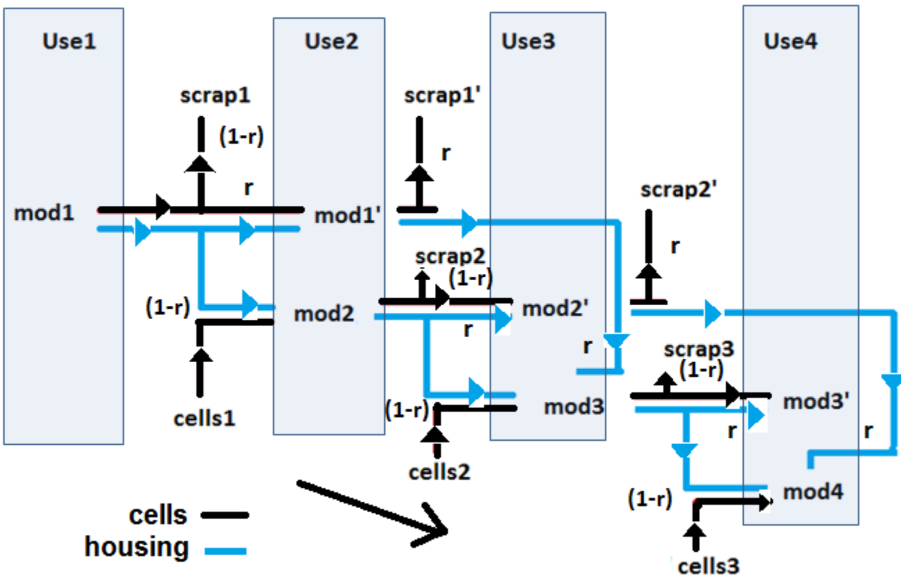
Averaged reuse rate

Taking the remanufacturing and the refurbishment of modules into consideration, it is necessary to evaluate the to what extent different components can be reused. Assuming the cells can be reused once, the maximum average reuse rate of cells would amount to 50%. However, if the functioning cell yield from the module only is 70% after first use, and an average of 50% of these can be used one more time, the resulting reuse rate for the cells in one average module is approximately 35%. The reuse loops with material flows are illustrated in figure 4.9.

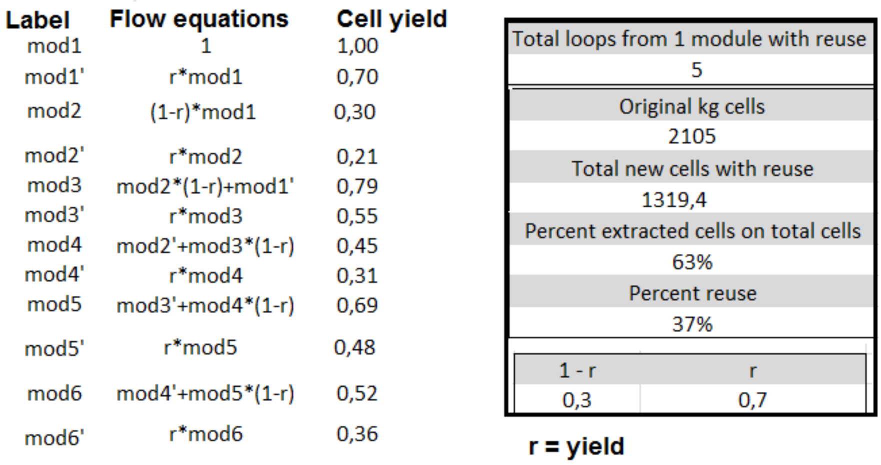
It should be noted, however, that in order to obtain these average results in all modules, a large fleet of used batteries would be needed. The inflow of new cells must also be guaranteed, since the cell reuse rate is different from the average module and pack reuse rate.

Second use example

UPS for small industries or large stores such as IKEA is a possible choice of a second life application for used automotive batteries. The battery will supply power during outages of 1 hour length, 10 times per year for 10 years, connected to the low voltage grid (400 V), with a power of 50 kW. The power requirement of 50 kW for 1 hour makes the need for 50 kWh



(a) Reuse loops for cells and module housing.



Label	Flow equations	Cell yield
mod1	1	1,00
mod1'	r*mod1	0,70
mod2	(1-r)*mod1	0,30
mod2'	r*mod2	0,21
mod3	mod2*(1-r)+mod1'	0,79
mod3'	r*mod3	0,55
mod4	mod2'+mod3*(1-r)	0,45
mod4'	r*mod4	0,31
mod5	mod3'+mod4*(1-r)	0,69
mod5'	r*mod5	0,48
mod6	mod4'+mod5*(1-r)	0,52
mod6'	r*mod6	0,36

Total loops from 1 module with reuse	
5	
Original kg cells	
2105	
Total new cells with reuse	
1319,4	
Percent extracted cells on total cells	
63%	
Percent reuse	
37%	
1 - r	r
0,3	0,7

r = yield

(b) Reuse equations for mass flows.

Figure 4.9: Reuse loops for one module unit, assuming a different reuse rate for module housing and cells. The cells could in the best case be used twice, and the housing is assumed to be reused for infinite number of loops. The cell and material flows are illustrated in (a), and the formulas for the mass flows are found in (b) together with the averaged percentage of reuse for the cells.

available energy storage capacity. With a SOC window of 60% this means 83 kWh total storage capacity. Every application would need 3 old 40 kWh bus batteries of 70% storage capacity. The total cycling would be 100 cycles which is marginal in comparison to the total number of 10000 cycles during the battery life making the application reliable if tested and diagnosed previously. The remanufacturing in this case would be minimal. The market is, however, small with presumably 10-20 applications to cover in Sweden, amounting to a fleet of at maximum 60 used bus batteries. The price of the battery could at maximum be set to 25% of the current market price [10].

This second life case is preferable compared to other larger UPS applications in which the additional installation equipment and cost makes the battery price neglectable in comparison, and the risk for dysfunction cannot be taken. In an LCA perspective the allocation of the saved new battery produced is difficult to determine. In fact the battery sent to second use could be evaluated on the basis on available storage capacity, the power, expected remaining life, consumer perception [Neubauer et al. 2012] or a coefficient of the new battery market price. The simplest approach is to assume that one old battery replaced 0.7 new batteries, and that the cradle to gate emissions from materials extraction could be avoided as a credit, given that the UPS would have been installed anyway, and that for maintenance the life time of the battery is set to 10 years even in the case of a new one.

If instead the original UPS application is expected to last 20 years and the predicted life of the used automotive battery lasts only half the time, the cradle to gate impact reduction of an automotive battery is only 35% compared to 70% according to the allocation method of [Cicconi et al. 2012]. The losses in electricity comparing the old and the new battery may be significant if the efficiency loss is high for the used battery, depending on changes in the material leading to increased internal resistance. The difference in losses on total charged electricity between a new and an old battery may be at least 9%, see table 4.9. In addition the capacity degrading may be at different rates for the old and the new battery and a linear approximation may be far from reality.

A possibility that can be considered is to make window change during the use phase, either for mitigating the gradual efficiency and capacity loss, or to make the battery last longer. The first design requirement of available capacity may than be dependent on many uncertain parameters, making the dimensioning difficult. This means that the first assumption of comparing the total capacities of the new and the old battery at present time may not be enough as a base for the dimensioning. As in the example in table 4.9 the initial capacity may vary with 50% depending on what dimensioning method used. The prediction models of battery life performance after automotive use will be needed for a more secure allocation and dimensioning.

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[10] Estimates from personal communication with Per Halvarsson, 2013

Table 4.9: Second use example for new and old battery in the same application, with a linear capacity degradation of 25%, and efficiency degradation of 5%. The losses are illustrative for the given efficiencies and number of cycles. The efficiency is applied both at charge and discharge of the battery. The maximum capacity takes capacity degradation, SOC window of 60% and efficiency loss into account. Instead the minimum capacity takes only the SOC window into account.

Parameter	**New battery Old battery**	
Cycles	20	10
Batteries consumed	1	2
Charging/discharging efficiency BOL	0.95	0.9
Charging/discharging efficiency EOL	0.90	0.85
Dimensioning output (kWh)	50	50
SOC window (%)	60	60
Min initial capacity (kWh)	83	83
Max initial capacity (kWh)	123	131
Total losses (kWh)	170	307
(%) Losses of total charged electricity	15	24
Electricity discharged (kWh)	1000	1000

Reuse and recycling assumptions for complete pack

Depending on the cost and difficulty of disassembly and remanufacturing of different parts, the concept of reuse is more or less convenient in relation to the value of the components. At current status the weak link in the battery is the lithium ion cells; the decision of size and life length of the battery pack is determinant for the service frequency for the vehicle. The most resistant components such as cases could be reused many times, assuming vehicle lifetime of 9 years, active cell life in vehicle service 3 years, the housing should for example be used as many as 5 times before being recycled. The cost of dismounting the contents and from the case together with transports should be lower than the cost of a new case.

The reuse rates in the models have been allocated on a basis of component life length expectancy in a simplified way. Three different life lengths have been used according to the component materials, dimensions and wear during the use phase in the vehicle. These very optimistic reuse rates have been set to give a best case scenario of reuse. For example the aluminium fins of the BatPaC construction are typically too thin to be disassembled many times, and the reuse could be zero, but on the other hand, recycling of the aluminium is likely to happen.

The highest reuse rate of cells has been set to 40%, with the assumed cell fault rate of 0.03 for the best case scenario. The constraint is set that one cell can be used at maximum two times. The EOL of the battery pack has been evaluated using general values for recycling and assumptions about reuse possibilities for various pack components. The recycling of the pack components was only considered to the extent of reducing the original extraction rates of materials, and so no values for energy or emissions during recycling, incineration or landfill are included.

The components in the pack that are static and are not subdued to any kind of movement, wear or corrosion have been given the life lengths displayed in table 4.10.

For the recycling, general averaged data have been assumed for the passive pack components, table 4.11 and for the cells no recycling was assumed in the total scenario. These assumptions have been made since data is missing and because it could be possible to recycle pack components at very high rates depending on the decision of the manufacturer. The cell recycling was excluded due to the high cost, and the probability that it will happen is low in the close future.

Table 4.10: Reuse rates battery components. The extraction rates assumed for the scenario of maximum reuse of passive battery pack components, based on the material thicknesses and aging during the use phase. The ESS system is set to last 3 years.

Battery component	**Extraction rate factor per ESS**	**Total years in service**	**Times used**
Pack housing	0.2	15	5
Module housing	0.2	15	5
Insulation	0.2	15	5
Copper connects	0.33	9	3
Steel connects and straps	0.33	9	3
BMS	0.33	9	3
Coolant	1	3	1
Cells	1	3	1
Thin (0.4 mm) cooling plates	1	3	1

Table 4.11: The recycling rates assumed for the scenario of maximum recycling of passive battery pack components, based on the extraction rates with reuse taken into account. No energy recovery of energy consumption is included for the waste management. Only the reduced material extraction is accounted for in the recycling scenario. The recycling rates are general average values commonly applied[Ashby 2012].

Battery component/material	**Recycling rate**	**BatPaC component**
Stainless steel	0.4	Housings, pressure plates and straps
Aluminium	0.55	Housings, cooling plates
PU	0	Thermal insulation for housing
PP	0.06	Housings
Copper	0.40	Connects
BMS	0	-
Coolant	0	-
Cells	0	-

4.6 Cell recycling models

The end of life (EOL) stage of the LCA is an important stage to assess since it can help decrease the impact of the material choices by recycling materials and allocating the emission between different products. However, it should be stated that great uncertainty is associated with the recycling step, since it occurs in the future, it is cost driven, new materials are constantly developed and the state of the battery when it reaches this stage varies.

Since recycling is both a current and future problem, comparison of one existing recycling method for NMC with one future method of LFP is of interest. For the current method more data exists, but for LFP it is also of interest to look beyond existing methods that focus on Co and Ni extraction. Therefore a hydrometallurgical method will be included for LFP. This choice will give perspective on possible future recycling alternatives.

Pyrometallurgical method

As a model for the pyrometallurgical process data from a report by Dunn, Gaines, Barnes, Wang & Sullivan [2012] was used. The report presents an assumption of the energy requirements for a pyrometallurgical recovery method, based on the process by Umicore. The data was presented in the form of energy/kg_{cobalt}, although the exact chemistry was unknown. It was also stated that the percentage of cobalt in the battery was 14%, information taken from a patent by Umicore [Cheret, Santen et al. 2007]. In order to apply this data to the NMC evaluated in this thesis the data was translated into the general form energy/$\text{kg}_{battery}$, which then was assumed to be a good approximation also for other types of layered oxide Li-ion batteries, like NMC.

The steps involved in the process were:

- Smelting, $0.21\,\text{MJkg}_{input}$.
- Leaching, $0.08\,\text{MJkg}_{input}$.
- Solvent extraction, requiring stoichiometric amounts of HCl.
- Oxidation, requiring stoichiometric amounts of H_2O_2.
- Firing, $1.18\,\text{MJkg}_{input}$, requiring stoichiometric amounts of Li_2CO_3.

The solvent extraction and oxidation steps were assumed to require zero energy input.

Hydrometallurgical method

For the LFP chemistry, where pyrometallurgy is of no interest due to the lack of valuable Co and Ni parts, a hydrometallurgical method was modeled as recycling method. With the aim to extract lithium as well as valuable copper and aluminium, the method chosen was a promising future one, solvent extraction. The data for this process was based on lab-scale test of this process performed by Kosaraju [2012].

The steps involved in the process were:

- Dismantling, cutting the cell and separating active material from foil, requiring HCl for leaching.
- Solvent extraction, requiring kerosene and Cyanex 272 mix for extraction.
- Lithium extraction, requiring HCl.

It is possible to extract iron with an additional leaching step, but this will be disregarded in this thesis. The pouch and the separator are also assumed not to be recycled, and could possibly end up in an incineration process to eliminate waste. This will not be included in the assessment. The foils are assumed to be recycled back to foils, which is somewhat misguiding. They are recycled in their original form, but the potential to use them is more limited since they are already cut.

Since the energy requirements for each step are highly dependent on the scale of recycling, and no large scale test have been made, it is assumed that no process energy is required. The savings can then be viewed in light of this, as potential savings. The main impact from this method is in the cost and environmental impact of the chemicals involved. It is assumed that 90% of the solvents and extractants are recycled in each cycle. To motivate this assumption reports show that large scale systems have stated recovery up to 97% (Dalal Engineering), while small scale have reported around 75-80%. Pharmaceutical companies have set a desired recovery at 90% [Rockwell Automation 2009], making this value a reasonable assumption for this future method. It should also be noted that additional energy consuming steps, apart from those mentioned above could be needed to ensure various things, for example that the solvent and binder do not get released with the waste water without processing.

Recovery rates

In the future of battery recycling the goal would have to be to recycle the constituents back to battery grade material. For the purpose of this thesis we will count material recycled to a lower grade, but with opportunity to be improved to battery grade material, as recycled. With this approach the energy cost of refining the material would be placed in the LCA of a battery using recycled materials. In the LCA the recovered material will be set as a negative contribution, and the size of this contribution will be equal to the energy consumption of the corresponding input material.

Some different recovery rates were used for the different materials and recycling processes. In the pyrometallurgical process it is assumed that either all or none of the material is recycled, the effect of this assumption will be tested in the sensitivity analysis. Most likely, there will be some slag left from the reactions occurring when pyrolized. The same assumption is made for the hydrometallurgical method, except for the electrolyte were some losses due to evaporation are assumed. For this process the assumption of 100% is more likely to be achievable, since all the materials are handled in their pure form, and thus no yields for reaction need to be taken into account.

Results

This chapter presents the results from the life cycle assessment of battery cells (section 5.1), modularization and pack design (section 5.2), use phase (section 5.2.1) and recycling (section 5.4). The energy during the cradle to gate of the components are analyzed, along with the chosen impact categories. The potential energy savings from recycling are presented separately.

5.1 Cell manufacturing and constituents

The cell and its material production are major components in the impact of the production phase of the battery system. The impact per cell is also largely independent of other parameters related to the whole ESS, making the cell assembly results applicable to other system configurations than the ones modeled here. Therefore the impact of different cell chemistries and process choices will be presented as a separate category, where the implication of changes in the cell will be in focus. The same cells will later be viewed in light of their place in the total system, see section 5.2.

5.1.1 Energy use for the cell components

The energy consumption during material extraction, production and cell assembly is an important step to analyze. Both the total amount used and the distribution between the different stages have implication for total impact and possible gains of recycling.

Figure 5.1 shows the energy use impact of the different cell components for the various chemistries, and the total energy consumption for one kg of battery cell. Independent of chemistry and production method, it is the lithium-based electrodes that have the largest impact. For this reason, the fact that LMO uses LTO anodes instead of graphite means a higher total energy consumption for this cell type. The production of one kg of cell required roughly 80-100 MJ for the graphite based cells, which is in line with, or slightly lower than previous work [Majeau-Bettez et al. 2011] [Notter, Gauch, Widmer, Wager, Stamp, Zah & Althaus 2010]. The results from the LTO based cells are slightly lower than previous work [Kushnir & Sandén 2011].

The total results for the different production paths give indications on the best approach for producing cells with different chemistries. For the cells using materials that need nano-sizing there is a clear advantage in using the wet synthesis. For the cell not needing nano-sizing, NMC, the impact is more equal between production paths.

The impact from the cell casing seen in figure 5.1 is mainly caused by the use of aluminium. More than 90% of the energy use for this component comes from the aluminium foil and its processing. The plastics and their processing play a smaller role, suggesting room for improvement if less aluminium is used. For the separator, the main energy consumption is

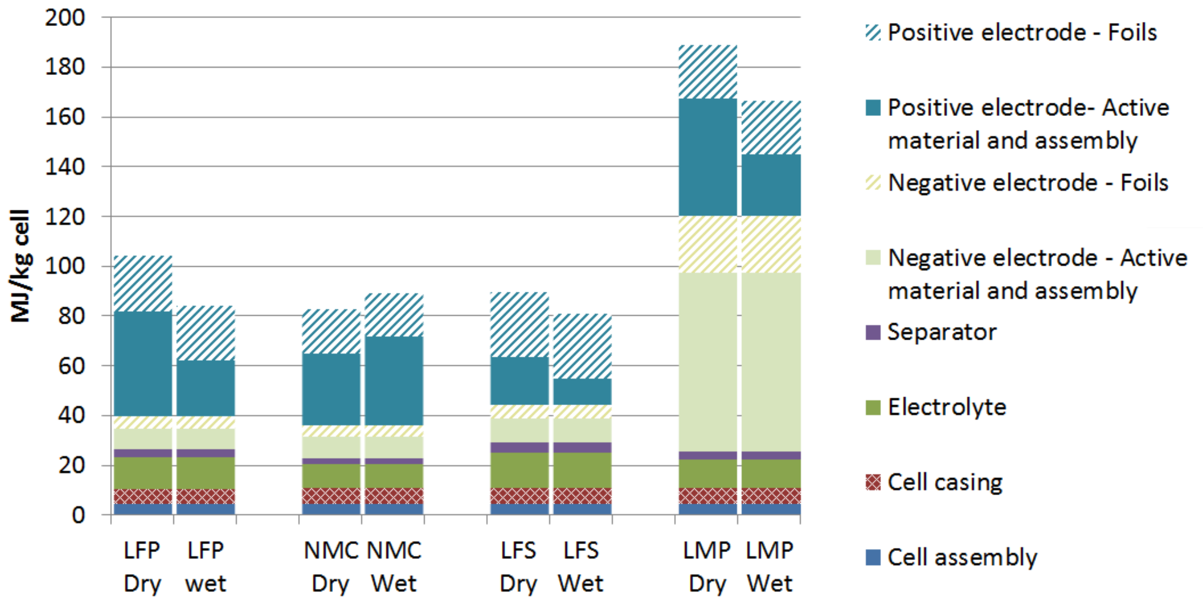


Figure 5.1: The energy consumption from extraction of materials to finished cell is shown for each cell component. All chosen chemistries are represented, with both wet and dry production alternatives for the cathode active material. The negative anode is graphite based for all chemistries except for LMP, where the anode active material is LTO. It can be seen that the electrodes consisting of active material and foil have large impact.

in the plastics, and only a little over 6% is from the production. Due to the way the electrolyte production was modeled, with no energy consumption for the mixing steps, all the energy impact is from the constituent materials and their production. The contribution from the solvent materials and the salt precursors is roughly equal, with a slightly higher impact from the carbonate solvents. The cell assembly with its energy consumption both from electricity and heat contributes around 5% of the total energy use, when looking at the production alternative with least total consumption.

Energy use of the electrode components

As shown in figure 5.1, the positive electrode is a key consumer of energy during the cell production. In figure 5.2 the impact of each of the components in the positive electrode is shown. This reveals the large part that the foils play when it comes to energy consumption. The assembly of the electrode is a minor part. It is also clear that the relation between energy from processing and energy from materials in the active material production varies depending on the type of production method used.

When the materials needs to be nano-sized, like for LFP, LFS and LMP, the process energy for the dry synthesis rises considerably due to the extra milling step. This difference is not present in NMC, here the simplicity of the dry process can be beneficial. The effect of assuming different amount of water as heating solution during the wet process can be seen in the difference between LFP and LFS wet, LFS is modeled as using less water per kg active material, and the energy use scales accordingly. The energy consumption for the LFP wet process is slightly higher than in previous studies, indicating a possibly over dimensioned assumption of the amount of water needed [Kushnir & Sandén 2011]. The dry process for layered oxides is fully in line with previous work. The indication of improvement when using a wet process on nano-sized materials is consistent with previous work [Kushnir & Sandén 2011].

The relative impact of the active material production and the active material precursors

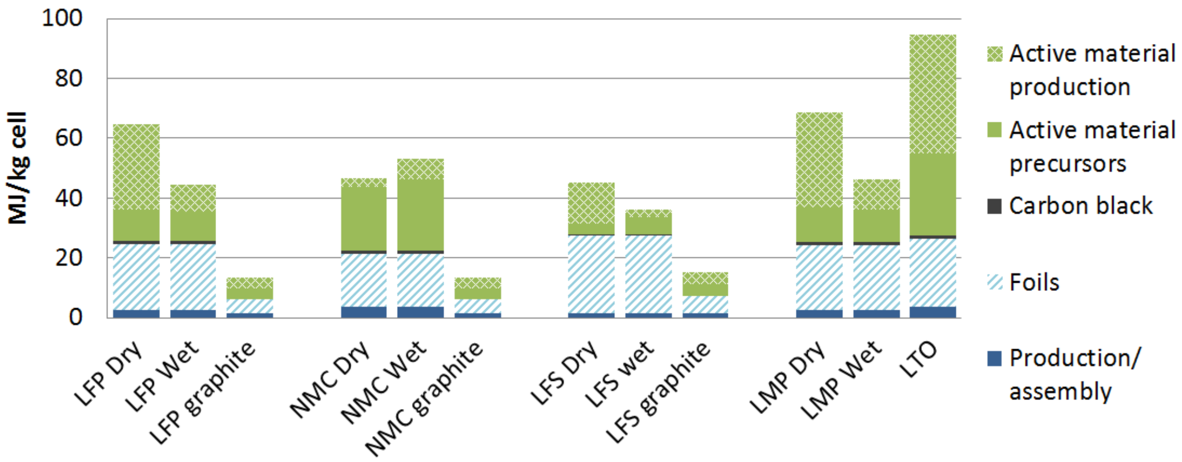


Figure 5.2: The energy consumption from extraction of materials to finished cell is shown different constituents of the positive and negative electrodes. The energy is calculated per kg of total cell, and thus the results reveal the relative impact of different electrode constituents for a certain chemistry, as well as the difference between chemistries. The foils and the active material stand for virtually all the energy consumption of the electrodes.

vary. For NMC the main impact is from the precursors, highlighting again the energy intense materials used in this chemistry. In the dry process over 70% of the active material energy is from Co and Ni precursors. In the wet process the chemicals for hydroxide production further increases the impact of the active material precursors, although less energy intense materials can be used as nickel and cobalt source, only contributing 30% of the active material energy consumption. Improvements to the process will only give minor benefits in this case.

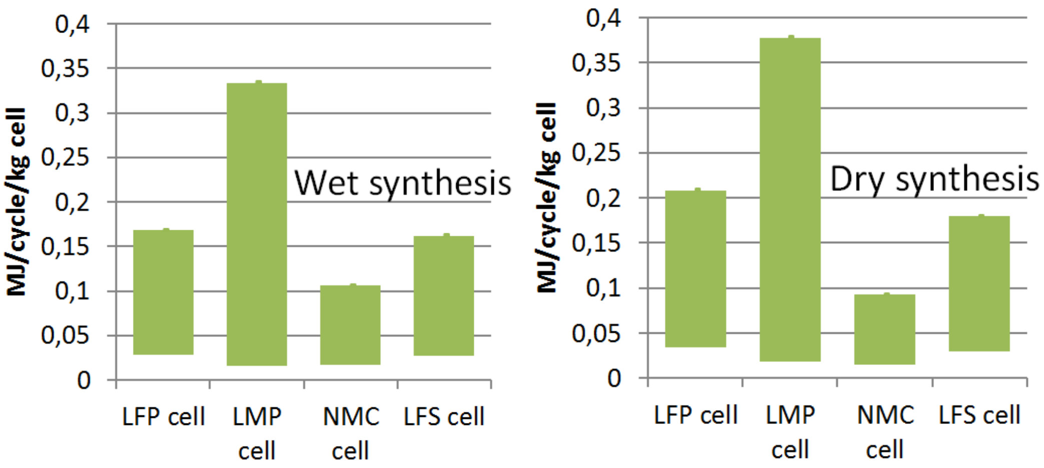
In contrast LFS has its main impact from the process. The active material also has a smaller total impact. LFP and LMP have a wet synthesis consuming energy close to that of NMC, but the contribution of precursors versus production is changed, making improvements in process equally beneficial to improvements in precursor alternatives. In these material there is also no dominating precursor, as Ni and Co are in NMC.

Switching focus to the anode it can be concluded that the graphite anode has a much smaller impact on the energy consumption than the cathodes. The relative contributions within the electrode between active material and foil is however similar. Changing anode to LTO, with its difficult production and demands on nano-size, greatly increases the energy consumption. This effect is due to the change of foil to aluminium, and the great increase in process energy and precursor complexity compared to graphite.

Looking again at the impact of the foils, the aluminium in the cathode electrodes has a larger energy impact than the copper in the anode. The positive aspects of using aluminium are not coupled to energy consumption, but rather to price, and aluminium is used were possible. An additional effect is also that the copper sheet can be thinner, and thus less material is used. In the electrodes the energy consumption is basically only from the aluminium foil and the active material, in average around 50% each depending on chemistry and production path. This result is consistent with that of Notter et al. [2010], showing the aluminium foil contributing more than 50% of the cathode impact.

Normalizing with available cycles

The energy consumption when producing a cell use should also be viewed in light of the possible life-length of the cell. Since the LTO anode provides the possibility of more cycles this can



(a) Best/worst case energy, wet synthesis. (b) Best/worst case energy, dry synthesis.

Figure 5.3: The production energy per kg of cell is presented normalized with the available cycles. Best case represents deep 3000 cycles for the graphite anode based chemistries (LFP, NMC, LFS) and 10000 for the LTO anode chemistry (LMP). Worst case is represented by 500 deep cycles for all. It is clear that a full utilization of the available cycles compensates the higher energy use of the LMP-LTO cell.

compensate the higher energy consumption during production. The impact of this normalization can be seen in figure 5.3, where the worst case performance has been set to 500 full cycles, and the best case to 10000 full cycles for LMP and 3000 full cycles for the other chemistries. Full cycles implies that the depth of discharge is equal to the cell capacity.

It is clear that a full utilization of the possible 10000 cycles for LMP with the LTO anode fully outweighs the larger energy consumption shown in figure 5.1. However, if this possibility of longer life-length is not utilized fully the anode choice cannot be motivated compared to the less energy intense graphite anode. However, the indication of prolonged system life that comes with increased cycle life can be of great importance to the viability of batteries as ESS. Previous work concludes that the impact of improved cycle life goes beyond the differences in energy use, since the benefits of having systems that last as long as the vehicle are very large [Kushnir & Sandén 2011].

Figure 5.3 illustrates the opportunities for improvement coupled with using materials that increase the life-length of the battery. The increased life can make the production cost per year equal to that of cheaper cells, and the costs of changing or updating the battery when it is placed in the vehicle will decrease, since fewer batteries will be needed. Therefore it is clear that large gains can be found in improving the life-length, and the added production costs must be viewed in light of this.

5.1.2 Impact categories of the cell components

To achieve a full assessment of the impact of the different production methods and their corresponding precursors, it is not enough just to look at the energy consumption. This since different precursors can be used, with more or less environmental impact.

The most illustrative results for the impact categories are presented in figure 5.4. The impact of the different components, for all impact categories, can be viewed in figure A.1. The electrodes dominate all of the impact categories, albeit to a varying degree, and will be broken down and discussed further. For reference it can be stated that the total GWP of 6-7 kg CO_2 equivalents for the cell is in line with other bottom up LCA results. Notter et al. [2010] have for example stated a 6 kg CO_2 equivalents use per kg of cell.

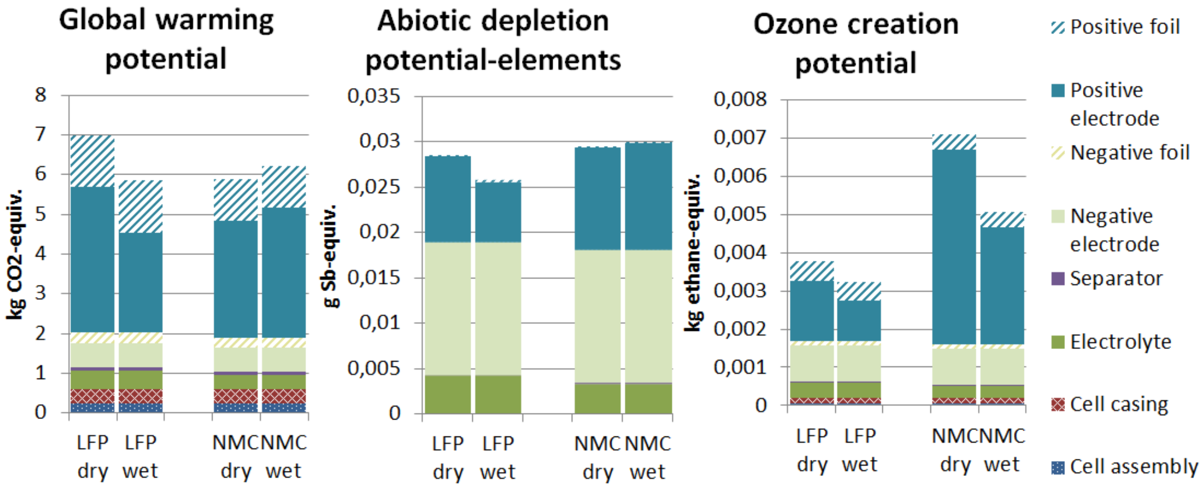


Figure 5.4: The impact of the different components of the different cell chemistries is shown. The impact categories represented are energy use, global warming potential, abiotic depletion potential of elements and fossil fuels, acidification potential, eutrophication potential, human toxicity potential, photochemical ozone creation potential. The electrodes can be seen to have the largest single impact.

Looking at the supporting components, the electrolyte has most of its impact linked to the acidification potential (AP) and abiotic depletion potential (ADP) of elements, but can be found to impact all categories. The ADP is linked in equal amounts both to the carbonate solvent and the precursors for the salt, which is also the distribution of impact for all the categories. The acidification comes mainly from the possible chloride emissions from the salt production, modeled as stoichiometric amounts of HCl. Improvement to the electrolyte can clearly be of interest, since it impacts all categories, and this could possibly be done by switching to materials with less impact than the currently involved carbonates and salts.

The separator has a very small impact, mostly linked to the use of fossil fuel for plastic production. This makes the main impact categories for this component global warming potential (GWP) and ADP of fossils. As with the energy consumption, the main impact from the casing is from the use of aluminium, giving it a slightly higher impact in the human toxicity potential (HTP) and GWP compared to other impacts. For HTP aluminium stands for 99% of the impact of the casing and for the AP for around 97%. In all other impact categories the impact of aluminium is closer to 90% of the casing impact, comparable with the energy percentage. The cell assembly mostly involves the use of energy and therefore impacts the categories coupled to fossil fuel use, GWP and ADP of fossils. Generally, as for the energy consumption, the impact of the passive components comes from the use of aluminium in the casing and from the materials in the electrolyte. These results are in line with previous studies, indicating that the supporting materials does not contribute greatly to the energy consumption or GWP [Dunn, Gaines, Sullivan & Wang 2012] [Notter et al. 2010].

Impact categories of the electrode components

The positive electrode dominates all impact categories, except for the abiotic depletion potential of elements. Here the copper in the negative graphite electrodes makes this component a key impact. This illustrates the scarcity issues, and possible gain of using aluminium foils instead of copper, although the energy impact of aluminium is greater. Beside the impact of the copper on the ADP of elements, the negative electrode contributes to ADP of fossils and GWP as well. Here the impact is shared by the copper foil and the graphite production. The negative electrode can also be seen to impact photochemical ozone creation potential (POCP) to some

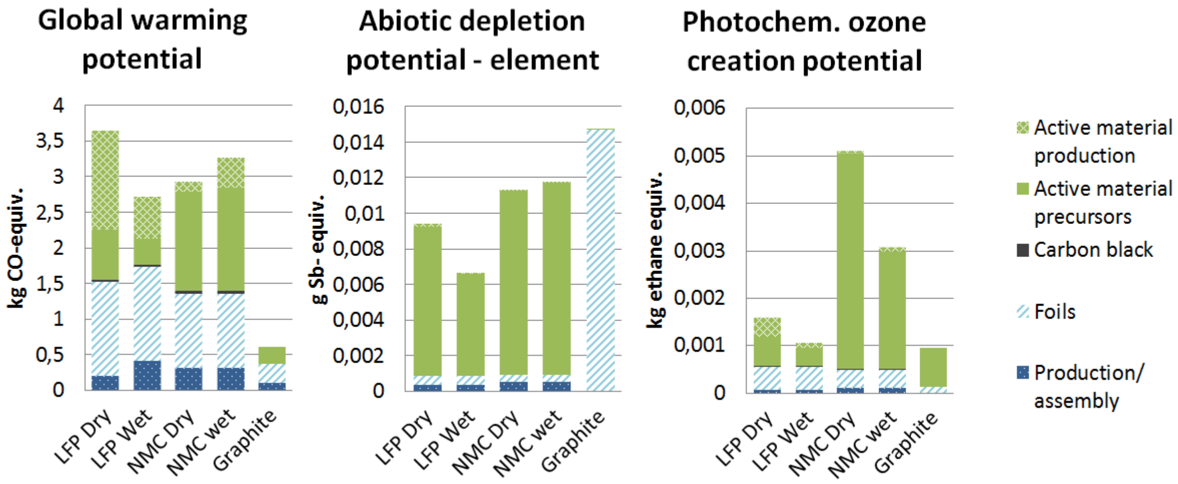


Figure 5.5: The impact of the different components of the positive electrode is shown, for different cell chemistries and production paths. The impact categories represented are energy use, global warming potential, abiotic depletion potential of elements and fossil fuels, acidification potential, eutrophication potential, human toxicity potential, photochemical ozone creation potential. The foils and active materials dominate, but the relative contributions vary.

extent, due to the emissions from graphite production.

As mentioned, the positive electrode is a key component influencing all of the impact categories to great extent. For a deeper understanding, the most illustrative impacts of different subcomponents in the positive electrode can be seen in figure 5.5. For the impact of the different components in all impact categories see figure A.2 in Appendix A. The aluminium foils are dominant for the GWP and ADP of fossils. The production of the active material, and also the assembly of the electrode, is an electricity and heat demanding step, and thus impacts the GWP and ADP of fossil fuels. The increased electricity use of the milling step in dry synthesis of LFP can be noticed. The effect of this can be mitigated by using electricity and heat sources with less carbon foot-print, like renewable sources.

The impact of the chosen conductive additives is quite small. The starch used in the wet process does, however, impact the eutrophication potential to some extent. It also required slightly more energy than the carbon black used as additive in the dry process.

The precursors for the positive electrode active material have high impact in almost all of the categories. Interesting to note is the difference in the impact when comparing NMC and LFP chemistries, LFP consumed more energy, but NMC impacts almost all other categories to a greater extent than LFP.

NMC has higher impact in GWP and ADP of fossil due to the energy intense precursors. Also in ADP of elements NMC has the largest impact, with the main impact for NMC being the impact from the nickel and cobalt, but also with contribution from the lithium. In AP NMC has its main contributions in the emissions from nickel production. However, it is possible that this impact is too high, since the materials are modeled based on metallic nickel, see Appendix A.The human toxicity potential and photochemical ozone creation potential are other categories were the NMC active material has a large impact, especially for dry synthesis. Again it is the nickel oxide that gives the large impact.

The large impact of the dry processing for both NMC and LFP on the EP is due to the choice of diammonium phosphate as phosphate source for LFP and again the nickel oxide for NMC. For LFP the impact in ADP of elements comes from the use of lithium, with slight impact also from the phosphorous source in the dry synthesis case.

It can be interesting to note that on a per kg basis aluminium foil has the largest impact in the GWP and ADP of fossils categories while copper only influences ADP of elements. Nickel and cobalt impact both GWP and ADP of both fossil and elements. Nickel has a large impact also in AP, EP, HTP and POCP.

It is clear that there can be interesting conclusion drawn from looking at the impact categories, since they illustrate the benefits of choosing common and non-toxic elements. While the energy use for LFP and NMC cells are similar, favoring NMC, the impact of using LFP is smaller for virtually all impact categories assessed in this report. This conclusion is validated by previous similar studies, comparing NMC and LFP [Majeau-Bettez et al. 2011].

Improvements when using $\mathbf{LiMnPO_4}$ and $\mathbf{Li_2FeSiO_4}$

The impacts if LFS and LMP are not presented in detail, since they are modeled in much the same ways as LFP, with the main differences in the active material precursors. Therefore, a comparison with the impact of the LFP components are more interesting. For graphical representation see figure A.3 in Appendix A.

Using the high capacity LFS leads to a need for less active material in general. Due to this, the impact of the materials is lower for LFS compared to LFP, although the synthesis may be similar. However, due to the lower density of LFS, and since the coating thickness is kept equal, the amount of inactive material is increased. As mentioned earlier the aluminium is the greatest factor of the inactive components of the electrode and hence an increase in aluminium will impact all categories. Regardless, a switch to LFS could in total be potentially beneficial, due to the lowered amount of active material. The impact of silica compared to any phosphorous source is also beneficial since silica has virtually no impact in any category. If the coating thickness can be made thicker, this would decrease the impact of the foils and other passive components, limiting this increase.

LMP and LFP were modeled as having equal production paths. Acquiring manganese precursors could require slightly more energy, giving this material a higher impact. However, the higher voltage gives reason to assume that this increase can be outweighed by performance, although this is not shown quantitatively. In the case modeled in this report, the main change between the LFP and LMP is not in the active positive material, but rather in the anode material.

Impact when using graphite versus $\mathbf{Li_4Ti_5O_{12}}$

Focusing on the impact of the anode, the graphite anode is a minor component in most impact categories. The copper foil does however make it a key component in the ADP of elements. The active material in the electrode, graphite, has similar impact as for example LFP in HTP and POCP, but no impact from the foil. In all other categories the impact is smaller than that of the cathode active materials.

The LTO anode has been evaluated in comparison with the graphite one. When the impact is normalized by available cycles (3000 for graphite and 10000 for LTO), LTO shows a doubled impact in most categories, see figure 5.6. The main difference is the decreased ADP of elements achieved when changing the foil to aluminium. The graphite material also impacts the POCP, and this impact is reduced with LTO. However, there is a general increase in impact even when normalized by the cycles, and this is an indication that other aspects than energy use must be taken into account when switching to LTO. One explanation to the increased impact of LTO is the fact that more mass of active material is needed per kg of cell, since LTO has a lower capacity than graphite, 170 $^{\mathrm{mAh}}/_{\mathrm{g}}$ compared to 330 $^{\mathrm{mAh}}/_{\mathrm{g}}$ for graphite.

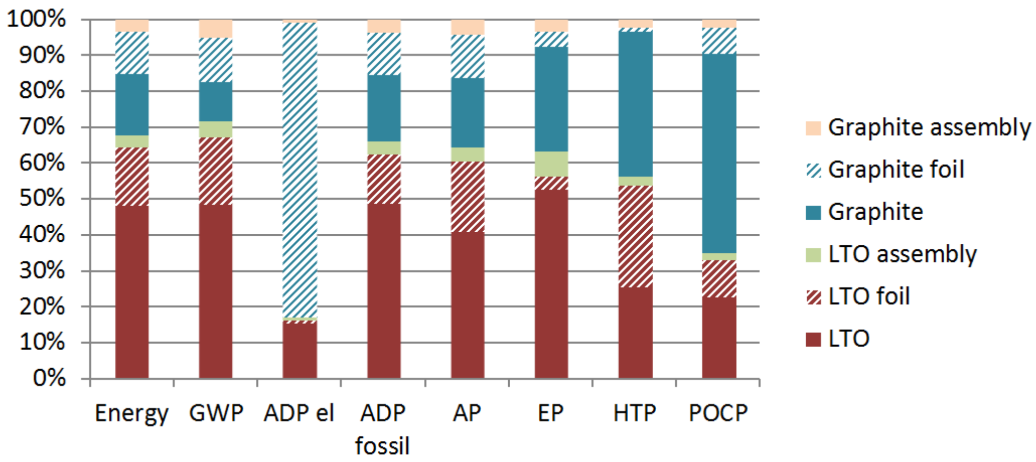


Figure 5.6: The relative impact of the different component of 1kg of graphite and LTO anodes are presented. For most impact categories the red LTO has a greater impact, most likely due to the need for more active material. Graphite has high impact on the ADP of elements due to the use of copper.

5.1.3 Applying weighting methods

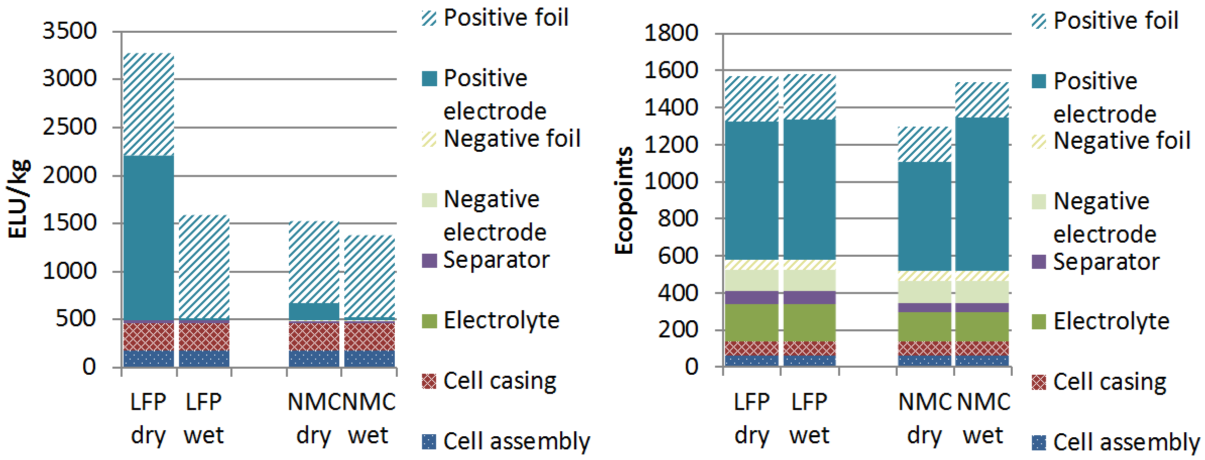
The impact of different cell components can also be viewed in light of a weighting method, where all impact categories are summed into one impact value. This can give an insight into the effects of all the impact categories, depending on what your focus is. The two weighting methods, EPS and EI99, where presented in section 2.2.

Figure 5.7 shows two different ways of summing the impacts. EPS puts high penalty on the use of EU-27 electricity, since this mix includes hard coal and lignite with large ELU/MJ, and therefore LFP produced with dry synthesis has a high impact due to the electricity used for milling the material. The NMC precursors give slightly higher impact compared to LFP precursors, but also here it is the electricity that contributes most. It should also be noted that aluminium foil has a large impact on EPS score, due to its production with hard coal and lignite energy sources.

Looking at the EPS score for wet synthesis, the LFP material is beneficial compared to NMC, but this result is balanced by the need for more passive material in the cell, due to the lower density of LFP. This leads to the need for more aluminium, which in turn gives a high EPS score. LFP with wet synthesis is however more comparable to the results of NMC, with the main contribution from the foil. The cell casing also impacts in this weighting, since it contains aluminium. The anode graphite, and the electrolyte impact very little.

Looking instead at the results from the EI99 weighting the different chemistry alternatives are more equal. For NMC, dry is more beneficial since the wet process uses more energy, and most importantly uses chemicals like ammonia to produce the precursors. This even though the precursors themselves have a larger impact when using dry processing. Due to the dry precursors being modeled from metals this difference might be even larger. In general, higher energy use both from electricity and heat have a great impact on this weighting method. Again, the wet processed LFP active material has less impact than NMC, but this is compensated by the need for more passive material. The more simple precursors of LFP dry now give a larger benefit since EU-27 electricity and natural gas heat are more equally weighted. Compared to NMC it is, however, the larger total use of energy that makes the weighted result for LFP worse for both production paths.

Both weighting methods emphasize the importance of considering the energy consumption. Depending on how different energy sources, like natural gas or coal based sources, are valued different materials will have more or less weighted impact. Depending on where focus is placed,



(a) EPS weight.

(b) EI99 weight.

Figure 5.7: Summed total impact of all categories, with different weight methods applied. Both results for the EPS and EI99 methods are shown. In EPS, LFP dry is clearly less beneficial. In EI99, the different chemistries and production paths are more equal.

the fact that NMC has higher impact than LFP in basically all impact categories becomes more or less important. In the weighting methods discussed above the larger energy consumption of LFP makes the NMC favorable. For production this is a guide that will optimize the production cost today. On the other hand, it is possible that this choice would not be sustainable over a longer period of years.

5.1.4 Implications for future chemistries

Looking into specific examples of future chemistry candidates, the results from the Li-ion chemistries can suggest some implications for other chemistries as well. Since the electrode active material plays a large role, and since the amount of inactive materials could be decreased, Li-S could be one technology largely beneficial for environmental impact.

Additionally, the impact on some of the categories can be decreased when going from metal based cathodes with costly precursors to simple and cheap sulfur. Further evaluation on each category would be needed to assess this in detail, especially to evaluate the impact of sulfur. It should be noted that if Li-S is shown to require a supporting structure of some sort, this could increase the weight and therefore impact the gravimetric energy and power density, as well as adding energy consuming materials to the process.

Na-ion as an alternative would most likely not influence the impacts of the cell to great extent, since the impact of lithium is such a small component. The increased weight of using Na-ion could instead impact the use phase negatively and using more aluminium would increase the energy need, since this foil type was shown to have greater impact than copper foil. Most likely it would be the economic benefits of using Na-ion chemistries that would guide towards the implementation of this type, and this is of course in practice a factor of great importance. It should also be taken into consideration that the need for other anode materials than graphite might impact the life cycle.

Since the active materials, and the electrodes in general have such a large impact, organic based cells or electrodes could present large improvements to the impact of the cell. If the need to use foils can be reduced this would be an added benefit. If organic electrodes would be possible would become more important to assess other components in the cell apart from the electrodes. Organic electrodes could potentially be easier to recycle, however, the decreased value and hazard of the active material might lead to a decrease of recycling also for other components.

The impact of improving the cycle-life is clear when analyzing the results from using LMP with LTO. This indicates to how much energy and impact the materials can cost if they give a long cycle-life. For the very unstable Si anode, tough the theoretical capacity is great, the cycle life needs to be improved if this gain is to be utilized. The material also needs to be able to achieve good practical utilization of the theoretical capacity, as this is not achieved today. This is a general conclusion for all short lived chemistries, and must be viewed in light of the consumer benefits of having a long-lived system. Short life may not be desirable even if the production and material impacts are decreased.

If the solution to the stability issues for Si anodes is to be solved by nano-sizing it will be important to assess the energy needs to achieve this. Indications from the LFP cathode active material is that nano-sizing can greatly impact the energy use, depending on process path.

5.1.5 Sensitivity analysis and limiting assumptions

The use of aluminium in the electrode foils proved a large impact, especially when considering GWP, ADP of fossils and in the light of the EPS weighting method. However, we chose to model power optimized variants of the batteries, with active material thickness of only 35 μm on each foil. The original value of the coating thickness of 100 μm, given in the BatPaC software, was used to conduct sensitivity analysis, since it represent a high energy design. It showed that having a more energy optimized system, and thus allowing thick coating, can reduce the weight of aluminium and copper in the cell with 25% and 20% respectively. This would give the corresponding decrease to the foil impact in all impact categories. As illustrative examples, this would mean around 5 MJ less energy used per kg cell with LFP chemistry, or 0.3 kg of CO_2 equivalent for the GWP category. This corresponds to roughly 5% of the impact from the total cell. This impact is thus highly influential when designing of high-power cells.

The thickness of the aluminium in the foils is another factor that can influence the foils impact. The standard was 20 μm. To assess the impact of this choice the impact of changing to 15 μm and 40 μm was evaluated. The impact of changing the foil thickness is significant; for a decrease of 5 μm, that is a 25% decrease in material use, the decrease on the energy consumption for the whole cell drops with 6%. The impact on the GWP and ADP of fossils for the whole cell follows this results, with a slightly higher decrease (7%) in GWP due to the high CO_2 emissions from the energy sources used for aluminium foil production. Increasing the thickness to 40 μm gives an added energy consumption of almost 25% on the whole cell. This thickness is in no way unreasonable, since batteries scaled for higher power often required thicker electrode foils to ensure high current.

The change of the copper foil has less impact. Changing from 12 μm to 15 μm leads to an 1.5% increase of energy consumption for the whole cell. The effect on the impact category ADP of elements is, however, very large, since copper is the main contributor. The mere 3 μm increase leads to a 13% increase for the whole cell in that impact category.

The assembly of the cell is a crucial part of cell production, and has uncertain energy consumption. In the model used for the assessment, a total energy consumption of 2.27 $^{MJ}/_{kg}$ of electricity was used. With the appropriate assumptions, and bottom-up modeling, 10 $^{MJ}/_{kg}$ of electricity was stated as a maximum energy use during assembly. Conducting a sensitivity analysis between these two values shows a very large increase in energy use, GWP and ADP of fossils when increasing the assembly energy. The change is roughly a 20% increase in the energy use of the total cell, depending on the chemistry and process path.

For the wet synthesis the process is based on the assumption that the production energy is taken from the heating of a water solution. The amount of water needed to produce one kg of active material is therefore the most important factor for the energy need of the production step. It is possible that the water amount can vary greatly depending on chemistry. Assessing LFP, a 50% decrease of the water amount decreases the total energy consumption of the total cell production by 7%.

For LFP, LMP and LFS a conductive additive is assumed to be added to the active material during production. The type of material can affect the impact of the active material. Using starch, as in wet production, has a larger impact than the acetylene black used in the dry production. However, a 25% increase of the starch in the wet case only increases the energy consumption with 1%. Better knowledge concerning the precise type of additive needed, and the amounts that are required at large scale production, would improve the assessment.

Where the production of parts or constituent was kept to a general case the electricity mix used for cell production was EU-27, containing larger amount of coal-based sources than for example a Swedish mix. The effects of changing to a more carbon free electricity will influence the production of the materials and cell assembly, in particular the dry production of LFP, LMP and LFS since these use much electricity for milling. In the EPS weight this would mean that all the materials and production paths would have equal impact. In the impact categories it would mainly mean a decreased GWP and ADP of fossil. Choosing a more carbon intense electricity mix would instead increase the impact. In light of the electricity choice it should also be noted that all heating is assumed to be from natural gas.

In the LCA of the cell the yield for the active material production is assumed to be 100%. To test the impact of this assumption, the yield was changed to 95% [Majeau-Bettez et al. 2011]. Looking at LFP produced via wet path and NMC via dry, the energy consumption goes up with around 1.5%, thus not greatly impacting the end result. The effect is slightly higher in the impact categories where the cathode active materials dominates to greater extent.

For the production, only the effects of the precursors were analyzed. The emission of for example CO_2 from reaction balances were not included. This would mainly effect the impact of the dry production since the heating of the lithium carbonate precursor would lead to emission of CO_2 further worsening the GWP. The wet production would only lead to some sulfur based emission to water that are more likely to be handled, albeit with a slight energy cost.

Exclusion of the transportation may not contribute greatly to the energy use, but may shift the relative contributions of the different components. This depending on how high the impact of transportation is on that particular production part. This assumption should not be kept if site specific data are available for a certain battery or component. The 1% impact of the transport to the total gross energy demand [Rydh & Sandén 2005] is not equally distributed over components.

5.2 Battery pack and modularization impacts

The degree of modularization has been identified as an important parameter for safety and for the amount of passive materials in the pack. From an organizational point of view the modularity could enable reuse and facilitate the testing before a possible second life. Additionally for the sake of reducing the production costs the module size should fit multiple applications as stated in chapter 3. For the scenarios of selected modularization and sensitivity analysis of PCB, pack size and reuse, the cradle to gate results will be presented for the whole pack of NMC and LFP chemistry. The impact categories of focus are ADP elements and embodied energy (net calorific value) since they were found representative, and have shown the greatest changes in the different scenarios, while other impact categories are similar or less sensitive to the different designs. The complete set of results in all impact categories can be found in Appendix A.

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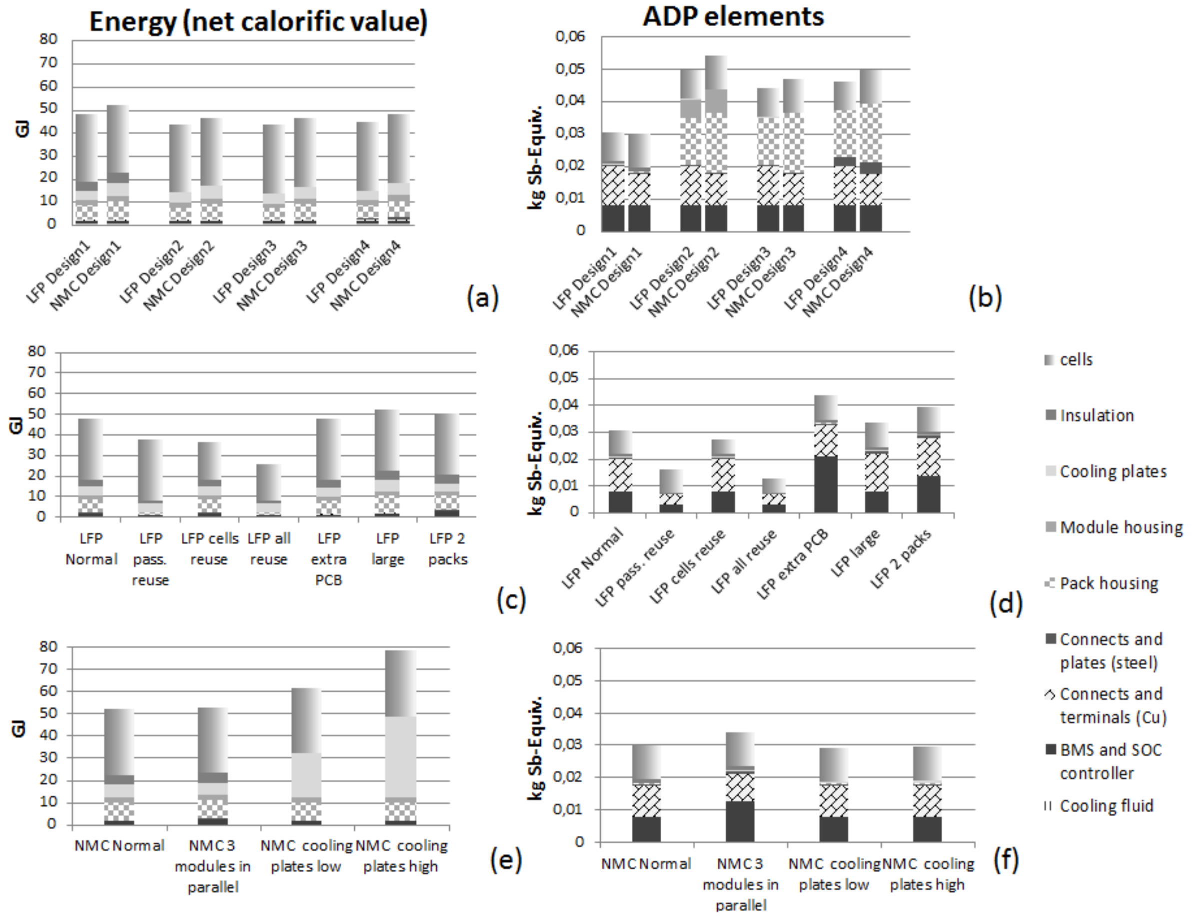


Figure 5.8: NMC and LFP pack cradle to gate impacts per component for different standard design alternatives and various extra scenarios represented by the categories energy and ADP. In (a)-(b) is shown a comparison between LFP and NMC standard designs. In (c)-(d) are found LFP extra design scenarios of reuse, pack size, 2 packs replacing one and extra PCB. In (e)-(f) the effects of NMC extra scenarios of added cooling plates, and module string parallel connection are shown.

Table 5.1: Total and normalized values for the energy and ADP elements impacts of the NMC and LFP packs, cradle to gate.

Impact	LFP pack	NMC pack
Energy (MJ)	47858	51860
MJ/kg pack	84.3	88.4
kg Sb-equiv.	0.0306	0.0301
kg Sb-equiv./kg pack	5.39E-05	5.14E-05

Impacts of standard designs and chemistry

The four standard designs presented in the inventory are here evaluated in terms of ADP elements and embodied energy for the NMC and LFP pack. As a first result, the NMC pack and the LFP pack show to have little difference in impacts both in the embodied energy, and in the ADP elements (figure 5.8 (a) - (b)). For the LFP pack, the maximum of 48 GJ embodied energy, 84 MJ/kg is very similar to the NMC pack with a maximum of 52 GJ and 88 MJ/kg. The results are not too far from the ones found in [Dunn, Gaines, Sullivan & Wang 2012] of 75 MJ/kg for the BatPaC model taking into account the medium high rate of modularization. For both packs the cells are dominant of 50% or more in the scenarios in which no reuse of cells is assumed, in all categories except HTP and ADP, where the steel casing has high importance.

Regarding the evaluated standard design choices, design 1-4, it is seen that on an energy basis they are all similar, except from design 1 which is higher due to the contribution of the thermal insulation here (PU). Supposing that this insulation would be removed, the energy impact for all the four standard designs would be almost equal (figure 5.8 (a)). For the different standard designs only the housing structure is changed in terms of materials, which is a contributing factor to the similar impacts.

For the ADP elements the clear advantage is given by design 1, since aluminium and PU do not contribute much to the mineral resource depletion. Instead the steel housings in design 2 contribute to high extent to the ADP elements impact (figure 5.8 (b)). This is because of additive metals such as the chromium and nickel present in the stainless steel. A steel alloy with fewer amounts of those components would have lower impact. The module housing of plastic (PP) and aluminium in design 3-4 have almost no contribution to the ADP elements category, while the added steel pressure plates in design 4 increases the impact (figure 5.8 (b)). To conclude the best designs from an energy point of view are design 2-4, the best one in ADP elements is design 1 which at the same time is the worst case for the energy. The worst case for ADP elements is design 2 due to the chromium steel. The designs 3 and 4 are medium good choices in both categories.

The ADP elements impacts are dominated by copper, BMS and stainless steel. Some difference in the amount of copper connects can be seen between the LFP pack and the NMC pack because of the different voltages of the modules, the NMC module being of higher voltage than the LFP module. For the stainless steel, NMC has a higher contribution due to its higher amount of housing materials deriving from the slightly larger cells (figure 5.8 (b)). On the other hand the energy category is dominated by the cells, making the design choices less important for the total impact.

Looking more at the passive pack materials, the actual composition of the plastics used for the housing could be evaluated further. A more resistant engineering plastic such as polycarbonate could possibly reduce the need for extra steel compression plates and reinforcements in the pack, meaning that the total cost, weight and environmental impact possibly could be reduced. The pressurizing plates of steel and steel straps are assumed to have always the same thickness. In reality the thickness could be adapted to the amount of cells in rows and in relation to the swelling of the cells, which means that the results may look different depending on the modularization. For a further improvement of the modeling of the insulation, the type of insulation plastic should be determined, since for example the ADP elements may vary quite much depending on the type of foam used.

Impacts of alternative designs

Having seen the trends for the impacts related to housing materials and chemistry, some alternative designs are considered for the component set up of design 1, comparing with the standard design 1 as a reference, for NMC or LFP chemistry with the impact properties described in table 5.1.

The reuse of the passive pack components set at a maximum rate enables the reduction of the total cradle to gate impact of the LFP pack by 22% in the energy category and by 57% in the ADP elements (figure 5.8 (c)-(d)) thanks to the minimized extraction of control system materials and copper and housings. The reuse of passive components is a relatively easy way to reduce the impacts of the whole pack. The adoption of reuse of different passive components need not be complicated on a technical level, but the logistics and organizational channels should be studied to see at what cost reuse is feasible and at what rate. Reuse is perhaps more viable than second life since it can be made at various component levels and within the same organization. The knowledge about remanufacturing and the legal permission to open and refurbish the modules will be needed. At present the manufacturer of the battery does not allow the vehicle manufacturer to open the modules which makes the reuse difficult.

The cell reuse is a more distant solution, with its requirements for advanced qualification of old cells. However from the assumption of 40% reused cells, a result of 25% reduction of energy, and 12% reduction of ADP elements is achieved. The total impact reduction is inferior to the one of the passive pack reuse. To arrive to a rate of 40% cell yield may be difficult in practice and so this result may be considered optimistic (figure 5.8 (c)-(d)). Making use of the reuse concept to a maximum extent, in the case of both passive pack materials reuse and cell reuse, the impact reduction can reach 47% for the energy- to a total net calorific value of $44.5\,^{\mathrm{MJ}}/_{\mathrm{kg\ pack}}$ and 59% for the ADP elements 2.2E-05 $^{\mathrm{kg\ Sb\ eq.}}/_{\mathrm{kg\ pack}}$. This reduction could be seen as a target for the battery life management (figure 5.8 (c)-(d)).

A sensitivity analyses was done by exchanging the normal PCB unit with a type of higher percentage of gold. The difference on the energy was minimal while for the ADP elements the impact was increased by 42% (figure 5.8 (c)-(d)) showing the importance of choosing the control units carefully. Since the SOC controllers and BMS are components subdued to little wear and aging during the battery life, reuse should be an aim, or recycling of the gold and other rare metals, in order to mitigate the impacts.

For the purpose of using one pack size for both NMC cells and LFP cells, the LFP pack will be oversized, and the related impacts are increased by about 9% (figure 5.8 (c)-(d)) both in energy and ADP elements giving an idea of the costs of interoperability from a material point of view. The result is highly dependent on the difference in dimension of the cells; here the NMC cells are considered 20 v% larger than the LFP cells.

For the special design of the two small packs in one, almost the double of control units is added to make the singular packs autonomous, and extra housing materials are needed. The energy impact is increased by marginal 4%, while the ADP elements impact is increased by 27% (figure 5.8 (c)-(d)). If this set up will be needed, it is recommended to perform reuse of the electronics and control system to minimize the impacts.

In some cases when the choice can be made to place the control units independently outside the packs, the amount of control units required may not be as high. The impact of the ‘two packs’ scenario thus depends on the alternatives of placement of the BMS.

For the interoperability of modules, it can become necessary to make a compromise in the cell interconnection, and go from three cell strings in parallel to three modules in parallel. The effects of this configuration with higher amount of SOC controllers are seen in the ADP elements, sensitive to the amount of electronics, by an increase of 12% (figure 5.8 (e)-(f)). .

Fast charging has implications on the durability of the battery, making it age sooner, resulting in the need for more packs during the vehicle life to keep a constant electric range. Additionally the fast charging needs to be compensated for with a more efficient cooling system, or by making the cooling system more powerful. Depending on the type of cooling structure used, more or less material, such as cooling plates need to be added. Especially the conductive cooling with solid aluminium plates can result in high amounts of added materials. Giving an idea of the fast charging implications from a material point of view, unit[84]kg (low) and unit[180]kg(high) extra added aluminium cooling plates result in 20% and 51% increased energy, while for the ADP elements the change can be neglected (figure 5.8 (e)-(f)). In this scenario, reuse should be a reasonable way to reduce impacts. If not possible, at least recycling of the cooling plates should be done.

In order to make the fast charging scenario more realistic, a more thorough calculation and possibly a real dynamic model should be built trying out the optimum between minimizing the amount of cooling materials and the power required from the pumps and fans, which were neglected for this model. In addition the pack casing increase due to the volumetric change should be taken into account for more accurate results, which would make the related impacts even higher.

As mentioned the second life may reduce the original pack impact with about 25%, when applicable. It should however be discussed at what rate the packs could be sent to second use to see how the environmental impact would change for the whole vehicle fleet. It is not likely that all the packs would be sent to second use, because of the degradation of cells and the cost of remanufacturing. If the 50% of used automotive packs are sent to second use, and have their impact reduced by 25%, we have an average impact for the battery fleet of 0.5+0.5(1-0.25) =87.5%, which is a reduction of 12.5%.

5.2.1 Use phase

The use phase is an important part of the total battery life cycle. The energy consumption of the 1080000 km use phase of the PHEV bus amounts to 1.95 GWh, see figure 5.9. This is lower than the hybrid reference bus and the standard diesel bus for the same driving pattern. About 60 % of the energy consumed derives from electricity, and 40 % from diesel. The contribution from the electric driving is 80% and from hybrid driving is 20%. The efficiency of diesel tank to wheel is assumed to be 35% and the efficiency grid to wheel is set to 70% of which 95% grid efficiency, ESS in average 90%, electric motor 92%, AC DC converter 95%, DC AC converter 95%. The fuel consumption is 0.31 l/km for hybrid mode, and 1.5 kWh/km for full electric mode. The results are a reduction of the energy consumption of the standard bus of about 63 %.

Use phase scenario full vehicle life

The efficiencies and the type of fueling of the power production technologies in the different electricity mixes affects the impacts of the PHEV driving significantly. The driving with Nordic electricity is a better choice for the PHEV bus, and can be used as a comparison to European electricity used for the most part of this thesis, see figure 5.10. The higher carbon content in the EU-27 mix makes it less beneficial than Nordic electricity mix advantaged by high hydro percentage, about 30%. The best case of PHEV use is thus Swedish hydro power, in all impact categories except for abiotic depletion elements where it has the highest impact. The Nordic PHEV driving is however better than both the standard bus driving and the hybrid bus in all categories (except ADP). It is about 150-200% lower than the impacts of the standard bus. The worst case of acidification is found for the EU-27 electricity mix PHEV driving, whereas the POCP and HTP are equal for the PHEV EU-27 and the standard diesel bus. In GWP the EU-27 electrification of PHEV leads to a lower impact than the hybrid bus which means that even in the worst case the GWP is reduced thanks to the PHEV bus.

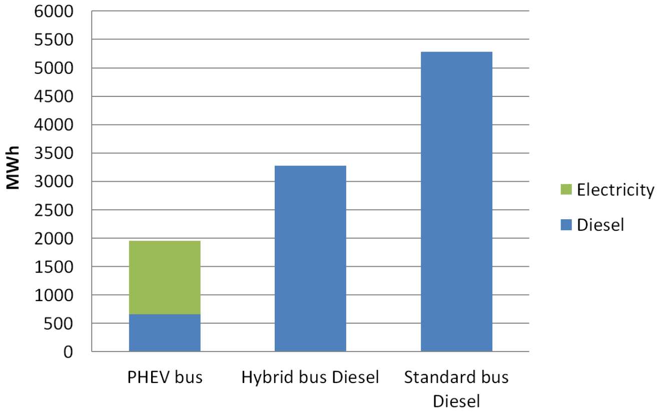


Figure 5.9: Energy supply Tank to wheel and Battery to wheel, during the whole use phase of the vehicle life for PHEV bus and reference standard (conventional) bus and hybrid bus, for the assumption of 80% electric mode and 20% hybrid mode for the PHEV bus.

Comparing the energy needed to produce the battery pack with the energy consumed during the use phase, it is seen that the battery with its around 50 GJ embodied energy is about 160 to 320 times smaller than the use phase of between 8 TJ to 16 TJ (figure 5.10, 5.8 (a)) depending on electricity mix. The number of batteries consumed during the vehicle life should be taken into account when comparing use phase with batteries produced. For the selected battery packs, a life of three years is assumed, thus only a third of the 9 years energy consumption may be related to each battery.

An important comment to the results is that the electricity is assumed to be averages for the selected regions. If instead marginal electricity would have been applied, the results could look different. The worst case Nordic marginal electricity would be similar or worse than the European average. The marginal electricity concept implies that the next unit of electricity supply in the merit order often is coal and natural gas depending on the time of the day and the period of the year. Hydro power and nuclear power are normally used to full extent during the day since their variable production costs are low. Adding the PHEV bus charging to this load during the day, would call in marginal extra production of for example coal condensing power. In an international grid perspective, the difficulty comes in identifying from where the charged electricity comes, since the grid includes many different producers in different nations. The last consideration in terms of electricity supply is the scenario of a large fleet of PHEV vehicles which, depending on the control strategies and time scheduling for the charging, could increase the total need for electricity supply within a region, as has been shown in a model for the city of Gothenburg [Steen 2012]. This means that the introduction of a large PHEV fleet can solicit to install new power production services. The consequence and the allocation of such a new installed power capacity to the grid need to be further investigated.

In order to make more precise assumptions about the electricity use, the recommendation is to make a model of the scheduled charging of the PHEV bus, compare it to the real time electricity production data of the specific area of vehicle operation and extract the actual technologies for the power supply. In this way both the exact electricity mix can be retrieved and the need for extra installed power supply capacity can be determined.

In the electrified drive line the conversion efficiency of the electricity to traction is of great importance to achieve the environmental gain. Adding the efficiency degrading of the battery to the evaluation could determine the point at which the full electric driving is beneficial. In fact the electric mode will lead to a reduced impact compared to the ICE mode only when the conversion efficiency of well to power plant to grid to wheel is better than the conversion efficiency of the diesel engine. Depending on the assumed electricity technology assumed and

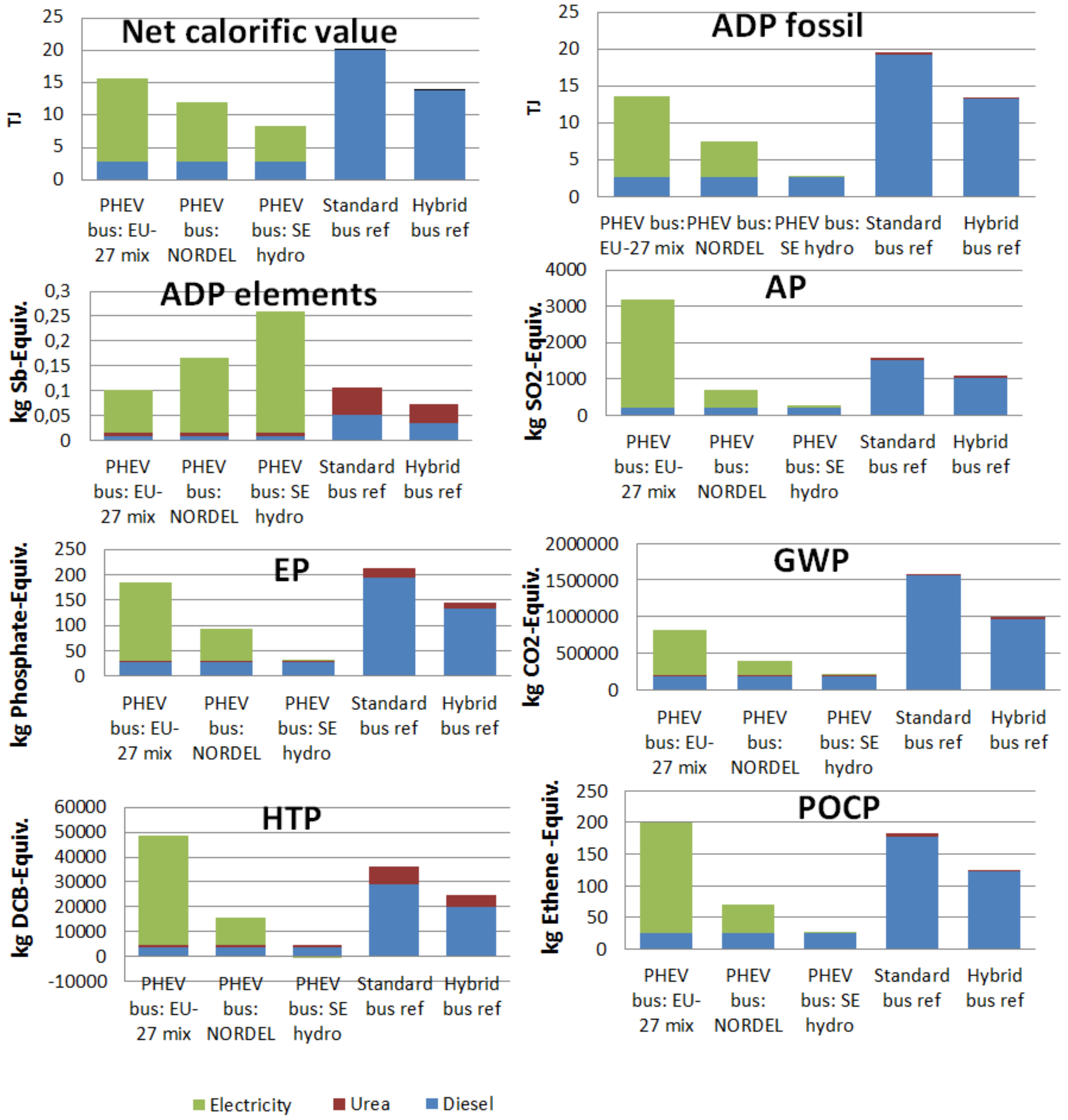


Figure 5.10: Impacts in various categories for the use phase of the PHEV bus well to wheel, 9 years, with different electricity mixes, compared to reference standard (conventional) bus and hybrid bus, for the assumption of 80% electric mode and 20% hybrid mode for the PHEV bus.

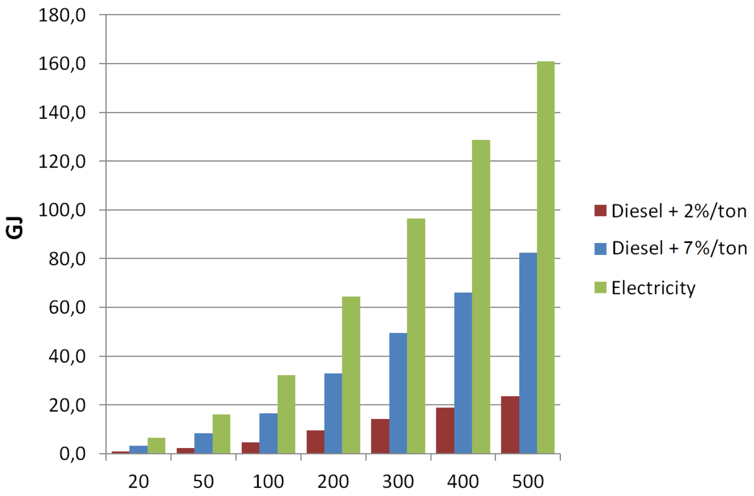


Figure 5.11: The energy consumption increase in relation to added weight on the vehicle for 2%and 7% diesel consumption increase per tonne added weight and proportionally increased electricity consumption.

its fossil fuel content, the allocation of marginal or average electricity the outcome could differ.

The battery weight contribution to the fuel consumption is marginal compared to the total electricity supply and diesel supply during the life phase. The increase in diesel consumption is set to a minimum of 2% per added 1000 kg extra weight and of maximum 7% per tonne extra weight. The electricity consumption increase is proportional to the relative increase in weight of the whole vehicle see figure 5.11. If the battery pack leads to an increase in the minimum vehicle weight, the best case scenario is that the fuel consumption is increased, and there is a marginally higher life cost of the vehicle. Considering an increased weight of 500 kg leading to a total energy consumption increase of 3%, the marginal change in fuel consumption is 663 l diesel and 52000 kWh electricity.

In the same way an increase of 1000 kg leads to an increase of 7-8% energy consumption as a best case. If instead the battery weight is added on the max loaded vehicle, the number of passengers allowed on the bus must be reduced to stay within the vehicle weight limits. This is the worst case scenario since a the service of the vehicle is reduced, and more buses are needed to cover the service for the number of passengers on the line. Adding 500 kg corresponds to a reduction of 7 passengers of 75 kg, 12% lost passenger capacity on a bus with 60 passengers and 12% more buses needed in the fleet to cover the function of a conventional bus. Similarly added 300 kg means 4 passengers or 7% lost capacity. In figure 5.11 the increase in energy consumption is illustrated. From increases of 20 kg that are the possible impacts of changes in modularization and to those of 500 kg that are the ones of over dimensioning in battery energy storage capacity or in the amount of cooling plates. The proportion of the energy consumption allocated to battery weight during driving and the embodied energy of the battery pack are of the same magnitude, assuming a fuel consumption increase of 2% to 7% the relative impacts are shown in figure 5.12.

For future evaluation of the use phase, it could be interesting to compare the impacts per person and distance for the PHEV bus with a PHEV car. In particular the embodied energy of the battery compared to the energy saved during the use phase should be interesting to see.

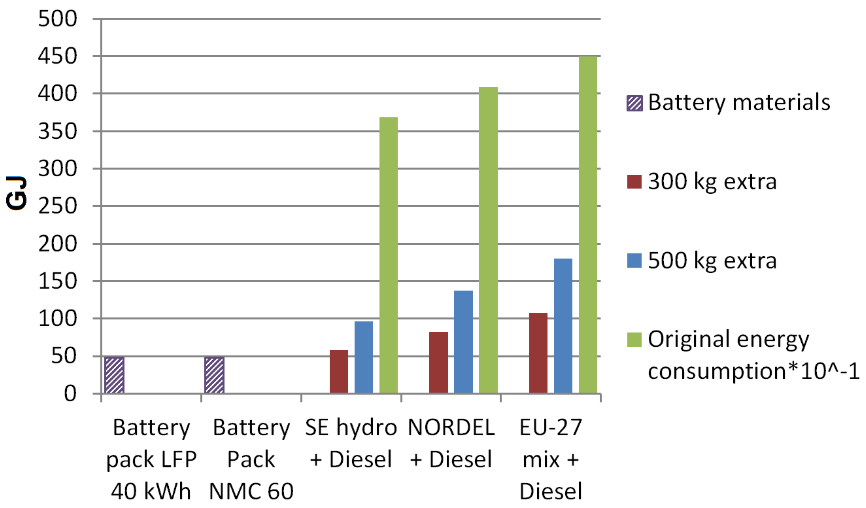


Figure 5.12: The energy consumption increase in relation to added battery weight on the vehicle and compared to the embodied energy in the battery pack. 2% diesel consumption increase per tonne added weight, set into relation with the total fuel and electricity that have been used during the ESS life in the vehicle. N.B. Scaled total original energy consumption by a factor of 0.1.

5.3 Pack life cycle

The total life cycle has been modeled for LFP with assumed reuse and recycle rates see 4.11 and 4.10. The results in figure 5.13 and 5.14, show that the reuse of passive components can reduce the total impact significantly. The use phase with the contribution of the electricity and diesel from carrying the pack has higher impact than the pack production phase in Energy, ADP fossil and GWP. For these impacts the reduction of the weight of the battery or the elimination of other components in the drive line could improve the total impact. The cells have the highest impact in POCP, AP and EP. The ADP elements impact can be improved by reusing pack components such as BMS. In AP the reuse of pack components could mitigate the use phase energy consumption.

Second life scenarios

The assessment of second life should be further investigated, with more exact data for the yield of functional batteries after first use, and calculations on the second life impacts for different options of applications. An evaluation of a new battery used in a stationary application could be beneficial; to determine the possible energy gain from the second life service. This should then be the reference to compare the impact of the refurbished vehicle batteries. Due to the battery weight the location of the second life application could be important due to possible emissions from transporting the used battery packs. The degree at which the transport factor influences the total impact of second life could imply constraints on the possible second life markets.

Going towards possible second life applications a standardized method for testing and diagnosing of the batteries should be established. It could also be of interest to investigate whether there are differences in diagnosing and testing of PHEV bus batteries and PHEV car batteries, and to determine whether one of them is be more suitable for second life, from both a cost perspective and a performance perspective.

For future batteries, the initial design of the cell properties could be made to support the automotive use followed by the second life stationary application. The hot-spots in the requirements for such secondary applications should be identified. The case may be that power

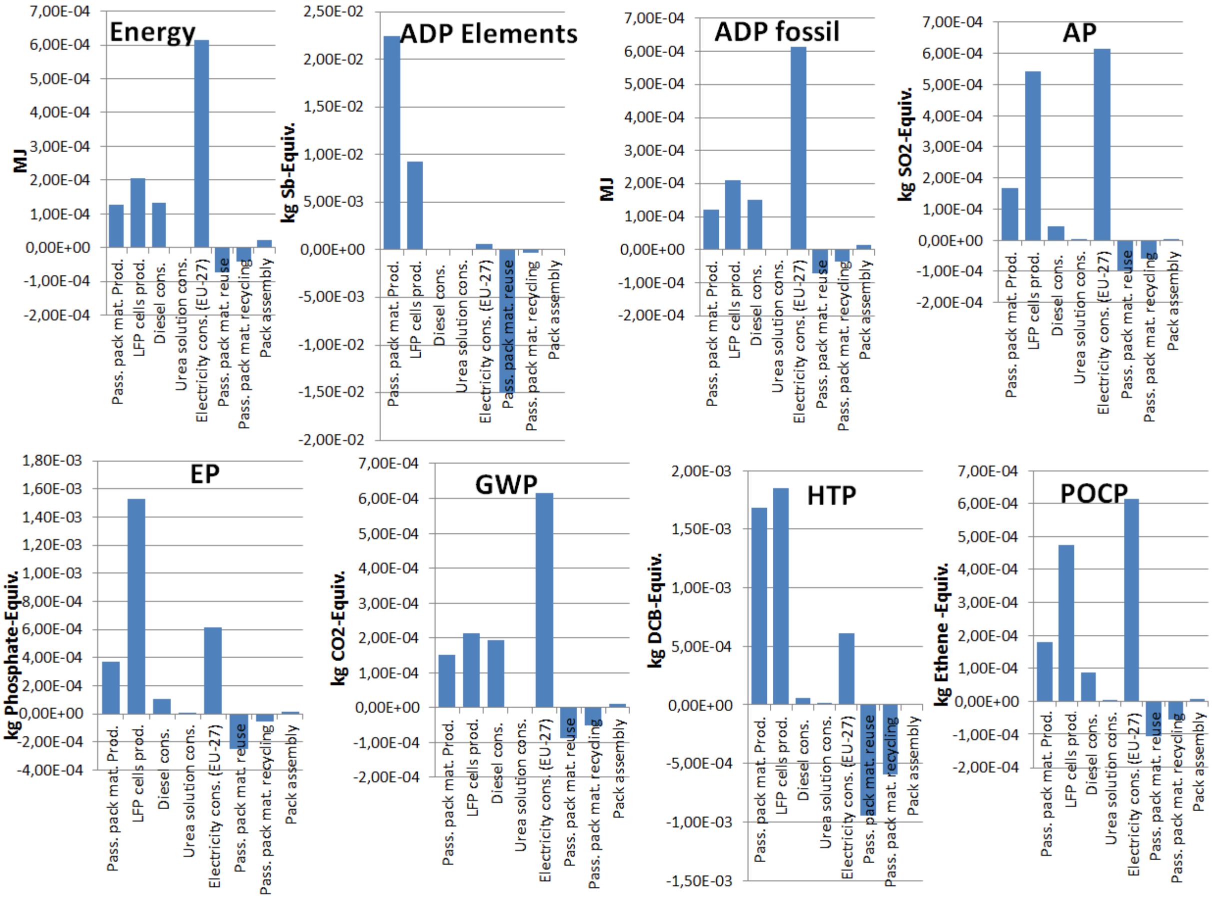


Figure 5.13: The aggregated results from production of cells and pack materials with use phase, reuse and recycling for LFP . The production is compared to the use phase with 7% diesel consumption increase per ton added weight and proportionally increased electricity consumption for 300 kg added weight due to the battery pack. The unit is per passenger and kWh electricity charged from grid to battery.

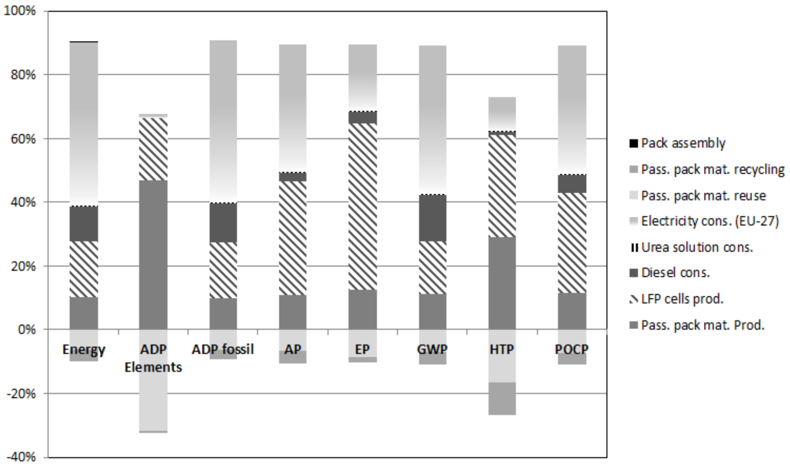


Figure 5.14: The aggregated results from production of cells and pack materials with use phase, reuse and recycling for LFP with the different components and phases in percentage of total impact for each category.

optimized batteries from PHEV bus applications could suit a certain type of application better, such as power quality applications, and that PHEV car energy optimized batteries could be used for other stationary applications such as UPS and batteries installed in apartments.

5.4 Battery material recycling scenarios

Recycling of the cell material is very chemistry dependent and thus hard to model. The results reflect the specific modeling choices, but give general indication. For the hydrothermal recycling, no process energy is included, making the results a comment on potential saving in the materials, and not actual energy savings associated with the method. The results of pyrometallurgical recycling will be shown for dry produced NMC cells, and those of hydrometallurgical recycling will be shown for wet produced LFP cells.

5.4.1 Life cycle impact assessment

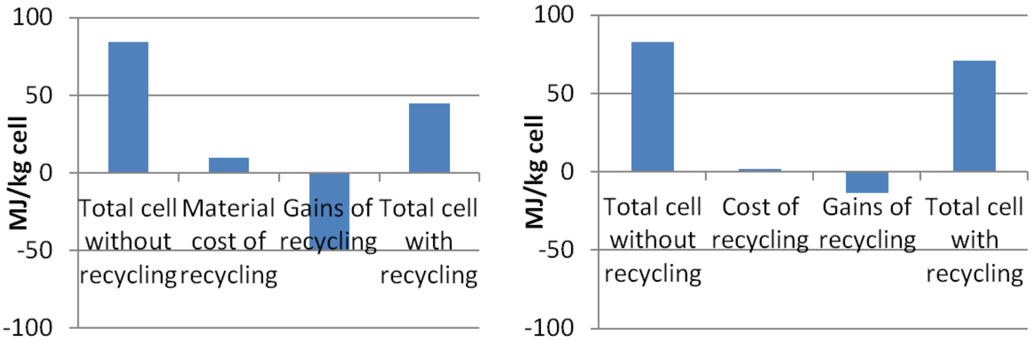
The effects of recycling different chemistries will be assessed in terms of energy saving compared to energy consumption during the recycling. Figure 5.15 shows the energy consumption of a cell produced from virgin material, the energy cost of recycling, the energy gain from accrediting the recycled materials negative energy consumption and lastly the total energy consumption if recycled materials are included. The figure includes the results both for NMC and LFP recycling.

The gain of NMC recycling is clear, but not a great contribution to the total cell production. This is mainly due to the small percent of the cell being recycled back into battery material. The rest is used for heating or goes to slag and is not accredited in this assessment. The energy cost of recycling is rather low, which can partly be explained by the use of all organic components as fuel. However, using the energy in these materials is a way of recycling them, although not back to battery grade. The gains from recycling NMC is distributed among the materials being recycling, namely cobalt, nickel and copper.

For LFP recycling the gain is larger, since much of the material is recycled to a reusable state. However, the energy cost of recycling is somewhat uncertain since only the chemicals needed are taken into account. The indications that there are potential benefits for the energy consumption in recycling is still clear, since the major impact of this recycling method is the chemicals. In light of the aluminium foils large contribution to several impact categories, one large gain of hydrometallurgy in comparison with pyrometallurgy is the opportunity to decrease this burden by recycling.

For the hydrometallurgical recycling of LFP the main gain comes from the recycling of the aluminium foil. Since the processing of the aluminium is a small part of its impact, this recycling will be effective even if the aluminium foil cannot be reused directly. The credit of lithium and the electrolyte are about half that of the aluminium each. The lithium gain is readily realizable, as the lithium is retrieved in a form that can be reused in battery material production. Lastly, a smaller gain is added from recycling the copper foil.

It is important to consider that recycling often is driven by price and not energy consumption. If legislations are passed to regulate recycling, the energy consumption might be a good guide to when it is beneficial to recycle. If not, the energy savings have to be viewed in light of cost. The saving from pyrometallurgical recycling may look small, but the value of the recovered material is high since copper cobalt and nickel are among the recovered metals. The hydrometallurgical method may look appealing from an energy perspective, but the chemicals involved are often very expensive, and the value of the recovered material is small.



(a) LFP recycling, hydrometallurgical

(b) NMC recycling - pyrometallurgical

Figure 5.15: The energy needed to recycle and the energy gained by accrediting the recycled materials negative contribution can be viewed in light of the total virgin cell production. The impact recycling would have on the total energy consumption can be seen as the right column.

Previous assessments of the effects of pyrometallurgical and hydrometallurgical recycling have indicated that hydrometallurgical actually may be less energy efficient than pyrometallurgical, due to the use of chemicals. Dunn, Gaines, Sullivan & Wang [2012] has taken larger consideration to the need for post-processing the materials, and included that energy, as well as including process energy. The resulting assessment shows hydrometallurgy requiring more energy than pyrometallurgy.

5.4.2 Sensitivity analysis and limiting assumption

For the pyrometallurgical approach, the whole cell is assumed to simply be placed into a furnace to be burnt and recycled. In the case of hydrometallurgical, a limitation is that no EOL processing is assumed for the components that are not recycled. That includes the pouch with its aluminium and the separator. Apart from the possible aluminium recovery, managing these components EOL would cost energy without adding value to the life cycle stage. Possibly, these components could be incinerated and used as heat for some of the other processes.

Since all the materials in the NMC recycling contribute equally to the gain of recycling, a lowered recycling rate for any of them would correspond to a reduction in the total gain with a third as much. Since the energy consumption of the recycling step is so low, a recovery rate of only 12% of the valuable metals would still validate the recycling path.

Discussion

The results in the previous chapter, and the models used to describe the ESS in this thesis, gives rise to some interesting points for discussion. Both the results and the models can have implication for future work, both new life cycle assessments and product development.

The results of the assessment of cell materials and production give indications of possible improvements that can be obtained when changing battery chemistry. It is clear that the choice of production method for the active material needs to be chosen to suit that particular chemistry. Both the energy intensity of the process itself, but also the available precursors impact the choice of most efficient production. Changing precursors affect the energy consumption, but can also greatly influence other categories, leading to a reduced total impact.

For materials that require nano-size, the benefits of using wet synthesis are clear. For other materials, the choice of dry processing is more reasonable, but still comparable to the wet method. Therefore all potential active materials, and possible precursors, need to be evaluated in detail before a process choice can be made.

Another indication is that the foils used as current collectors and support for the active material have a large impact on both energy consumption and some resource oriented impact categories. Copper has great impact of the ADP of elements, and has a high price. However, it should be noted that the choice of the thicker aluminium foil has larger impact on many of the other categories. Minimizing the thickness of the foils is of large importance when designing high power cells which, to a greater extent than energy optimized cells, use thicker foils. If a change in chemistry required a greater or smaller thickness of the foil, this should also be taken into consideration.

The results for the LTO anode, indicating the viability of increased energy consumption in light of longer cycle-life, are valid also in a more general case, with other cathode active materials than the future LMP chemistry. The most common cathode for the LTO today is LMO and not LMP, and the indications of the large impact LTO has on cell production would hold for this chemistry as well. The conclusion that it is of great importance to utilize the possibility of increased life-length is also valid for other cathode choices. This also gives indications to one route to improve the electrode impact, namely prolonged cycle-life. In addition, if the boundaries of the assessment are broadened, the decreased need for replacement and maintenance may positively influence more parts of the whole system.

The different housing material choices for the pack designs have shown few effects on the cradle to gate impact of the whole pack, but less than for example cells, copper connects and control units that are present in about the same amount for all the different standard designs. Firstly the similar impacts may derive from the fact that the aluminium, steel and plastics used all are common metals and materials with little risk for depletion and with few related toxic emissions during production and extraction. Secondly, all the pack designs have been made with the same requests on assumed strength and durability, to allow a long life of the passive components. As have been mentioned the embodied energy (cradle to gate) per volume of a material is positively correlated to the strength in terms of young's modulus, and so the request for strength and the dimensioning criteria makes it reasonable that the outcome is similar for all standard designs.

It would be interesting to investigate the actual thicknesses of the cases required to withstand a crash. The current designs for the models are not tested with finite element method and so the actual yield strength should be further investigated. The possibility to use less material for the housings should be evaluated, as the minimum material thickness required. Since it has been shown that module housing adds a high amount of material, due to the large surface. BatPaC has a standard set up of dimensions for housings, materials and connects, which should serve mainly to give directions for design of packs for cars. Typically the weight is doubled for the battery of the PHEV bus compared to the BatPaC standard system, and so the requests on the structure to withhold the weight of cells and modules may be higher. In order to take the environmental considerations into account during the first concept designs of the battery pack, part of the LCA evaluation could be integrated directly into CAD software, or into BatPaC. In this way construction, electric properties and ecodesign could be joined directly.

In the results the product manufacturing process energies of the pack passive materials have not been included, which gives a margin for errors, making the pack passive materials perhaps more equal to the cells in terms of energy.

Having seen that the reuse of cells and passive pack components may lead to a great improvement of the life cycle impacts in the best case, the actual component life lengths, the transports needed, and the feasible collection rates should be further investigated. For a realistic case the possible reuse rate may be a lot lower for various reasons.

For the driving the results show that the impact from energy consumption during the use phase related to the battery weight is similar to the energy needed to produce the battery. This means that reducing the weight of the passive materials in the battery can be an equally efficient measure from an energy point of view as reducing the production energy.

To achieve better accuracy, the actual increase in energy consumption due to added load on the bus should be simulated, or measured. After all, the linearization that is done in the assumptions is an approximation that could be done in a more precise way.

For the battery assumptions, the life length of the batteries needs to be validated with tests or case specific data, being an important parameter for the battery life cycle impacts, and a possible difference in life length between the selected NMC and LFP packs could make need for a different sizing of the packs.

Some impacts related to voltage mismatch could be reduced if choosing the battery early in the development phase, in order to optimize the interfaces between all the drive line components. This could also be achieved by keeping a close contact between the battery manufacturer and the vehicle manufacturer from start. In this way voltage levels may be kept similar for the whole drive line and less extra components will be needed to compensate for different voltage levels implying less weight and costs.

An alternative to fast charging would be to have a redundancy of battery packs that could be switched at the end of each service route, which would allow using slow charging and so prolonging the battery pack life. The comparison should be made in terms of costs and impacts to evaluate the optimum number of packs serving each bus, compared to the cost of shortening the battery life due to fast charging. To succeed with battery friendly fast charging, the cell aging properties needs to be further improved.

Given the importance of the cooling system weight and volumetric contributions for the battery pack, the choice of cooling structure should be made carefully, to not increase the amount of passive materials unnecessarily. The tradeoff between the cooling system efficiency and the weight related fuel consumption may need to be done. In general the type of infrastructure for the cooling system should be further investigated, there are many different options and to be tested is which one is the most efficient, from an energy and material point of view. It seems a good idea to give supporting structures such as the housings the function of heat exchangers.

Recommendations for future life cycle assessments

The results of this thesis are aimed at showing hot-spots and important stages in battery design and production. This is done without specific data, to keep the results are general as possible. The key points to assess in future LCAs are summarized below:

- Include transportation and geographical production details.
- Include case specific use phase to better assess the end of life opportunities.
- Assess a specific cell chemistry and production path.
- Assess the impact of different power optimization designs.
- Assess in detail the cooling system needed for fast charging and its impacts.

Generally, adding the transportation impact to the assessment would further improve the results. This does require some more data on production and assembly sites. Acquiring more of the production locations would also help achieve greater detail, and limit the need to use global or European averages.

Since the life-length of the battery in the vehicle greatly impacts the per km or per year impact of the battery, as well as possible replacements cost, it is a factor to assess in greater detail. Case specific driving cycles, coupled to a known chemistry and a certain life-length of the ESS could fully determine the impact of the battery compared to the use phase. In this thesis only indications of the most influential components are given, based on general driving cycles and an assumed system life-length in the vehicle. Future improvements could therefore include collecting case-specific data for modeling one known battery configuration.

On a cell level this would include choosing one chemistry and assessing the precise process steps taken to produce the active materials and other cell components. The precise weights of the different components could then be better assessed. This would settle what impact the components with high sensitivity, like the foils, actually have.

Site specific production data for the different production processes could be useful to assess the importance of geographical location of the manufacturers. Finding a more detailed description of the production path could help determine the possibilities to improve, and more precisely where in the production line improvements would be most beneficial. Having known precursors with known production location improves the accuracy of the results, since site specific data and extraction methods can be used. A sensitivity analysis between different manufacturers of battery cells is of interest when choosing supplier. The dilemma with the cell production industry is that specific data rarely is disclosed, making evaluation difficult for an external party. The production paths for the active material is in this thesis modeled as proxies for wet and dry production, and more detailed steps could be added for greater detail into this step. A further assessment of the changes to the production path when changing chemistry would also be beneficial.

In this thesis some steps have been added to the model to ensure more power optimized systems, and in particular power optimized cells. For this purpose the thickness of the active material was decreased. To further evaluate the different energy impacts when power optimizing the thickness of the foils should also be changed. A comparison with an energy optimized cell would then be of great interest. It can also be of interest to compare different degrees of energy and power optimization, and different methods to achieve them.

The cell assembly is a step surrounded by great uncertainty and a wide range of data. A detailed assessment of actual energy needs during this step is therefore of great interest and could improve the assessment further.

Similarly, data for the assembly of the pack and manufacturing of other pack components such as housings should be collected, for the results to become more precise. Adding the actual recycling of passive pack components such as housings and cooling plates would also give more accurate results. Especially interesting is the possibility of recycling the gold in the PCB and the related potential of reduction in impacts from the control system electronics. The same is valid for the possible reuse rates that should be further investigated. Depending on the likeliness of second life, the allocation of the replaced new batteries can be included in the total lifecycle, finding a way to divide the impacts between first and second life actors.

Data for the energy consumption during the use phase should be validated with measurements for all the reference vehicles, with the actual number of passengers to achieve more accuracy in the assessment. The actual amount of added battery that increases the marginal weight of the vehicle should also be determined to improve the results.

The actual power needed for the ESS cooling has been excluded in this thesis, which may have a varying degree of impact depending on the amount of cooling plates and the cooling efficiency. It can also be of value to specify what type of cooling system that is used in the vehicle, to get a better assessment of the impact.

Conclusions

In the ESS, the cells have a large impact on the total life cycle. The results from examining the different components in the cell are therefore of great interest since this can suggest where there is most room for improvement. When choosing cell chemistry it is important to consider the type of impact. The layered oxide example NMC contains elements with larger impact in most categories, even though the total energy consumption is similar to for example the phospho-olivine LFP. For LFP the impact is divided between precursors and processing making the choice of processing and suitable precursors more open for fine tuning. NMC has less room for improvement since the process impacts very little.

The results of the LCA for the cells also indicate that the foils have a large impact. This makes it interesting to investigate the critical thickness needed for these foils, and the possibility to have a smaller total amount in the whole cell. For current chemistries it is still the active material that has the highest impact in the LCA of the positive electrode, but when the impact of the active materials is decreased as in LFS, the foils will need to develop as well to decrease the total impact significantly.

If the thickness of the foils are increased to enable higher power the impact is large, especially when considering energy consumption and global warming potential. This has implication when designing high power systems, since the foils then might need to be thicker to increase the current capacity of the cell.

The electrolyte has the largest impact apart from the electrode, and development of this component, especially when it comes to the acidification impact should not be neglected. However, if using the weighting factor EPS, the electrolyte has little importance for the total impact of the cell. If the focus instead is in the lines of the EI99 weighting method, the electrolyte does again matter. This implies that there is a need to have a clear picture of what the goal of possible improvements is, since the most important factors vary with weighting methods. This also holds true for the electrodes.

The assembly of the cell, the separator and other passive components have a small impact in all weighting methods. The fact that the cell casing has such a small impact on the total cell leads to the conclusion that a decrease in cell size leading to a change in the amount of pouch materials will not yield great improvements to the life cycle. Actions to achieve smaller amount of active materials are more valuable. Improvement to the graphite electrode is of smaller benefit than improving the cathode, especially when focusing on the EPS score.

Investigating the impact of using an anode with longer life-lengths illustrated the benefits of increasing this property. This can be used as a guide when discussing the possible life-length benefits of an anode or cathode change, in light of for example increased energy consumption. To increase the viability of battery systems in vehicles life-lengths closer to that of the vehicle life may be desirable, adding consumer benefits to the possible environmental benefits of longer life.

After the cells, the most critical components are the control units and the copper connects. Although their weight percent is very low, the related impacts are significant. As shown in the sensitivity analysis the type of printed circuit board and its content of rare metals highly influence the results. As follows it is relevant from an environmental perspective to try to reduce the amount of these components, and to select the printed circuit board to have less possible gold content. Reuse of the electronics is also a good idea, since they suffer little wear during the battery use. Both these actions would save both costs and environmental impacts. Attention should be paid when using multiple packs for one bus to not use multiple control units for the mentioned reasons.

The impacts of choices of various pack designs in terms of housing materials have little influence compared to the impact of the electronics, the cells, and the choice of total capacity. The choice of pack modularization has shown to have an impact in terms of weight; the larger modules the lighter pack. The possibility for second use and reuse is dependent on the module size where a smaller module size will be beneficial in terms yield rate. However, the number of parts to administrate and disassemble makes the remanufacturing more costly, as well as increases amount of housing materials and connects. More research on this topic is needed for an optimal trade off.

On a higher system level, the battery pack should be seen as an integrated part of the vehicle, meaning that many choices can be done to decrease the environmental impacts, taking into account voltage matching, weight and number of passengers versus capacity of the pack, fast charging implications and design and disposition of components to enable reuse and second use. Reuse of pack components and cells has shown to be an efficient measure to reduce the battery life cycle impacts if it can be done at high rates. Especially the reuse of passive pack components seems a recommendable choice, without risk of affecting safety or performance.

A weight increase of 300-500 kg, for example caused by an increased battery pack weight, leads to an energy consumption contribution similar to the one of the production of the battery pack. Additionally, this increase could result in a reduced number of passengers which reducing the battery weight an important factor to consider. The interfaces between battery and drive line should be optimized, especially in terms of voltage, to avoid extra weight from other components such as converters.

The cooling system is an important part of the ESS and the actual integration of the structure varies from case to case. The results from changing the thickness of cooling plates for fast charging indicates an increase in energy use both in pack production and use phase due to the added weight of the system.

As a last conclusion, recycling cells and cell material will most likely become increasingly important. The assessment in this thesis shows that there are environmental gains when recycling, both with pyrometallurgy and hydrometallurgy. The gains must however be placed in context of economic gains, and this is the current limit both for lithium extraction as an addition to pyrometallurgy, and to hydrometallurgy. The energy savings of aluminium recycling in the hydrometallurgical route are large, although they were not assessed in relation to a possible increase in energy use. If recycling is not viable, reuse of the cells may be an alternative to lower the impact of the production phase.

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Appendix

Modeling data for cells and electrodes

Table A.1: The table present the assumptions made on recovery rates for the different recycling methods. In most cases 100% or 0% is assumed, but for the electrolyte some unavoidable losses are assumed.

Positive electrode	wt% LFP	wt% NMC	wt% LFS	wt% LMP
Active material	56.90%	66.47%	38.42%	59.77%
Carbon black	3.84%	4.48%	2.59%	4.03%
PVdF	3.20%	3.73%	2.16%	3.36%
Aluminium foil	36.06%	3.73%	2.16%	3.36%

Negative electrode	wt% Graphite	wt% LTO
Active material	28.44%	58.77%
Carbon black	0%	3.96%
PVdF	1.50%	3.30%
Copper foil	70.06%	-
Aluminium foil	-	33.96%

Cell assembly	wt% LFP	wt% NMC	wt% LFS	wt% LMP
Positive electrode	35.0%	40.2%	26.35%	37.2%
Negative electrode	39.1%	38.7%	44.19%	37.5%
Electrolyte	18.0%	13.9%	20.73%	17.1%
Separator	3.9%	3.1%	4.62%	3.7%
Casing	4.0%	4.1%	4.1%	4.5%

Table A.2: Summary of all materials involved in cell production. Models for some materials during the LCA are given, as well as references for LCA data and materials choices.

Component	**Precursors**	**kg in/kg component**	**Modeled as**	**Data reference**	**Materials choices reference**
LFP wet	LiOH	0.46		Ecoinvent	[Chen & Whittingham 2006]
	H_3PO_4	0.62	85% in H_2O	Ecoinvent, industrial grade	[Chen & Whittingham 2006]
	$FeSO_4$	0.96		Ecoinvent	[Chen & Whittingham 2006]
LFP dry	Li_2CO_3	0.47		Ecoinvent	[Jugović & Uskoković 2009]
	FeC_2O_4	0.91	$FeSO_4$	Ecoinvent	[Jugović & Uskoković 2009]
	$(NH_4)_3PO_4$	1.07	$(NH_4)_2PO_4$	Ecoinvent, as P205	[Jugović & Uskoković 2009]
LMP wet	LiOH	0.46		Ecoinvent	From LFP
	H_3PO_4	0.62	85% in H_2O	Ecoinvent, industrial grade	From LFP
	$MnSO_4$	0.96	Modified Mn conc.	Majeau-Bettez-Ecoinvent	From LFP
LMP dry	Li_2CO_3	0.47		Ecoinvent	From LFP
	MnC_2O_4	0.91	$MnSO_4$	Majeau-Bettez-Ecoinvent	From LFP
	$(NH_4)_3PO_4$	1.08	$(NH_4)_2PO_4$	Ecoinvent, as P205	From LFP
NMC wet	LiOH	0.25		Ecoinvent	[Myung et al. 2005]
	$NMC_{1/3}(OH)_2$	0.95			[Myung et al. 2005]
	$NiSO_4$	0.26	Modified metallic Ni	Majeau-Bettez+Ecoinvent	[Myung et al. 2005]
	$CoSO_4$	0.26	Modified metallic Co	Majeau-Bettez+Ecoinvent	[Myung et al. 2005]
	$MnSO_4$	0.24	Modified Mn conc.	Majeau-Bettez+Ecoinvent	[Myung et al. 2005]
	NaOH	0.87	50% in H_2O	Ecoinvent, production mix	[Myung et al. 2005]
	NH_4OH	0.73		Ecoinvent	[Myung et al. 2005]
NMC dry	LiOH	0.25		Ecoinvent	[Wang et al. 2004]
	Ni_2O_3	0.29	Oxidized Ni metal	Ecoinvent	[Wang et al. 2004]
	Mn_2O_3	0.27		Ecoinvent	[Wang et al. 2004]
	Co_2O_3	0.29	Oxidized Co metal	Ecoinvent	[Wang et al. 2004]
LFS wet	LiOH	0.30		Ecoinvent	[Dominko et al. 2006]
	SiO_2	0.37	Quartz sand	PE	[Dominko et al. 2006]
	FeCl 40% in H_2O	1.96	40% in H_2O	Ecoinvent	[Dominko et al. 2006]
LFS Dry	Li_2CO_3	0.46		Ecoinvent	[Huang et al. 2010]
	FeC_2O_4	0.89	$FeSO_4$	Ecoinvent	[Huang et al. 2010]
	SiO_2	0.92	Quartz sand	PE	[Huang et al. 2010]
Graphite		1.00	Battery grade graphite	Ecoinvent	
LTO	TiO_2	1.20	TiO_2	Ecoinvent, chloride path	[Verhulst et al. 2003*b*]
	LiCl	0.27		Ecoinvent	
Electrolyte	$LiPF_6$	0.13			[Nelson et al. 2011]
	LiCl	0.28		Ecoinvent	
	PCl_5	1.37		Ecoinvent	
	HF	0.79		Ecoinvent	
	EC	0.44	Ethylene glycol	Ecoinvent	[Nelson et al. 2011]
	DMC	0.44			[Nelson et al. 2011]
	methanol			Ecoinvent	
	phosgene			Ecoinvent	
Separator	Polypropylene	0.80		PE	[Nelson et al. 2011]
	Polyethylene	0.20		PE	[Nelson et al. 2011]
Cell casing	PET	0.13		PE	[Nelson et al. 2011]
	Polypropylene	0.05		PE	[Nelson et al. 2011]
	Aluminium foil	0.82		PE	[Nelson et al. 2011]
Electrode assembly	Active material	See A.1		-	[Nelson et al. 2011]
	Carbon black	See A.1		PE	[Nelson et al. 2011]
	Polyvinylidene fluoride	See A.1	Polyvinylfluoride, at plant	Ecoinvent	[Nelson et al. 2011]
	N-methyl-2-pyrrolidone	See A.1		Ecoinvent	[Nelson et al. 2011]
	Aluminium foil	See A.1		PE	[Nelson et al. 2011]
	Copper foil	See A.1	EU-15 Copper sheet	ELCD/ECI	[Nelson et al. 2011]

Modeling data for pack components and materials

Table A.3: Summary of all materials involved in pack and their database, mass compositions are found in appendix A, tableA.4, A.5. * The module and pack housings have different materials in different designs but the mass composition is never blended.

Component	**Precursors**	**kg$_{material}$/ kg$_{component}$**	**Modeled as**	**Data reference**	**Material choices reference**
Pack housing and Module housing alternatives*	Stainless steel	1	Stainless steel cold rolled coil (304)	Eurofer	[Nelson et al. 2011]
	Aluminium	1	Aluminium sheet	EAA	[Nelson et al. 2011]
	PP	1	Polypropylene injection moulding part	PlasticsEurope	[Klason et al. 2008]
Insulation	PU	1	Polyurethane foam	PlasticsEurope	[Klason et al. 2008]
Steel straps/Plates	Stainless steel	1	Stainless steel cold rolled coil (304)	Eurofer	[Nelson et al. 2011]
Cooling plates	Aluminium	1	Aluminium sheet	EAA	[Nelson et al. 2011]
Copper connects	Copper	1	Copper mix 40% recycled	PE	[Nelson et al. 2011]
BMS and SOC controller	PCB low gold	0.1	printed wiring board, through-hole	Ecoinvent	[Majeau-Bettez et al. 2011]
	PCB high gold		printed wiring board, through-hole mounted, unspec.,solder mix	Ecoinvent Ecoinvent	
	Stainless steel	0.5	Stainless steel cold rolled coil (304)	Eurofer	
	Copper	0.4	DE: Copper mix 40% recycled	PE	
Fuel	Diesel	1	Diesel mix at refinery	PE	[Volvo Buses 2013*a*]
Urea solution (AdBlue)	Urea	0.325	Urea	Ecoinvent	[Tennants Distribution Limited 2008]
	Water	0.685	Water	Ecoinvent	
Cooling fluid	Ethylene glycol	0.5	Ethylene glycol	PE	[Nelson et al. 2011]
	Water	0.5	Water (desalinated; deionised)	PE	
Electricity	European average	-	EU-27 Electricity grid mix	PE	
	Nordic average	-	NORDE: electricity, production mix	Ecoinvent	
	Swedish hydro power	-	SE: Electricity from hydro power	PE	

Table A.4: Summary of all materials involved in LFP Pack design. GaBi databases and precise material properties found in appendix A, table A.3. Extra denoted design options where the materials are constant, but amount of packs (Extra 1) and size of the pack (Extra 2) are changed.

Component	**Design 1 Al**	**Design 2 steel**	**Design 3 steel-Al**	**Design 4 steel-plastic**	**Extra 1 Al 2 packs**	**Extra 2 Al large**
Pack [kWh]	40	40	40	40	40	40
ESS [kg]	568.1	594.3	573 .4	595.9	583.2	600
Spec. energy Wh/kg	82.3	78.1	81.4	77.9	79.9	66.7
Cells [kg]	434	434	434	434	434	434
Cell [g]	670	670	670	670	670	670
Cell [Ah]	20	20	20	20	20	20
Cell [Wh]	66	66	66	66	66	66
Cell [V]	3.3	3.3	3.3	3.3	3.3	3.3
SOC controllers [kg]	1.73	1.73	1.73	1.73	1.73	1.73
BMS [kg]	4	4	4	4	8	4
Connects Cu [kg]	3	3	3	3	2.18	2.3
Terminals Cu [kg]	1.8	1.8	1.8	1.8	3.54	1.8
Steel plates and straps [kg]	2.7	2.7	2.7	15.3	5.4	3.53
ESS case [kg]	37.2	81.3	81.3	81.3	40.74	47.1
Module house [kg]	11.13	32	11.13	21	11.13	14.07
Thermal conductor (Al) [kg]	25.6	25.6	25.6	25.6	25.6	31.86
Coolant [kg]	8	8	8	8	8.74	10.8
Thermal insulation [kg]	38.7	-	-	-	42	48.54

Table A.5: Summary of all materials involved in NMC Pack design in BatPaC. GaBi databases and precise material properties found in appendix A, table A.3. Extra 1 denotes that the materials are kept constant, but three modules are parallel connected.

Component	**Design 1 Al**	**Design 2 steel**	**Design 3 steel-Al**	**Design 4 steel-plastic**	**Extra 1 Al parallel mod.**
Pack [kWh]	60	60	60	60	60
Spec. energy $^{Wh}/_{kg}$	114.8	108	113.4	107.4	114.2
ESS [kg]	586.7	619.7	593.1	622.7	589.7
Cells [kg]	421	421	421	421	421
Cell [g]	650	650	650	650	650
Cell [Ah]	25	25	25	25	25
Cell [Wh]	95	95	95	95	95
Cell [V]	3.8	3.8	3.8	3.8	3.8
SOC controllers [kg]	1.73	1.73	1.73	1.73	5.18
BMS [kg]	4	4	4	4	4
Connects Cu [kg]	2.3	2.3	2.3	2.3	1.93
Terminals Cu [kg]	1.5	1.5	1.5	1.5	1.52
Steel plates and straps [kg]	3.53	3.53	3.53	20.1	3.53
ESS case [kg]	47.1	102.15	102.15	102.15	47.1
Module house [kg]	14.1	40.7	14.1	27.1	14.1
Thermal conductor (Al) [kg]	31.9	31.9	31.9	31.9	31.9
Coolant [kg]	10.8	10.8	10.8	10.8	10.8
Thermal insulation [kg]	48.5	-	-	-	48.5

Vehicle and driving parameters

Table A.6: Average data collected for the driving phase, vehicle data, distances. Fuel consumption and electric consumption are intended for all electric driving and all diesel mode driving. The data derives from calculations, literature and personal communication in 2013.

PHEV Bus - Parallel hybrid configuration, regenerative braking	**Data**	**Reference or Personal communication (PC)**
Max weight	19000 kg	[Volvo Buses 2013*a*]
Average weight	14500 kg (estimate)	Johan Johansson
Curb weight	12000 kg (estimate)	Johan Hellsing
Max passengers	90	[Volvo Buses 2013*a*]
Average passengers	33	Calculation
ICE	Volvo D5K 5 l 240 hp	Volvo Buses
Average load diesel consumption	0.31 l/km (estimate)	Johan Johansson
Standard bus average load diesel consumption	0.5 l/km (estimate)	Johan Johansson
Urea consumption (all buses)	5.7 v% (estimate)	Lisbeth Dahllöf
Average load electricity consumption	1.5 kWh/km (estimate)	Pontus Enhager
Electric efficiency grid to wheel	0.71 (estimate)	Edward Jobson
Battery efficiency	0.92 (estimate)	Edward Jobson
Diesel efficiency tank to wheel	0.30 (estimate)	Pontus Enhager
Electric mode	80 % (estimate)	Edward Jobson
Driving distance per year	120000 km/year	Calculation
Approximate driving cycle	Braunshweig city driving cycle	[Barlow et al. 2009]
Average driving speed	21 km/h	Estimate
Service time per day	16 h/year	Estimate
Service days per year	350 d/year	Estimate
Vehicle life	9 years (estimate)	Jens Groot
Batteries per bus	3 batteries (estimate)	Jens Groot
EM max power	150 kW	[Volvo Buses 2013*a*]
Battery SOC window	40 % (estimate)	Jens Groot
LFP battery available capacity	16 kWh	Calculation
LFP battery total capacity	40 kWh	Calculation
NMC battery available capacity	24 kWh	Calculation
NMC battery total capacity	60 kWh	Calculation

Reuse options on a system level

Table A.7: Options of system levels for reuse or second life and remanufacturing. The table illustrated how different components can be reused (marked with x) or have the need to be changed in different combination. Depending on the state of health of different battery components one of the 16 scenarios is possible for reuse of second life.

Reuse scenarios	**ESS**	**Battery pack**	**Module**	**Cell**
1	x	x	x	x
2	x	x	x	change
3	x	x	change	change
4	x	change	change	change
5	change	change	change	change
6	x	change	x	x
7	x	change	change	change
8	x	x	change	x
9	change	x	change	change
10	change	x	x	change
11	change	x	change	x
12	change	x	x	x
13	change	change	x	x
14	change	change	x	change
15	change	change	change	x
16	change	change	change	change

Supporting figures - Results

The following figures are the complete graphical representation of the results presented in chapter 5. All scenarios and impact categories are included.

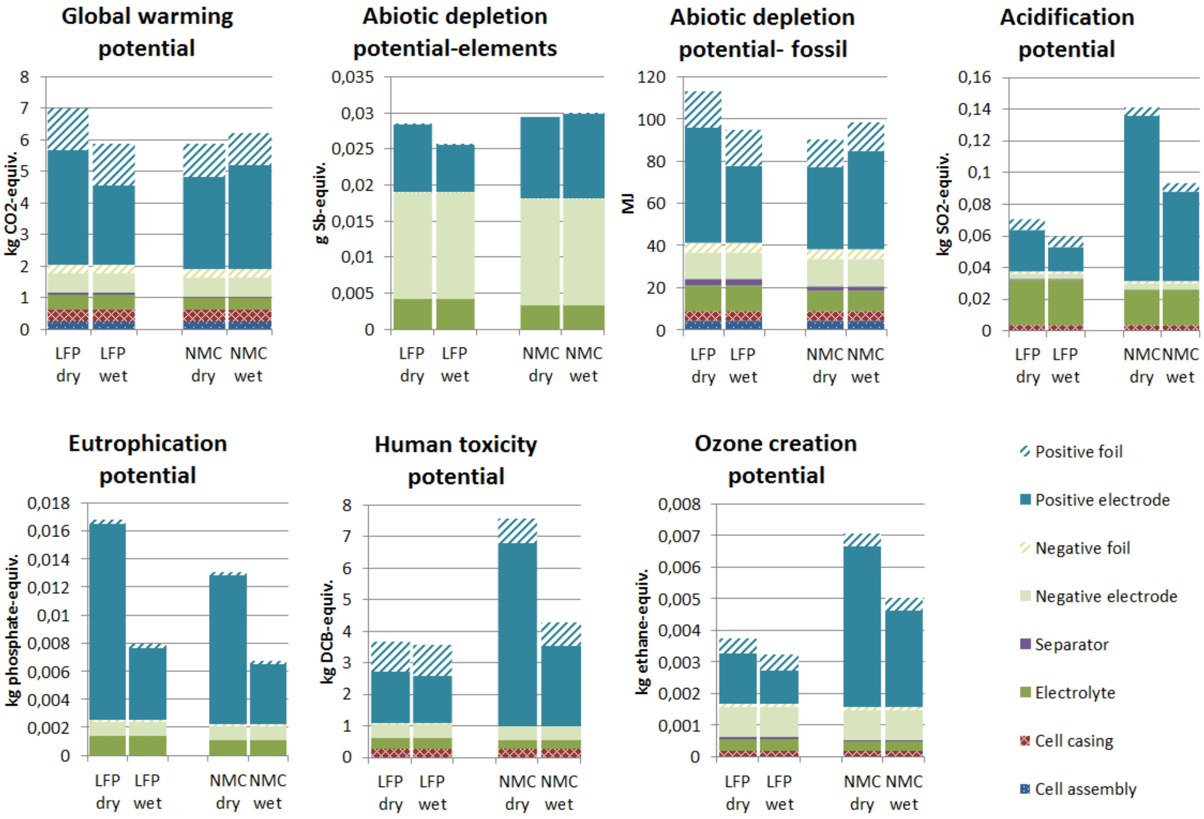

Figure A.1: The impact of the different components of the different cell chemistries is shown. The impact categories represented are energy use, global warming potential, abiotic depletion potential of elements and fossil fuels, acidification potential, eutrophication potential, human toxicity potential, photochemical ozone creation potential. The electrodes can be seen to have the largest single impact.

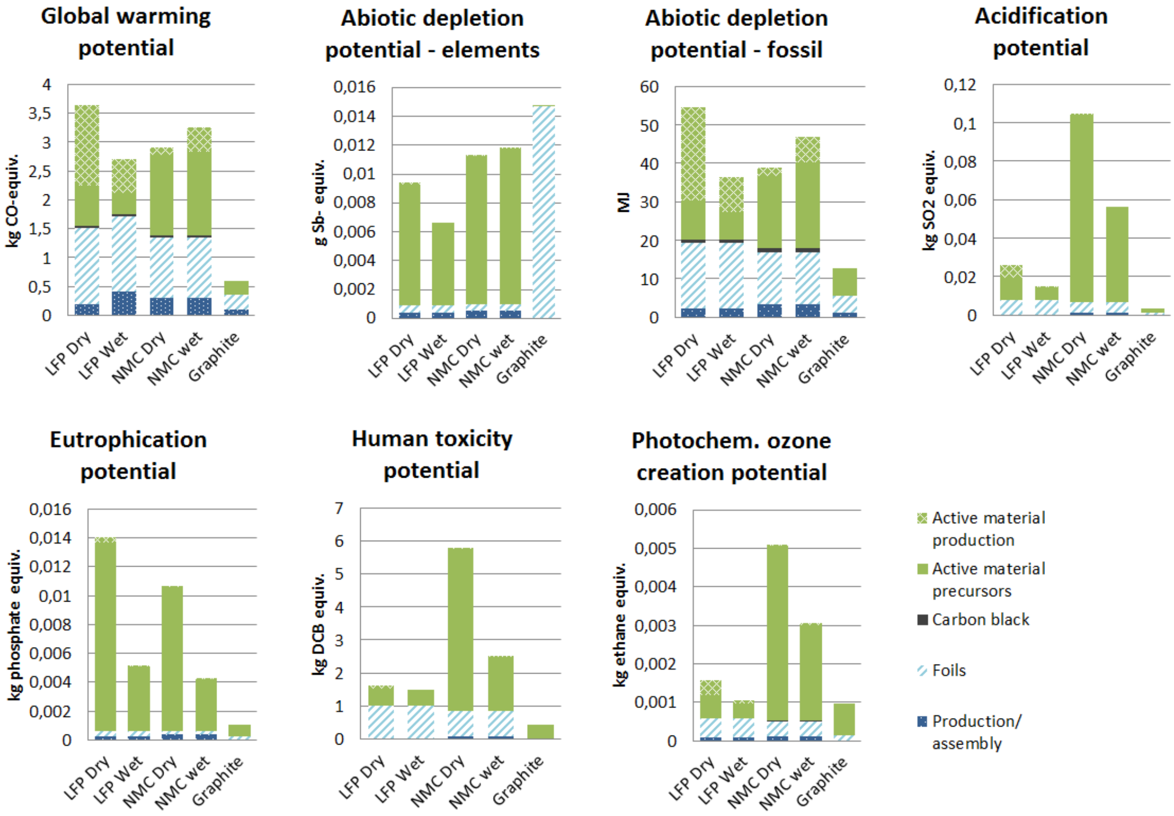

Figure A.2: The impact of the different components of the positive electrode is shown, for different cell chemistries and production paths. The impact categories represented are energy use, global warming potential, abiotic depletion potential of elements and fossil fuels, acidification potential, eutrophication potential, human toxicity potential, photochemical ozone creation potential. The foils and active materials dominate, but the relative contributions vary.

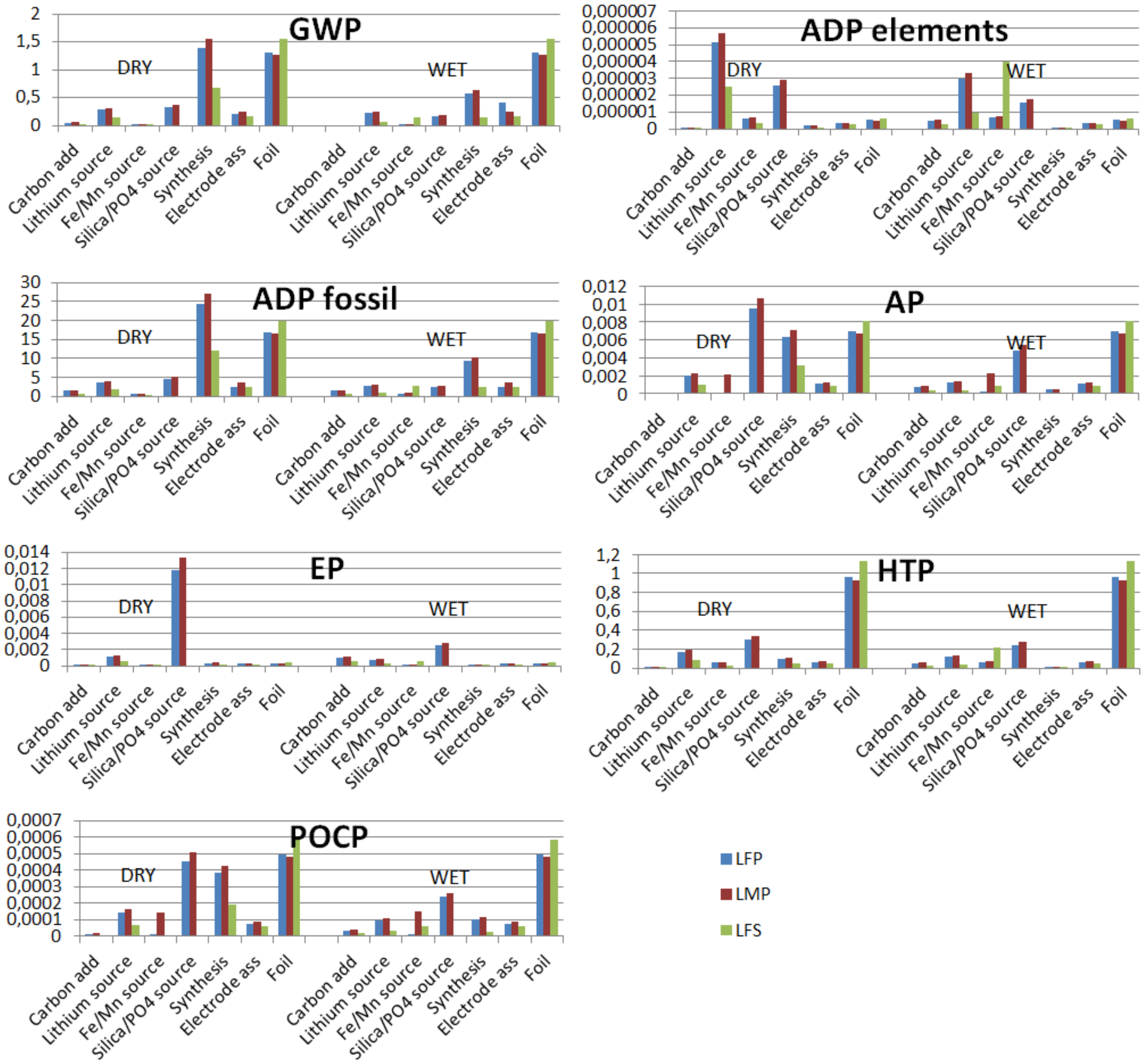

Figure A.3: Impacts of LMP and LFS compared to LFP.

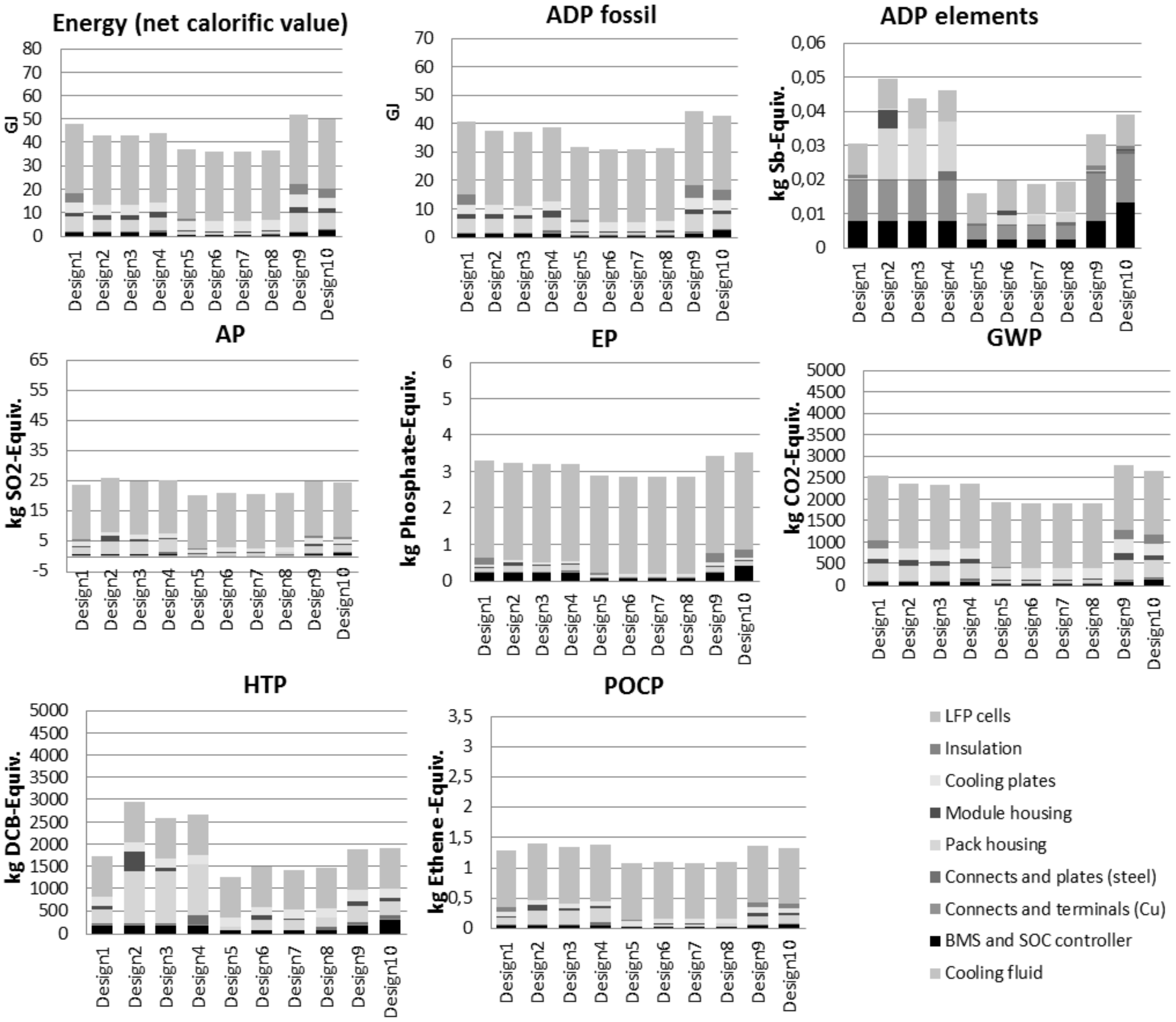

Figure A.4: Material choices and impacts per component of battery pack design alternatives with and with out reuse for LFP. The first 1-5 designs are shown with normal conditions, design 5-8 are the same as the first 4 but with highest possible reuse rate of passive components. Design 9 and 10 are equally configured as Design1, but the design 9 with extra large fit of cells in modules, and the last design 10 with two packs of 20 kWh coupled to one ESS of 40 kWh. For exact material composition see figure A.4

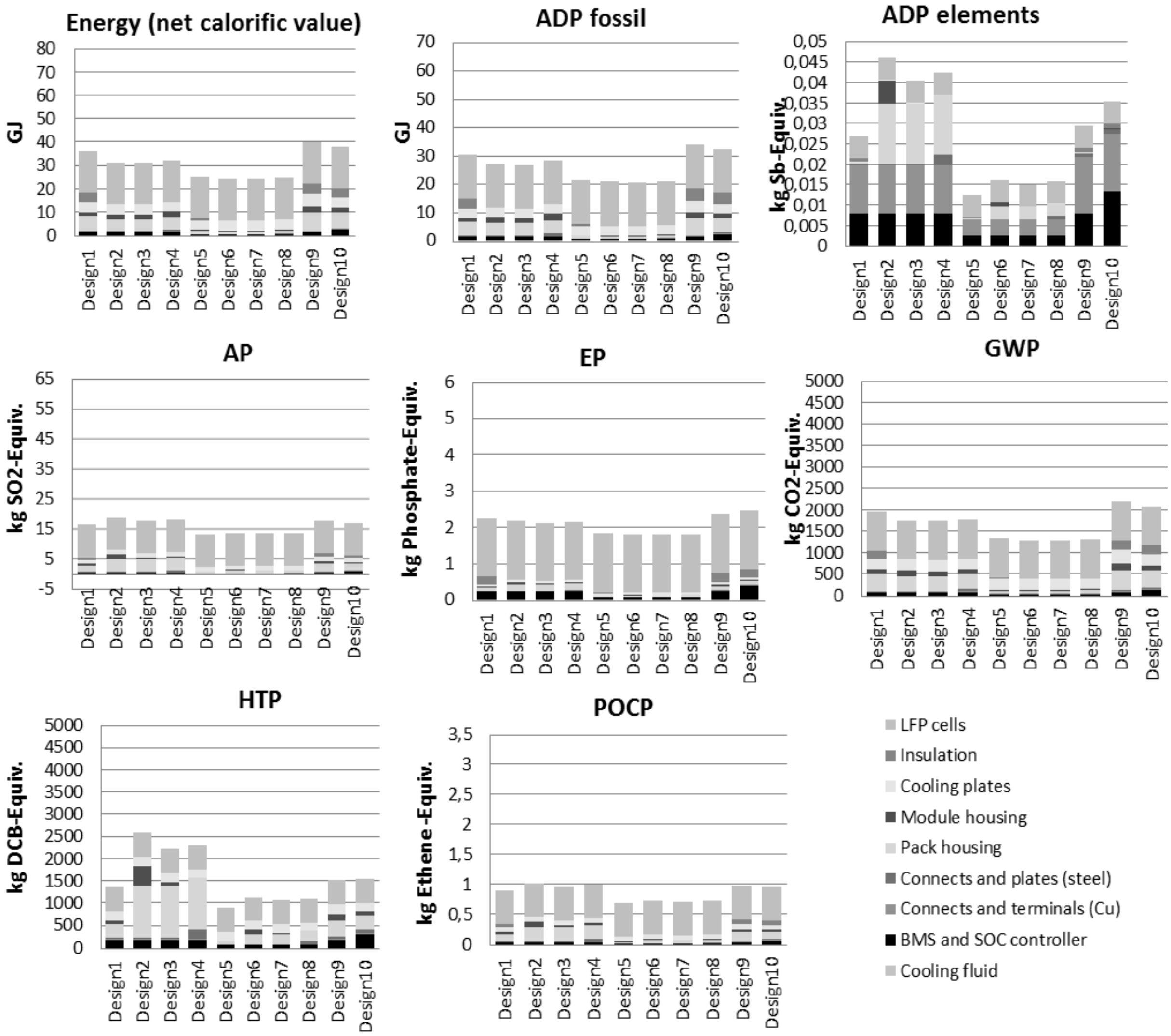

Figure A.5: Material choices and impacts per component of battery pack design alternatives with 40% reuse of cells and with and without reuse of passive components. The first 1-5 designs are shown with normal use conditions, design 5-8 are the same as the first 4 but with highest possible reuse rate of passive components. Design 9 and 10 are equally configured as Design1, but the design 9 with extra large fit of cells in modules to simulate LFP cells in a pack designed for NMC cells, and the last design 10 with two packs of20 kWh coupled to one ESS of 40 kWh. For exact material composition see table A.4 in chapter 4.

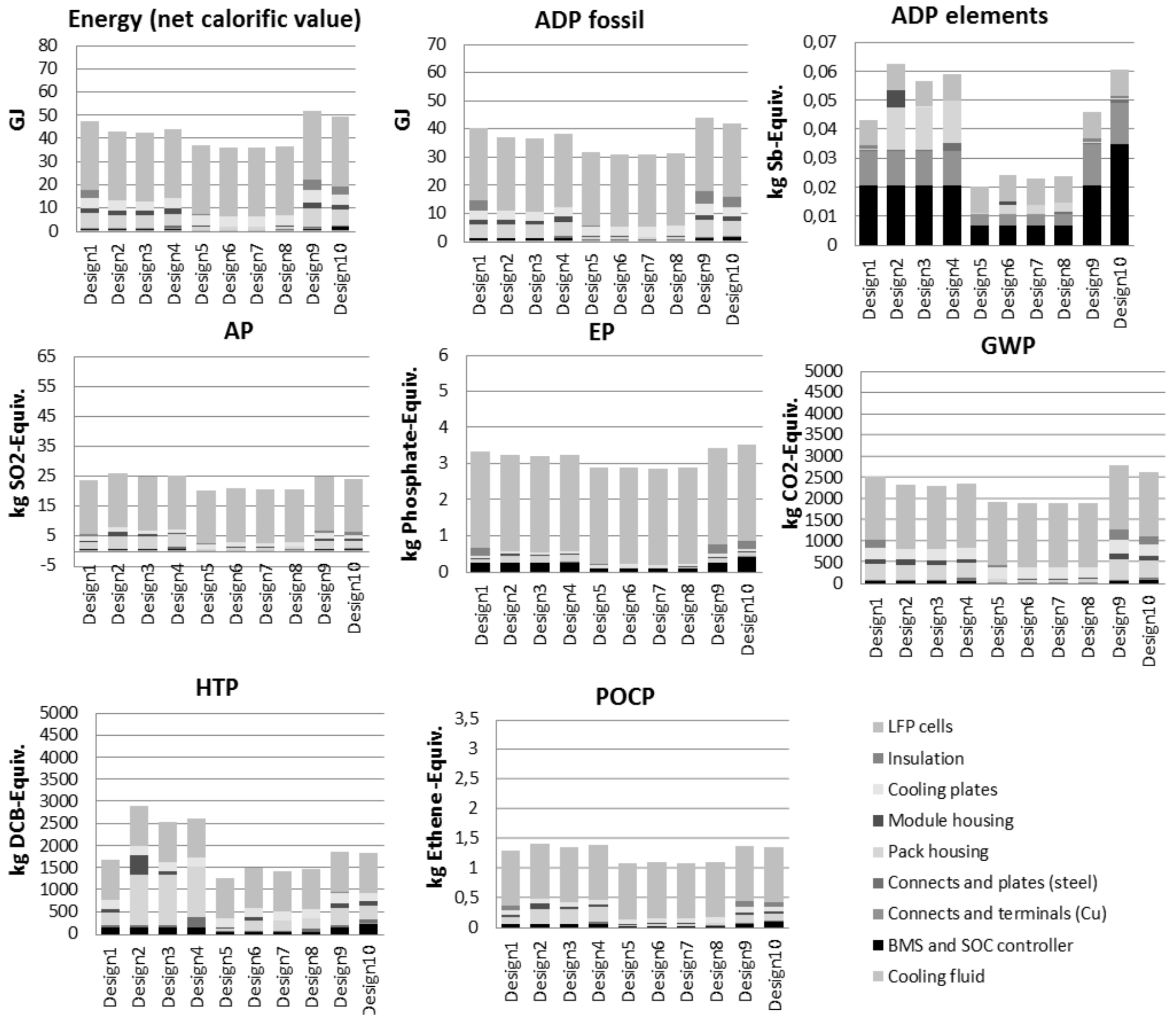

Figure A.6: Material choices and impacts per component of LFP battery pack design alternatives with and with out reuse. The PCB chosen has a higher gold content than usual. The first 1-5 designs are shown with normal use conditions, design 5-8 are the same as the first 4 but with highest possible reuse rate of passive components. Design 9 and 10 are equally configured as Design1, but the design 9 with extra large fit of cells in modules, and the last design 10 with two packs of 20 kWh coupled to one ESS of 40 kWh. For exact material composition see table A.4 in chapter 4.

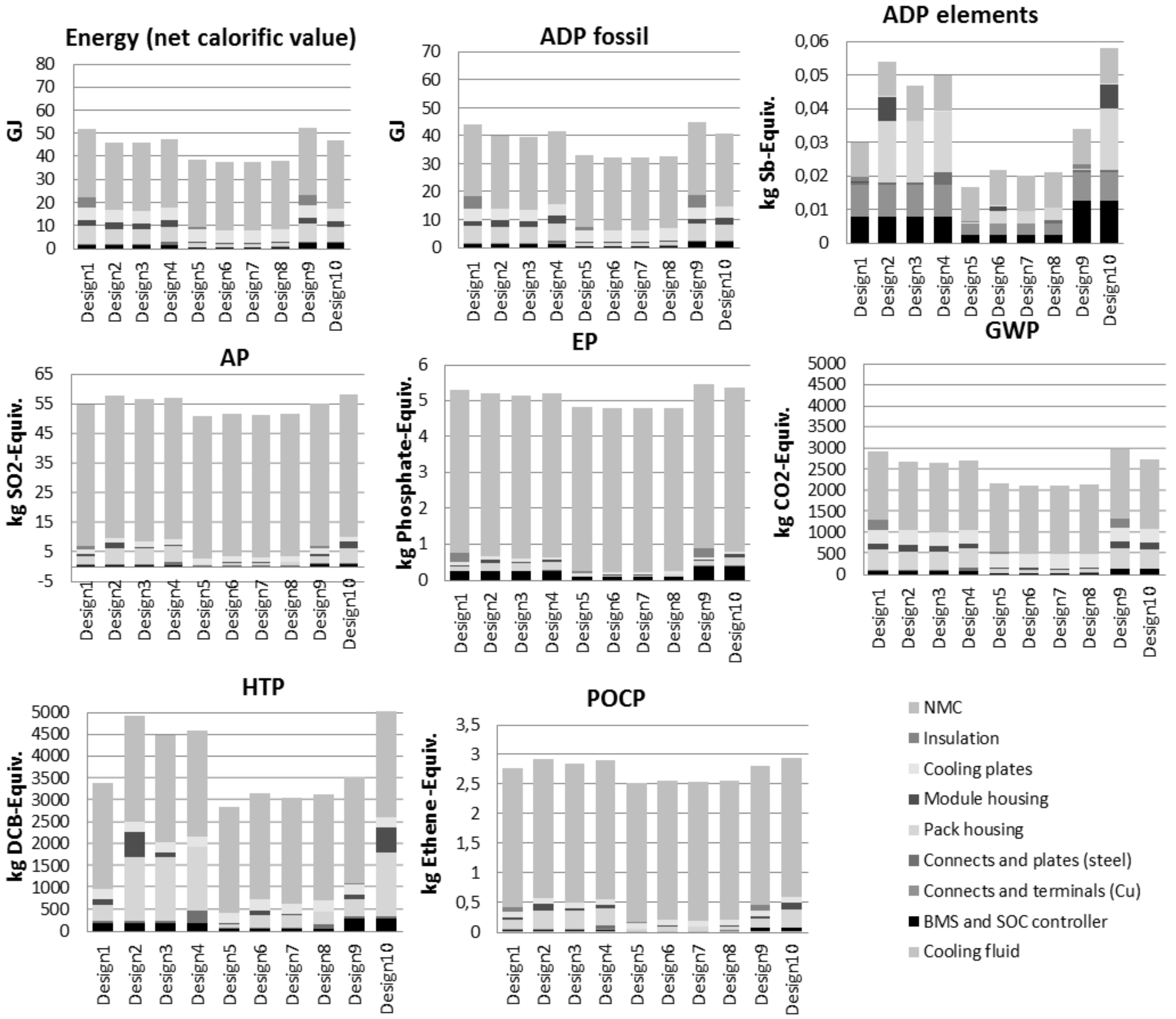

Figure A.7: Material choices and impacts per component of NMC battery pack design alternatives with and with out reuse. The first 1-5 designs are shown with normal conditions, design 5-8 are the same as the first 4 but with highest possible reuse rate of passive components. Design 9 and 10 are equally configured as Design1, and Design 2 but for 3 parallel connections on module level. For exact material composition see table A.5 in chapter 4.

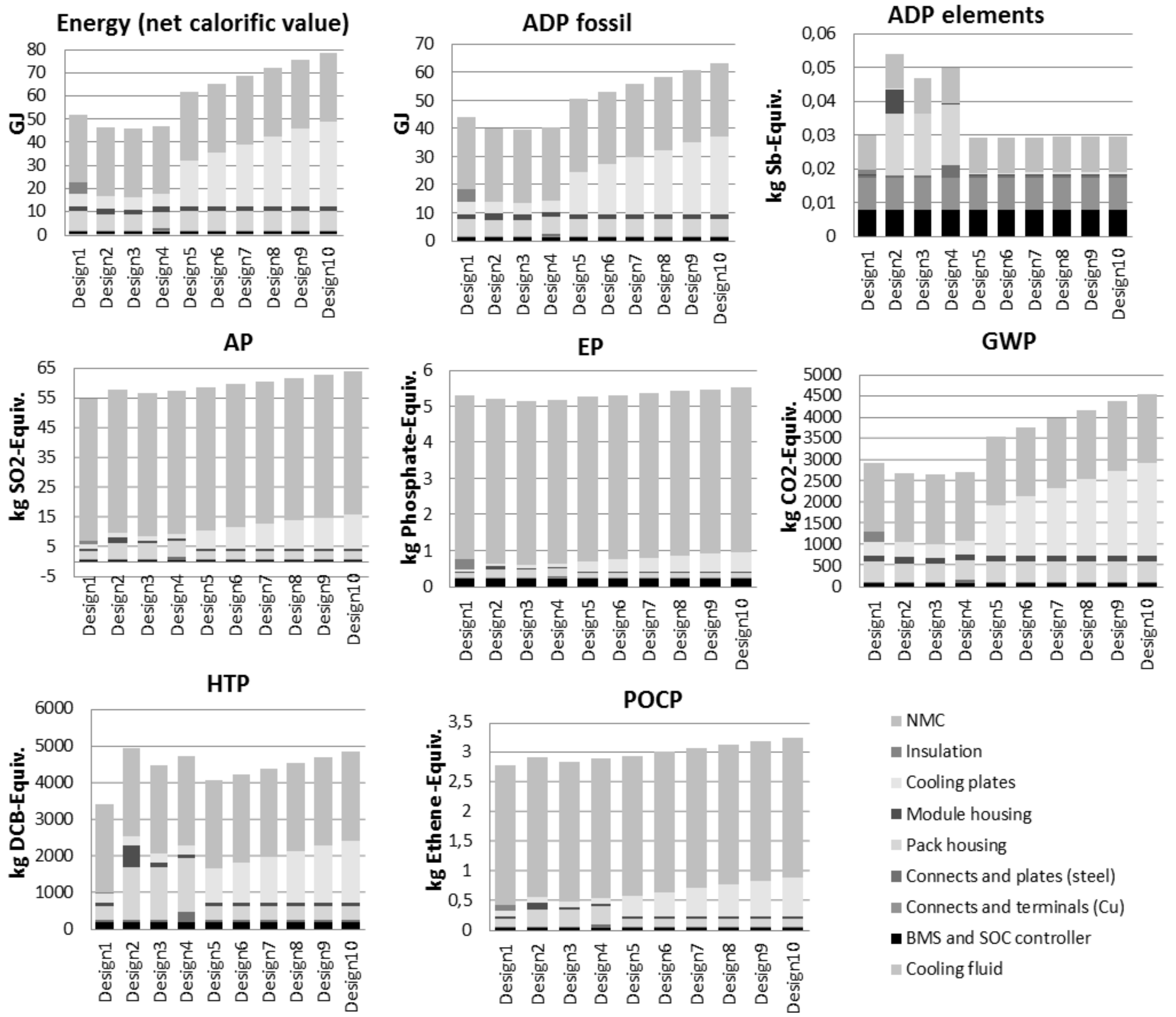

Figure A.8: Material choices and impacts per component of NMC battery pack design alternatives with and with out reuse. The first 1-4 designs are shown with normal design conditions for the all aluminium pack, design 5-10 are the same as the design1, but with increased amount of cooling plate material gradually from 84 kg to 181 kg. For exact material composition see table A.5 in chapter 4.

Impact per kg for different cell components

The data in the following figure can be used as reference if different wt% of the components are used compared to the values in this thesis.

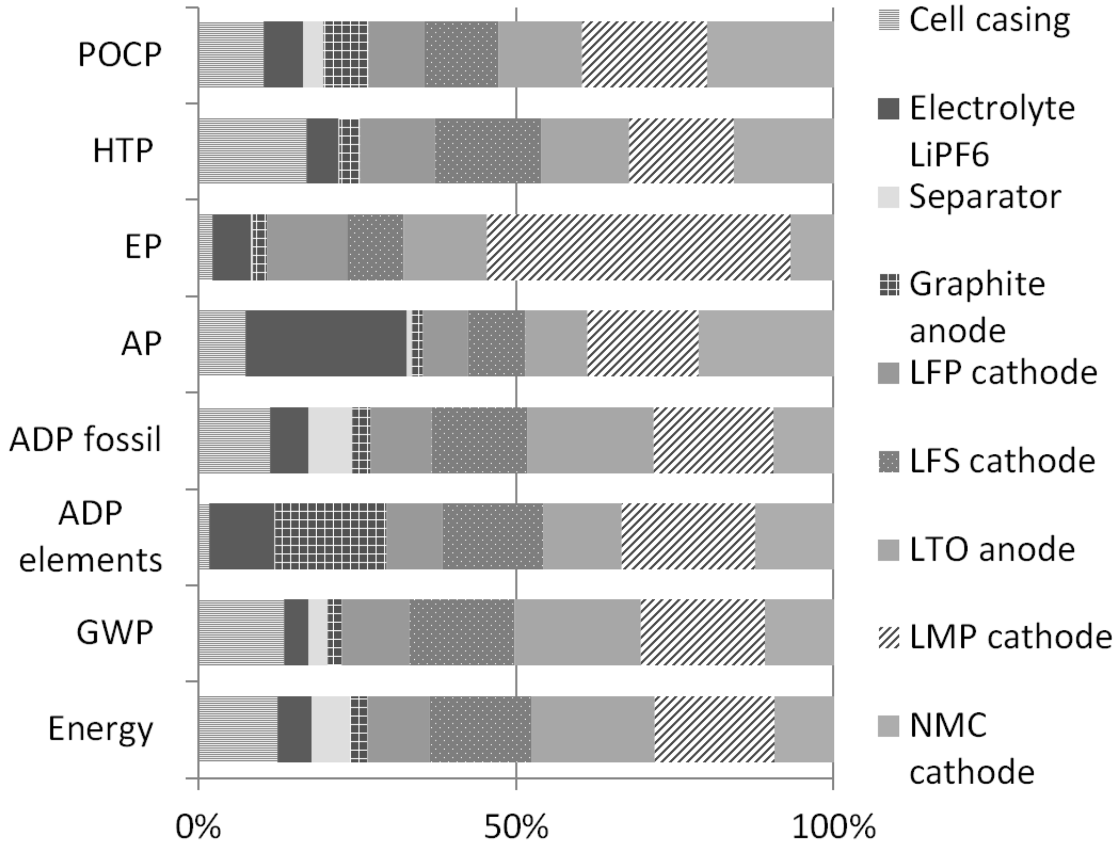

Figure A.9: The relative contribution of one kg of each of the cell components in given. The figure illustrates what components inherently impact what categories, independent on how much is used in the cell.