Life Cycle Assessment of an Organic Redox Flow Battery

by

Roel Maria Ralf Willem Degens

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Thesis committee:	Dr. Carlos Blanco,	Leiden University, 1st supervisor
	Dr.ir. Lydia Stougie,	TU Delft, 2nd supervisor

Executive summary

Energy storage systems can play a vital role in the implementation of a sustainable energy grid by allowing the wide scale implementation of fluctuating renewable energy sources like wind and solar. Therefore it is expected that in the coming years, the total amount of energy storage systems will drastically increase. Analysing the sustainability of these storage systems before widespread implementation is therefore of great importance. In this thesis such a life cycle assessment has been conducted to assess the environmental sustainability of one type of energy storage system: the Organic Redox Flow Battery produced by the Baliht research group.

In the first part of this research the important aspects on life cycle assessments of energy storage systems and more particularly of batteries have been analysed. From the literature analysis it is concluded that there are already a lot of different life cycle assessments on energy storage systems but it is difficult to compare the results of these studies. Modelling decisions as well as different functions of the energy storage system are aspects that make this comparison difficult. To get better and more comparable results it is therefore recommended to include important battery specifications in the functional unit. Next to that a cradle to grave approach was conducted to grasp the full life cycle impacts. Lastly a detailed reportage of the life cycle inventory was conducted.

From the results it is concluded that extra electricity input needed due to inefficiencies as well as the production of the battery are the biggest contributors for the total environmental burdens of the battery. Improving the round trip efficiency of the battery can therefore greatly improve the environmental performance of the battery. Due to the relatively low round trip efficiency, the total results are very dependent on the electricity source of the battery. Connecting the battery to a renewable energy source is therefore crucial. In the production phase of the battery, a large amount of impact comes from the battery stack as well as the inverter. This is related to the graphene in the electrode, and the copper in the current collector and inverter. Reusing or extending the lifetime of these components can greatly enhance the environmental performance

Compared to a Lithium Ion Battery and a Vanadium Redox Flow Battery, the Organic Redox Flow battery has a lower environmental impact. Many of the emissions in the Lithium Ion Battery and the Vanadium Redox Flow battery come from the production of scarce metals like lithium, cobalt, and vanadium. The absence of these metals and the use of more abundant materials like iron and carbon in the Organic Redox Flow Battery makes the battery a lot more sustainable.

In the last part of this research the effect of maintenance of the electrolyte has been analysed. For the electrolytes there were three different strategies for battery maintenance: 1) fully replace the electrolyte, 2) separate the inert active material and replace it with fresh active material, and 3) separate the inert active material and chemically reactivate it. There is currently still a lot unknown in terms of different battery aspects that can impact the total environmental performance. Therefore a statistical approach was taken to analyse under which conditions, which maintenance strategy has the best environmental performance. It was concluded that chemical reactivation strategy is the best strategy in terms of environmental performance of the battery. It is also shown how such a statistical approach to LCAs can be very powerful to gain valuable information of the product system.

Acknowledgements

"The important thing is not to stop questioning. Curiosity has its own reason for existing."
-Albert Einstein.

With this thesis a long journey comes to an end. A journey that started as a little kid, wondering why the sky is blue and the grass is green, and now ends by finishing my master's degree Industrial Ecology. I like to take this opportunity to express my gratitude to all the great teachers that helped me on this journey and always sparked my curiosity. Finishing my master's degree would not have been possible without your guidance.

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Abbreviations

Abbreviation	**Description**
DHPS	7,8-dihydroxyphenazine-2-sulfonic acid
EoL	End of Life
ESS	Energy Storage System
EU	European Union
GW	giga watt
HER	Hydrogen Evolution Reaction
kWh	Kilowatt hour
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LIB	Lithium-ion Battery
OER	Oxygen Evolution Reaction
ORFB	Organic Redox Flow Battery
VRFB	Vanadium Redox Flow Battery

1

Introduction

1.1. Problem introduction

Modern society is currently heavily dependent on a reliable supply of energy. The current energy system is heavily based on fossil-based fuels like natural gas, coal, and oil [Rahman et al., 2020] which is considered to be unsustainable due to their limited availability [Höök and Tang, 2013], their negative impact on human health [Lelieveld et al., 2019], and their effects on climate change [Mora et al., 2018]. Therefore, there is a need to change towards more sustainable energy systems based on renewable energy sources. The implementation and integration of these renewable energy sources into the energy system have some challenges involved in terms of efficiency, reliability, and stability. These challenges mainly arise due to the intermittent nature of these renewable energy sources [Olabi et al., 2021]. Solar panels only produce electricity when the sun is shining, while wind turbines only produce it when the wind is blowing. These challenges can be addressed by energy storage systems (ESSs) which can act as a catalyst for the implementation of these renewable energy sources [Koohi-Fayegh and Rosen, 2020].

The European Union has identified energy storage through batteries as one of the main pathways for a low carbon economy [Andrey et al., 2020]. Therefore the EU is currently investing a lot of research and development on ESSs to find cost-effective, reliable, safe, and environmentally friendly ESSs. The most utilized form of energy storage in the European Union is pumped hydro storage. Pumped hydro storage is a well-established and commercially acceptable technology that has been used since the 1890s [Rehman et al., 2015]. Drawbacks of this technology are their dependence on a suitable geographical location and high investment costs [Javed et al., 2020]. Therefore the EU is currently looking for other types of ESSs and has identified battery storage as a promising technology [Andrey et al., 2020].

Currently, the most used battery storage system is that of Lithium Ion batteries (LIBs) [Andrey et al., 2020]. LIBs have proven to be commercially effective and a lot of research is being conducted to further improve these types of batteries [Li et al., 2018]. Major drawbacks of LIBs are their safety and sustainability issues. LIBs currently use flammable liquids which could result in major accidents in case of battery failure [Chen et al., 2021]. The LIB furthermore uses scarce metals like lithium, cobalt, and nickel which are currently mined in inhuman conditions and could have a major impact on the environment. For the cobalt mining industry, there are many reports of child labor in the Republic of Congo. There are furthermore lots of health and safety concerns for the miners due to exposure to lung contaminating and eye irritating mineral dust. Furthermore, there are many concerns about the pay wage for these miners, where it is reported that the cobalt miners are not capable of feeding their family [amn, DZAKPASU, 2021, Kara, 2018, Nordbrand and Bolme, 2007]. For these reasons, there is a lot of interest in other types of battery storage that don't use these metals. Flow batteries are considered a promising candidate. There are many variations of flow batteries, with the Vanadium Redox Flow Battery (VRFB) and Zinc Bromide battery the most mature versions. A more thorough explanation of flow batteries can be found in chapter 2.

One promising type of flow battery is the Organic Redox Flow Battery (ORFB). This battery uses organic materials and water-based electrolytes. This makes the battery safe and potentially more sustainable and could make a big impact in creating a low carbon-based economy [Hu et al., 2017, Winsberg et al., 2017]. Next to this, the battery has a modular design making it easier to adapt the battery to the function it's needed to fulfill, while also allowing for battery maintenance. This could increase the lifetime of the battery, potentially lowering the total amount of resources needed for the battery. How the ORFB functions will be discussed further in section 2.5.

1.2. Research gap

In the literature, there are multiple publications that assess the environmental sustainability of ESSs. In a recent publication, Rahman et al. [2020] made a review on different assessment techniques for ESSs. The most common method used for this is Life Cycle Assessment (LCA). In the review they analysed 33 LCAs conducted on a multitude of different ESSs. Determining the environmental sustainability of ESSs is therefore not something brand new. In the review, there isn't a single LCA of organic redox flow batteries reported. If a search on the different online search engines (google scholar, scopus) for the keywords *LCA, Life Cycle Assessment, Organic Redox Flow Battery* is conducted only two relevant articles [Di Florio et al., 2022, Zhang et al., 2022] can be found, both of which focus on a different configuration of ORFB. Because of the reasons mentioned above, it is claimed that the new ORFB is sustainable with a low environmental impact [Winsberg et al., 2017]. This claim hasn't been researched and thus hasn't been proven so far. The lack of research on the environmental sustainability of this new type of battery has been identified as the main research gap.

In the research from Rahman et al. [2020] it is also concluded, that the results from the different LCA studies can vary tremendously because of a multitude of modeling decisions made in the different studies. Hiremath et al. [2015] showed that the impact on GW can variate between 177 g CO_2-eq./kWh and 810 g CO_2-eq./kWh for Li-ion batteries and between 201 g CO_2-eq./kWh and 937 g CO_2-eq./kWh for VRFB. Having this broad range of results can complicate conclusions made from these LCA studies. For instance, Hiremath et al. [2015] concluded that LIB have a lower impact on global warming, while Fernandez-Marchante et al. [2020]concluded the opposite. A second knowledge gap that has been identified is the availability of guidelines for the conduction of LCAs on batteries and ESSs.

1.3. Research goal and questions

The goal of this study is to assess the sustainability of this battery, find hotspots in the production process of the battery, and use this information to further improve the environmental performance of the battery. This study also tries to identify good practices for the LCA of batteries and ESSs.

To achieve these goals an LCA will be conducted on a case study of a project that is currently happening in the harbor of Ibiza, Spain. In this project, the ORFB is used as a charging station for the charging of electric ferries.

From the research goal, the following main research question is developed:

What are the environmental impacts of an Organic Redox Flow Battery over its entire life cycle?

In order to answer this research question, it is subdivided into multiple sub-research questions:

1. *How can the LCA of Organic Redox Flow Batteries best be conducted?*
2. *How does the ORFB function and what are other relevant energy storage technologies?*
3. *What are important aspects contributing to the environmental performance of the battery?*
4. *How does the environmental performance of an ORFB compare to other types of batteries with similar functions?*
5. *How can maintenance operations improve the environmental performance of the battery*
6. *How can the environmental assessment for batteries, energy storage systems, and in general be further improved?*

1.4. Connection with the Industrial Ecology program and societal relevance:

The industrial ecology master's degree evolves around the assessment of the sustainability of a multitude of products, product systems, production methods, and other aspects of our complete economic system. This research topic has an excellent connection with the program because it uses a holistic approach to determine the environmental sustainability of a promising emerging technology. It can furthermore help with the implementation of a greener electricity grid and improve the knowledge in the field of ex-ante LCAs on ESSs.

As described in the problem introduction, energy storage can have a tremendous impact in tackling the intermittency of wind and solar energy production. The International Energy Agency expects a rise in worldwide storage capacity from 5 GW in 2020 to a total capacity of 585 GW [IEA, 2021]. Analyzing at an early stage of deployment which ESS performs best and what limits certain ESSs can have a huge impact in this sector and is therefore very relevant for society.

1.5. Readers guide

This thesis is divided into several chapters. In the next chapter, an introduction to LCA, energy storage in general, and a more detailed overview of ORFBs is given. After this, a it is described how the LCA model of the battery is constructed. In chapter 4 the results from the LCA model are analysed. In chapter 5 the limitations of the study are discussed and future recommendations on LCAs of batteries are given. In the final chapter, the main research question is answered and further research recommendations are given.

2

Theory

The first step in this research is (1) to gather information about LCA in general and to obtain more information on LCAs of ORFBs and ESSs, and (2) to get a better understanding on ESSs and the ORFB from the Balith research group. This chapter will also answer the first two research questions.

2.1. Introduction to Life Cycle Assessment

Life Cycle Assessment (LCA) is an ISO standardised quantitative analytical tool [ISO, 2006] to assess the environmental burdens of products at all stages in their life cycle. ISO 14040 defines LCA as "the compilation and evaluation of the inputs, outputs and potential environmental impacts of a product system throughout its life cycle". LCA therefore not only analyses the environmental impacts of a product at its use stage, but also the production stage, including resource extraction, material production, and product production. Life cycle analysis furthermore includes the environmental emissions of a product's end of life stage [Guinée and Lindeijer, 2002].

Because LCA uses such a holistic approach to assess the environmental burdens of a product system, it is a strong tool to analyse which product is more environmentally sustainable. Using LCA can detect and avoid 'problem shifting'; Shifting environmental impacts from one stage of the product chain to another (e.g. from use phase to production phase). Another benefit of using LCA is its ability to give insight in which processes contribute the most to the environmental burdens of a product system [Hellweg and Milà i Canals, 2014]. This can help tremendously in finding hotspots in the product system. This information could be used to develop the product system, reducing potential future impacts (e.g. choose between multiple options of materials or production methods for the same material).

LCA studies follow the same framework (see figure 3) standardised by ISO [2006]. The first step in an LCA is the Goal and Scope Definition. In this step the product system is defined. Aspects of the products systems are for instance: The function of the product, the functional unit, the different alternatives, the geographical scope, the temporal scope, the technological coverage etc. In the second step, the Inventory Analysis, the product system is modelled. In this step, system boundaries are defined, flowcharts are completed, and data on the different processes is gathered, calculated and implemented into the model. The main result of the Inventory Analysis is an inventory table with all the environmental externalities associated with the functional unit. In the Impact Assessment, these environmental externalities are further processed using different models to assess the impact of a product system on different impact categories (e.g. global warming, acidification, eutrophication) [Guinée and Lindeijer, 2002].

The results from these three steps are interpreted and assessed in the Interpretation phase. In this step the quality of the research is discussed as well as a final result/recommendation is made [Guinée and Lindeijer, 2002]. The results from the LCA can be used for a multitude of applications including product development and improvement, strategic planning, public policy making, and marketing.

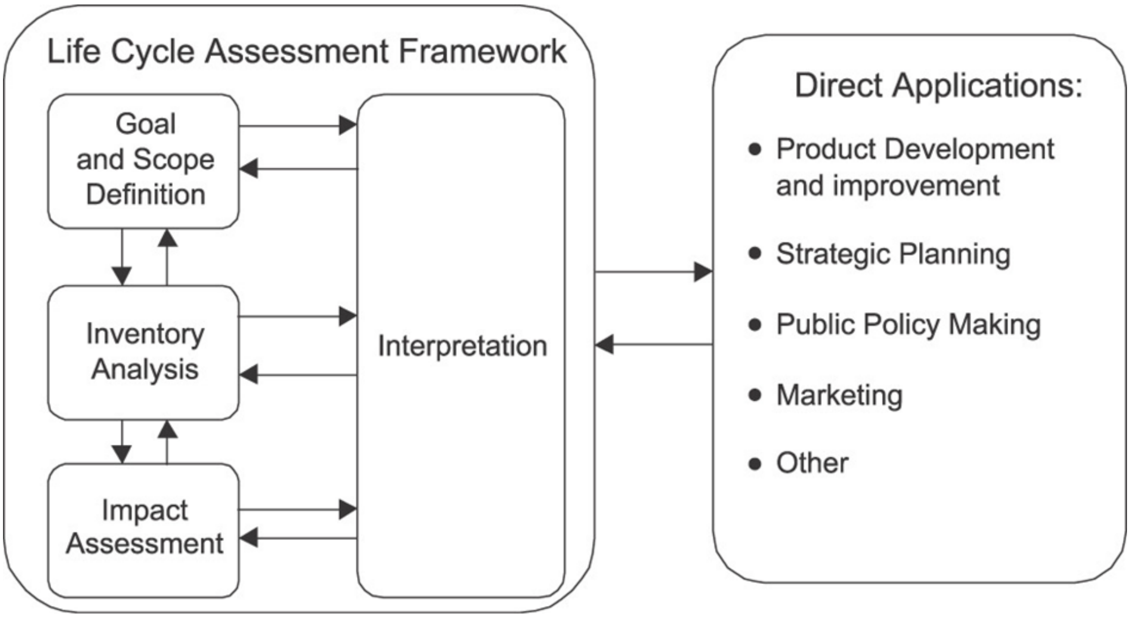

Figure 2.1: Life Cycle Assessment Framework and its direct applications [ISO, 2006]

2.2. Ex-Ante LCA

2.2.1. Introduction to Ex-Ante LCA

Currently most LCAs conducted are retrospective in which they analyse the environmental footprint of a product system once it is fully developed and operational. These retrospective ex-post LCAs are useful if a decision has to be made between two fully developed alternatives in the current market. These LCAs are however not useful in determining the best alternative in future markets and for product systems that are not yet fully developed.

For emerging technologies, these conventional LCAs only give insight on the current performance of the emerging technology. These emerging technologies are currently only working on a small lab/pilot scale and are not fully optimized yet. In order to assess the potential of an emerging technology, it would be powerful to analyse the environmental impact of the emerging technology in a fully developed market system in the future. Ex-ante LCA is a method in which this is addressed.

Ex-ante LCA uses modelling techniques to construct future scenarios in which the emerging technology is fully developed and uses these scenarios as input for the LCA. There are multiple factors of the emerging technology that can develop over time and potentially change the environmental performance of the battery. The emerging technology could for instance increase its efficiency in terms of energy or material usage. Another aspect of emerging technologies is that the current market is often not designed for the new technology. This could lead to inefficiencies in regards to the current technology. Once the emerging technology is fully developed, the complementary systems could also be more adapted towards the emerging technology resulting in better performance/a higher efficiency of the new product system. Lastly the background system could change drastically over the upcoming years. This can have a tremendous impact on the environmental performance of a product system. An example for this is the change of the current electricity markets from a fossil based market towards a renewable based marked. Electricity intensive product systems could currently have a bigger environmental impact compared to less electricity intensive products with higher emissions at point of use. This might change however if the environmental impact of the electricity mix gets lower and lower.

2.2.2. Probabilistic approach to LCA

Although it is powerful to “predict the future” using ex-ante LCA, the method comes with a lot of uncertainties. It is therefore important to critically scrutinize the modelling decisions and how they impact the outcomes of the LCA [Cucurachi et al., 2018, van der Giesen et al., 2020]. Instead of "predicting the future", ex-ante LCA can be better used to analyse under which conditions the emerging technologies can be successful. This information can be used to find potential bottlenecks, guide research and development, and advice in the decision making process.

One option to analyse emerging technologies is to change from a deterministic approach to LCA towards a probabilistic approach. Using this method, instead of using a fixed value for the LCI inputs, a range of inputs is given with a certain probability distribution. This input probability can effect a parametric input [Huijbregts et al., 2003], e.g. the energy/material consumption of a process gets lowered due to efficiency improvements , or a different technological pathway [Arvidsson et al., 2018, Cucurachi et al., 2018, Valsasina et al., 2017], e.g. the production pathway for a specific product can change.

Lots of LCAs on emerging technologies use a scenario set approach where different technological pathways with their uncertain corresponding parameter inputs are analysed by applying a deterministic approach to each scenario. In a framework given by Blanco et al. [2020], a deterministic approach towards the LCA for new emerging technologies is given. Using this framework, it is possible to analyse the effect of several technological pathways combined with parametric uncertainty. Using this method can be very powerful in determining which technological pathway has the best (environmental) performance under which conditions. In this thesis, such an approach is used to determine which maintenance option is best for the ORFB.

2.3. Environmental assessment of Energy Storage Systems

Currently there are a lot of studies highlighting several environmental benefits of ORFBs. These studies all highlight that an in depth LCA has to be conducted to analyse the actual environmental benefits of ORFBs. Currently only few LCAs on ORFBs have been conducted. Di Florio et al. [2022] assessed the environmental impact of an organic redox flow battery using anthraquinone disulfonic acid and hydrobromic acid as redox couple and compared it to a VRFB. In their analysis they showed that the ORFB scores better than the VRFB. For the ORFB, the energy efficiency at the use phase is most contributing to the environmental performance of the battery. Next to that Zhang et al. [2022] calculated the environmental impact of a flexible organic redox flow battery and compared it to a flexible Li-ion battery. They concluded that the Li-ion battery scores better than the analysed ORFB battery. The battery they analysed however, had a different set of electrolytes. Next to this, the scale and function of the battery is different compared to the ORFB by baliht.

There are several research gaps/inconsistencies revolving the methodology of environmental LCAs and energy storage. Pellow et al. [2020] highlighted that different studies on LIBs use different approaches in their LCA on several aspects like the functional unit of the LCA, the scope of the LCA, or how different use phase inputs are calculated. It is important to communicate the decisions made in the LCI and discuss how these decisions impact the total results.

Next to the different modelling aspects it is also important to mention that the function of the analysed energy storage system can have a big impact on the total results. This is usually not included in the functional unit, but can be very important when comparing multiple ESSs. Dieterle et al. [2022] recommends to include the power and energy capacity as well as important technological and temporal aspects of the battery in the functional unit. Other recommendations are to conduct a full life cycle from cradle to grave including replacement/maintenance of components, and the LCI input should be reported transparently.

using this information sub-research question 1 can be answered:

1. How can the environmental sustainability of Organic Redox Flow Batteries be conducted?

The best method to analyse the environmental performance of the ORFB is with the LCA methodology. There are multiple studies already conducted on several types of ESSs, but the amount of LCAs on ORFBs is limited. While performing the LCA it is important to look at the full life cycle and conduct a cradle to grave approach. Furthermore it is important to clearly report how the LCA is conducted. Next to this it is also important to report the function of the battery system together with the key parameters of the battery because this can have a large impact on the total results and makes comparison between ESSs a lot easier. The following key important parameters for the battery are identified: 1)battery capacity in kWh, 2)battery power in kW, 3)the round trip efficiency of the battery in %, 4)the Depth of Discharge of the battery in %, 5)lifetime of the battery in years, 6)Total cycle life of the battery or the amount of cycles per year,

2.4. Energy storage

2.4.1. Energy storage systems

As discussed in the introduction, energy storage can play an important role in the decarbonization of the energy grid. Fluctuating energy production methods like solar and wind energy can have a positive impact by reducing the number of greenhouse gasses produced upon energy generation. These energy production technologies also demand a lot in terms of flexibility of the electricity grid. In order to have a functioning power grid, the demand and supply of electricity have to be in equilibrium at all times. If there is a mismatch between load and demand the power grid will fail which could lead to tremendous amounts of economic damage. With only a small market penetration of renewable energy supply, the fluctuating energy generation of these renewables is manageable. With a high market share of renewable energy sources, electricity grid management gets more and more demanding. In such an electricity grid, short-term fluctuations, medium-term fluctuations, and network congestion are challenging aspects that could lead to the failure of the energy system. For PV panels, short-term fluctuations are caused by local cloud cover which could cause a rapid ramp up or ramp down of electricity generation. For wind energy, wind speed predictions are difficult and a sudden change in wind power can change electricity generation drastically. There is furthermore the possibility of a total stop of wind electricity production if wind speed gets too high and wind turbines are shut off due to rotary speed limitations. Medium-term power fluctuations are caused when over a longer period of time electricity generation is too low/high. Network congestion is caused when the current electricity supply is too high for the current infrastructure to handle [Moseley and Garche, 2014, Zsiborács et al., 2021].

ESSs can help in tackling these problems and stabilizing the electricity grid by storing energy at times when energy generation exceeds energy demand, and discharging this stored energy at times when demand exceeds generation. Decentralized energy storage can furthermore store electricity at the source of production, lowering network congestion. Next to these functions, an ESS is also capable of dealing with random fluctuations in both the supply as well as the demand side [Ausfelder et al., 2017]. Therefore, the implementation of ESSs can offer various advantages like less electrical energy loss, reduction of voltage fluctuations, increased reliability, power quality improvements, energy cost reductions, and increased customer satisfaction.

The way these ESSs operate can vary depending on which ESS is used. Their main functioning method is similar. Energy storage systems can operate in two different modes or stages. The first stage is the charging stage in which the ESS converts energy, usually electricity, from one form into another and stores it. The second stage is the discharging stage. In this stage the stored energy is released back into its original form [Gharehpetian and Mousavi, 2017, Guney and Tepe, 2017].

The different ESS can be categorized according to the form in which the energy is stored. An overview of different ESS and their classification can be found in figure 2.2 [Zhao et al., 2015]. All these different ESSs have their own advantages and disadvantages in relation to specific characteristics of the battery. Key characteristics for ESSs are: power density, specific energy density, capacity, efficiency, cycle life, price, availability of raw materials, and response time [Evans et al., 2012].

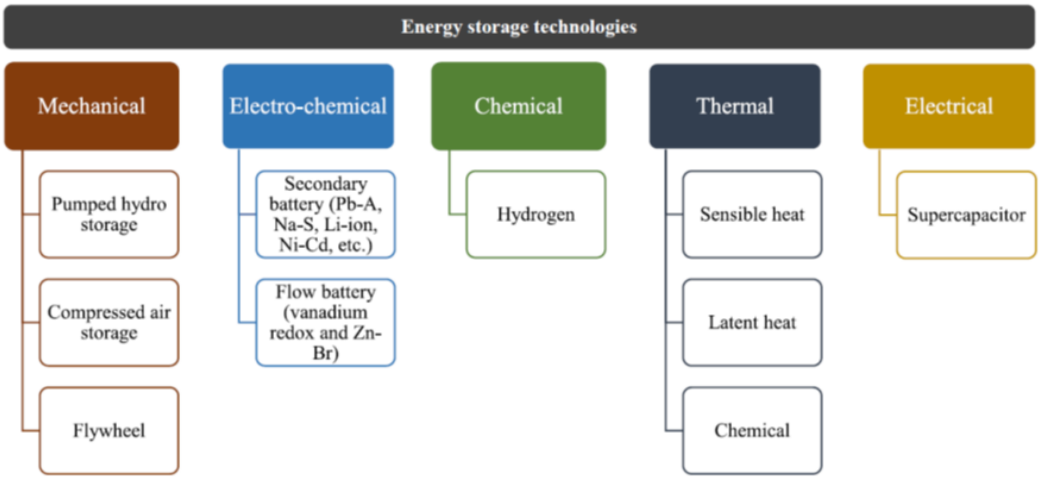

Figure 2.2: Different types of ESS, characterized by their form of energy storage [Zhao et al., 2015].

2.4.2. Redox Flow Battery

One subgroup of ESSs are so-called Redox Flow Batteries. A flow battery is a type of battery that operates slightly differently compared to the conventional LIB used in phones, laptops, electric cars, and other devices. The main difference between a flow battery compared to the LIB is that a LIB has the active/storage material incorporated into the electrode, whereas a flow battery has the storage material dissolved in an electrolyte, stored in two external tanks [Nguyen and Savinell, 2010]. In other words, the energy compartment and power compartment of redox flow batteries are separated.

A schematic overview of a redox flow battery can be found in figure 2.4. A redox flow battery consists of two electrolytes, called analyte/catholyte or posolyte/negolyte, which are stored in an external reservoir/tank. The electrolyte and their reservoirs make up the energy compartment of the battery. The power compartment consists of one or multiple battery stacks. Next to that, there are also some peripheral components (pumps, piping, energy management system, etc.) to ensure a good battery operation. This is also known as the Balance of Plant (BoP).

In a flow battery, the two electrolyte solutions are pumped into the battery stack which contains multiple battery cells. Each battery cell consists of two electrodes that are separated by an ion conductive membrane which forces the electrons (e^-) through an external circuit (see figure 2.4). When the electrolytes are pumped through the battery cell they will flow past the electrodes where the active materials in both electrolytes react and electrons are released on one side of the battery (the anode) and consumed at the other side of the battery (the cathode). These reactions are also known as half-reactions and together form a redox reaction, hence the name Redox Flow Battery. The generated electrons can be moved through an external circuit where the energy of these electrons can be used as electricity during discharge. At the same time, ions (usually H^+ or OH^-) diffuse through the membrane to maintain charge equilibrium.

In a redox flow battery, multiple of these individual cells are stacked together in series via bipolar plates to form the battery stack. This is done to increase the overall voltage of the battery which also increases the efficiency and functionality. Next to the membranes, electrodes, and bipolar plates, there is also a current collector, an isolation plate, an end plate, and a stack frame in every battery stack.

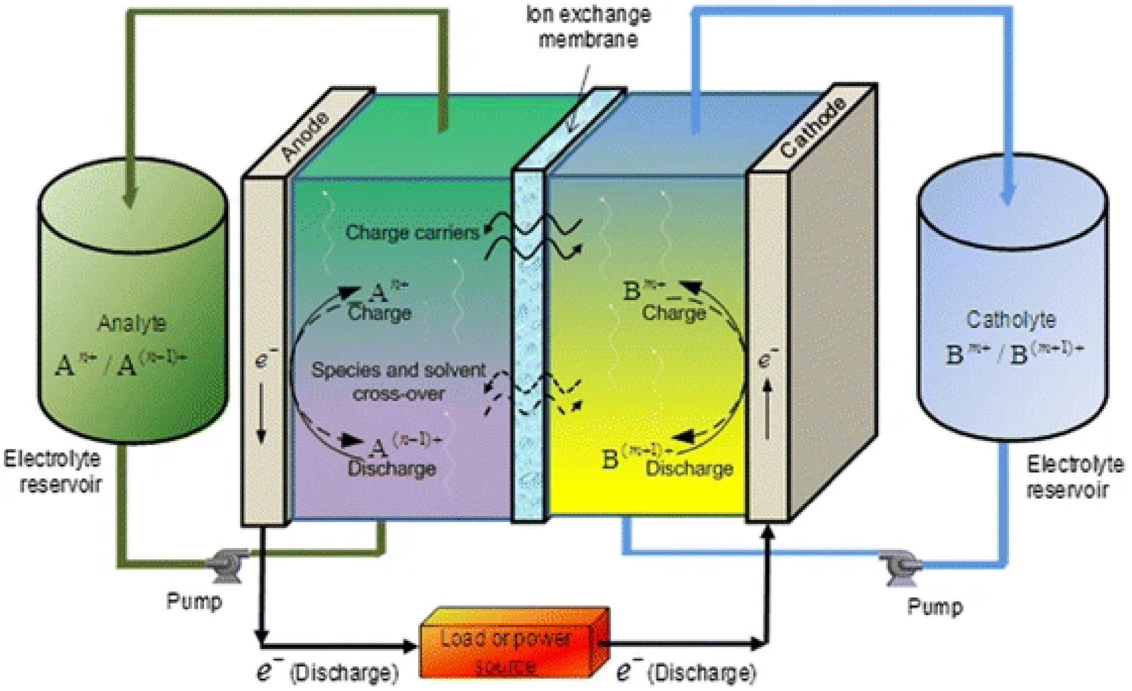

Figure 2.3: Schematic overview of a flow battery [Weber et al., 2011].

Due to the specific design of flow batteries, in which the storage material is not stored internally but externally in an electrolyte in an external tank, flow batteries have some advantages in terms of modularity. The first major advantage of this set-up is that it is easier to scale up the total energy or total power capacity of the battery. In order to increase its energy capacity, a larger volume of electrolyte can be used. This can theoretically be done up to very large quantities, making the battery suitable for large-scale energy storage. If a higher power supply is needed, the stack size can be increased [Nguyen and Savinell, 2010, Skyllas-Kazacos and Grossmith, 1987, Weber et al., 2011, Zhou et al., 2006]. For conventional batteries like the LIB, a completely new battery stack would be needed if a bigger power or capacity is needed. Because of its modular design, it is also relatively easy to replace/repair specific parts of the battery if maintenance is required. A long life cycle, quick response time, and increased safety are other advantages of this type of battery [Duduta et al., 2011, Wang et al., 2013].

Currently, the most mature and installed types of flow batteries are the VRFB and the Zinc-Bromide battery. Although the VRFB and Zinc-Bromide batteries are currently well-established types of batteries, they have some major drawbacks. The most important ones come from their expensive and resource-limited active materials which are dissolved in hazardous and corrosive electrolyte solutions. These batteries furthermore suffer from low current performances [Darling et al., 2014, Soloveichik, 2015]. To tackle these issues, the development of a new type of redox flow battery using abundant and sustainable materials is in progress: The Organic Redox Flow Battery (ORFB) [Hu et al., 2017, Parasuraman et al., 2013, Rychcik and Skyllas-Kazacos, 1988, Winsberg et al., 2017].

2.5. The BALIHT ORFB

2.5.1. Key characteristic and function of ORFBs

The Baliht battery is a new Organic Redox Flow Battery that aims to be economically feasible, has safe operating conditions, and aims to have as little environmental impact as possible. The battery uses aqueous electrolytes which can potentially be produced from lignin, a waste product from the paper and wood industry. Next to active

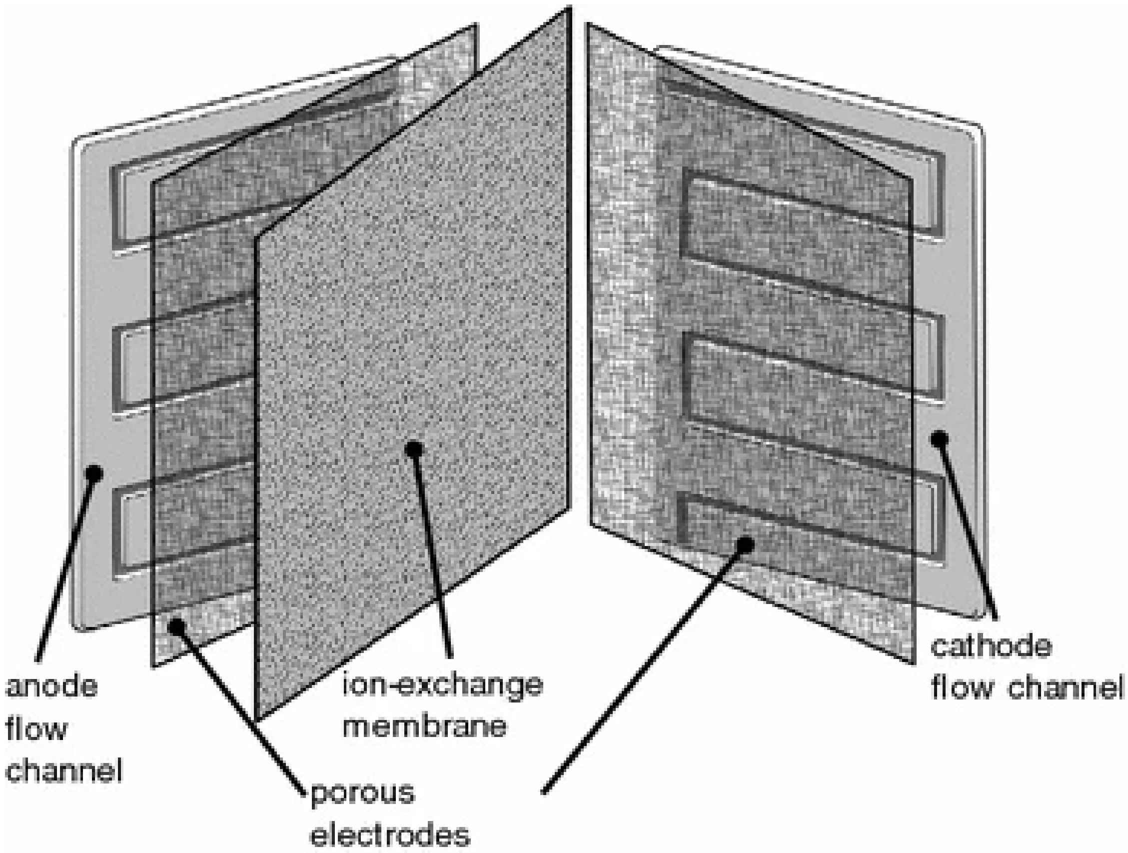

Figure 2.4: Schematic overview of a redox flow battery cell [Weber et al., 2011].

material being made out of renewable materials, these electrolytes, and the battery as a whole aim to operate at high temperatures (80 °C). Usually flow batteries have significant heat production and cooling is needed to decrease electrolyte degradation. Being capable of operating at this high temperature can decrease the energy losses needed for cooling and increases the efficiency of the whole system.

The ORFB has some specific key characteristics that allows for a specific function of the battery. The ORFB and flow batteries in general have a low energy and power density compared to other types of energy storage systems. High energy and power densities are important in applications where weight of the battery is an important aspect. An example of this is the mobility sector and ORFBs are therefore not suitable for electric vehicles. Due to their potentially high total capacity, and long cycle life and quick response time, ORFBs are great candidates for stationary energy storage applications to support the electricity grid. Some examples of possible applications for the ORFB are in sustainable energy production facilities, in power charging stations, to supply large industrial sites, and in micro-grids [Sánchez-Díez et al., 2021]. Similar type of batteries that can also have this function are LIBs and VRFB [Hesse et al., 2017].

2.5.2. Configuration of the ORFB

The energy subsystem of the Baliht battery consists of two aqueous electrolytes and the storage tanks in which the electrolytes are stored. The active materials in the Baliht ORFB are *7,8-dihydroxyphenazine-2-sulfonic acid (DHPS)* and *potassium ferrocyanide*. From these two electrolytes, the DHPS is the organic molecule that can be produced from lignin. During charge and discharge, the nitrogen groups of the DHPS can react with a hydrogen ion (see 2.5). Due to the availability of two nitrogen groups, the DHPS can react with two hydrogen ions which significantly increases the energy density of the molecule. The benefit of using potassium ferrocyanide is that it is a stable complex that uses iron, a widely abundant material on earth. During charge and discharge the active materials have the half-reactions depicted in figure 2.5.

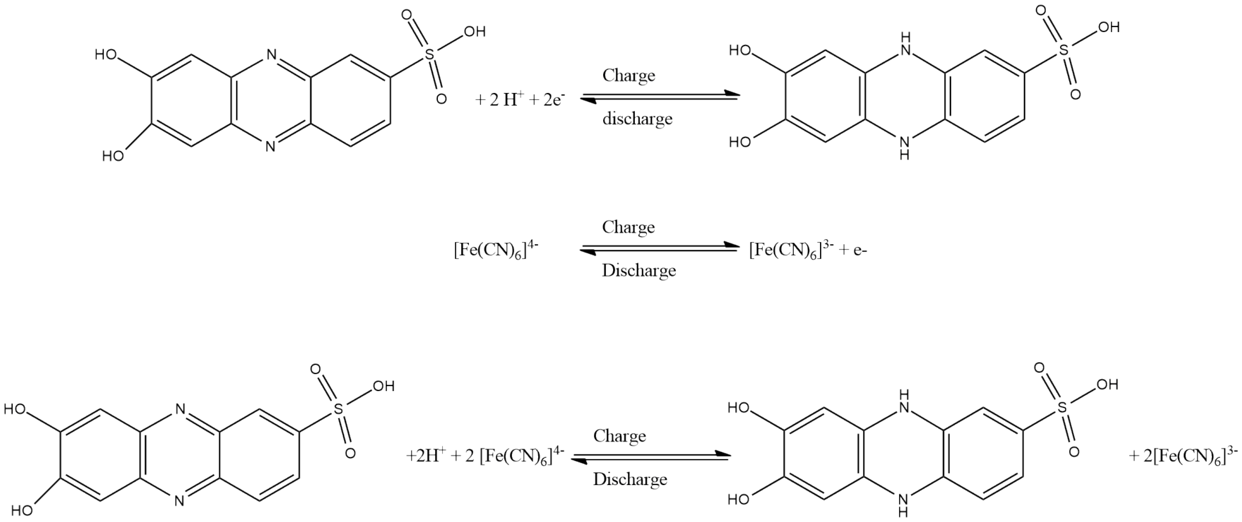

Figure 2.5: Half reactions and full reactions of the DHPS-Ironcyanide redox pair [Romadina et al., 2021].

2.5.3. Battery degradation

In a battery, degradation can occur to all components. Battery degradation lowers the overall performance and should be minimized. Battery degradation can have an effect on the electric efficiency of the battery, can lower the capacity of the battery and can even lead to critical failure of the battery. In a LIB such failure can be incredibly dangerous and could have catastrophic consequences due its flammable components. This is, luckily, not a problem for an ORFB, but should nonetheless be prevented. In figure 2.6 an overview of all types of degradation that can occur can be found. In the next few paragraphs a short description of the most important degradation mechanisms for the Baliht battery is given. After that, an overview for maintenance options for the electrolytes are given.

For each component, there are different mechanisms resulting in battery degradation. In ORFBs the main components that cause battery degradation are its electrodes/bipolar plates, the membranes and the active materials in the electrolytes. For the electrodes and membranes, the degradation mechanisms are mechanical degradation and (electro)chemical degradation [Briot et al., 2022, Collier et al., 2006, Derr, 2017].

For the electrolytes in ORFBs, degradation occurs mainly due to side reactions and active material decomposition. These degradation mechanism are dependent on which active materials are used as well as the conditions of the electrolyte solution (acidic or alkaline). The most prominent side reactions occurring in ORFBs are the Oxygen Evolution Reaction (OER) and the Hydrogen Evolution Reaction (HER). These side reactions are a result of the electrochemical splitting of water in the electrolyte while charging the battery. The effect of these side reactions is depicted in figure 2.7. During charge of the battery, the active material in one of the electrolytes gets fully converted while the active material in the other electrolyte only gets partially converted because some electrons are consumed during because of the OER/HER reaction. During discharge, the available charge in the not fully converted electrolyte is lower, resulting in some capacity loss [Páez et al., 2021].

Active material decomposition leads to a direct loss of active material due to decomposition reactions of the active material which results in capacity loss. For the posolyte, the ferrocyanide has been proven to be very stable in alkaline solutions [Páez et al., 2020]. Since the battery operates in an alkaline environment, available hydroxide ions can however still substitute cyanide ions leading to inactive iron hydroxides or iron pentacyanides [Luo et al., 2017]. An overview of the degradation reactions of the DHPS in the negolyte can be found in figure 2.8 and occur to the charged state of the DHPS. These compounds show a lower solubility and lowered/no electrochemical activity and thus lower the capacity of the battery [Wellala et al., 2021].

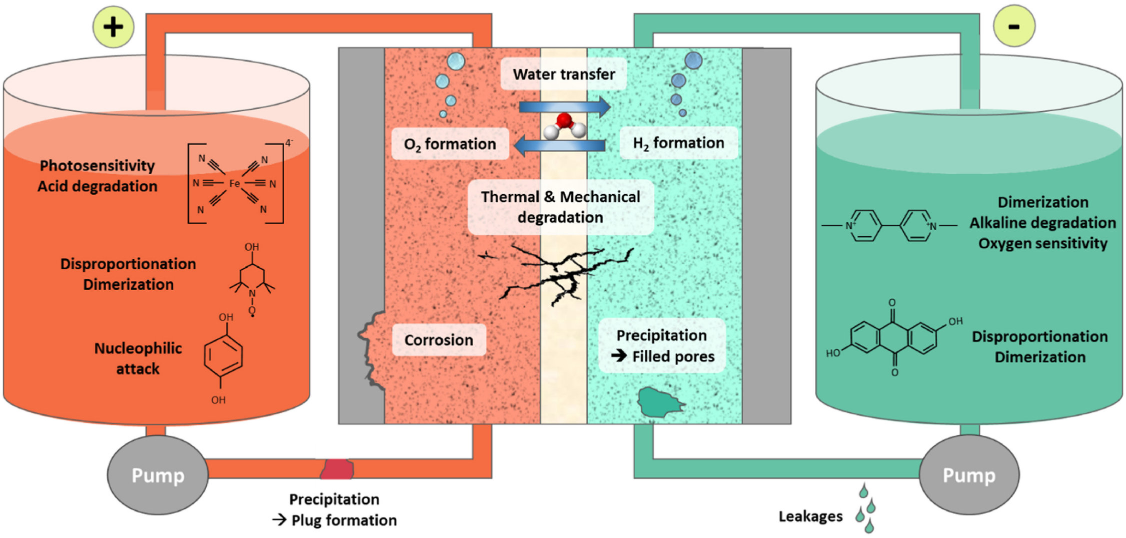

Figure 2.6: Most important degradation mechanisms in ORFBs (not specific to Baliht battery) [Briot et al., 2022].

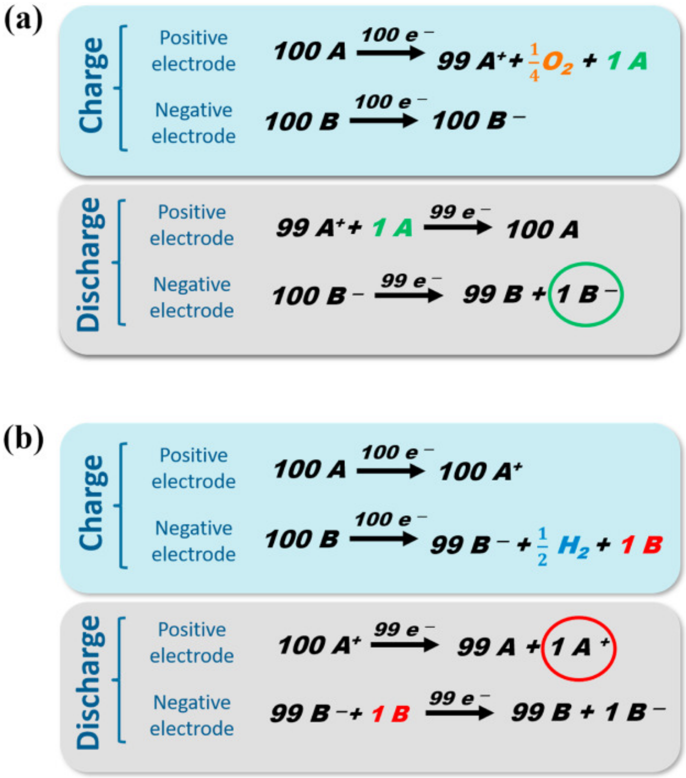

Figure 2.7: Schematic overview of the effect of the OER and HER on battery capacity [Páez et al., 2021]

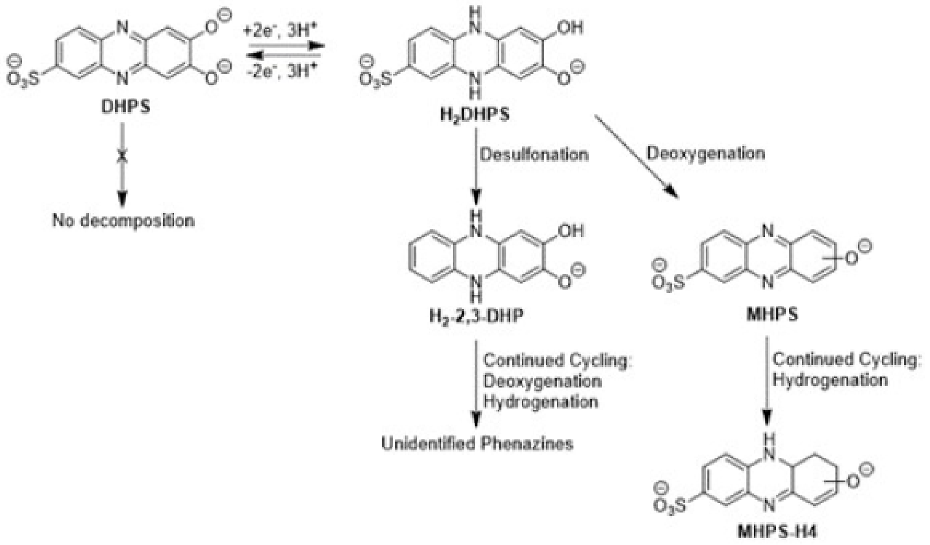

Figure 2.8: Decomposition pathways DHPS [Wellala et al., 2021]

2.5.4. Maintenance operations of the electrolytes

Because of the modular design of flow batteries, its easy to target a specific component for maintenance. Therefore, component specific maintenance procedures can be planned to counteract the loss of battery performance. In this research only the effect of electrolyte maintenance on battery capacity is researched and presented. There are a multitude of possibilities to repair other parts of the battery, but this would go beyond the scope of this master thesis.

As mentioned above, the main degradation mechanism in the electrolytes leading to capacity fade are side reactions (OER/HER) and electro-active material decomposition. The main problem occurring due to side reactions is an unbalance in the available charge available in both electrolytes. Luckily, this can be counteracted by a procedure introduced by Páez et al. [2021]. In this procedure they describe how an electrochemical re-balancing cycle can counteract the unbalance and restore the capacity. This procedure is considered to be easily applicable and cheap and can greatly enhance the cycle life of the battery.

Counteracting electro-active material decomposition is slightly more difficult and dependent on which material is used in the battery. The best method is to prevent the decomposition in the first place by applying conditions these reactions don't occur; e.g. For the negolyte, the decomposition reactions only occur from the charged state, and thus it can be chosen to not leave the battery in its charged state for an elevated period of time. Decomposition is, however, not unpreventable and will happen either way. To counteract this, three different maintenance procedures have been identified similar to Rodby et al. [2021]. The first and most straightforward option is to fully replace the electrolyte solutions with fresh new electrolyte solutions. The benefit of this method is that it's easy to execute and has a large capacity gain. The second option is to separate the inert active materials in the electrolytes and replace them with fresh active material. This method uses less materials compared to the first option. A potential drawback of this method is that it could potentially be difficult to fully separate the inert material from the electrolytes leaving some still in the electrolyte solution. This could potentially lower the solubility of the active material and thus lowering the capacity gain. The third option is to separate the inert material from the electrolyte solutions and chemically reactivate them. This can lower the resource consumption even more, but it might be difficult to fully convert the active material to its starting material. This could also lower the capacity gain.

2.5.5. Summary on Energy storage and the ORFB

The second sub-research question can now be answered:

How does the ORFB function and what are other relevant energy storage technologies?

An ORFB is a flow battery which consists of the following sub-units: 1) An energy sub-unit, 2) a power sub-unit, and 3) BOP/peripheral components. The energy sub-unit consists of two electrolytes which are stored in storage tanks. The power sub-unit consists of one or multiple battery stack(s). The main components in the battery stack of the ORFB are 1) the bipolar plates with electrode layer, 2)membranes, 3)current collector, 4) isolation plate and 5) end plate. The peripheral components are there to regulate the battery operation and consists of a battery management system, piping, pumps and electronics.

An important aspect of the ORFB is the separation of energy unit and power unit. This allows for scaling the two sub-units towards its function and for maintenance operations. Because the ORFB can be scaled to fit towards a specific function, the battery can be used in a variety of ways, but due to specific parameters of the battery it is best used for large stationary energy storage functions. Examples of where the battery can be used are next to sustainable energy production facilities, in power charging stations, to supply large industrial sites, and in micro-grids. Similar types of batteries that can also fullfil this function are LIBs and VRFB.

3

Methodology

In this chapter the LCA of the ORFB is given. In this thesis, the LCA has two different stages. At first an LCA of the battery is conducted without any maintenance operations and compared to LCA of a LIB and a VRFB. This is done to answer sub-research question 3 and 4. After this, the LCA is further developed and connected with a use phase model to assess the effect of electrolyte maintenance of the battery.

3.1. LCA Goal and scope definition

3.1.1. LCA Goal definition

The goal of this LCA is to assess the environmental sustainability of the Organic Redox Flow Battery developed by the Baliht research group. In this LCA the environmental burdens of the ORFB will be analyzed and a contribution analysis will be conducted in order to find hotspots in the life cycle of the ORFB. It is furthermore analysed how certain battery parameters impact the total results of the battery. Using this information, advice on the development of the ORFB can be given to improve its environmental performance. In order to better understand the environmental performance of the ORFB, the results are compared with a LIB and a VRFB. It was chosen to compare it with these two types of batteries because they have a high market share, and have similar functions to the ORFB (see previous chapter). Next to this, the effect of different maintenance operations are analysed to assess what maintenance operations are best. By conducting the LCA, sub-research question 3, 4, 5 and 6 will be answered.

3.1.2. Scope definition

In this LCA, the environmental impact over the entire life cycle of the battery is analysed and thus a cradle to grave approach is taken. The ORFB is currently in development and a pilot plant is constructed in Ibiza. The battery itself is produced at the facilities of CMBLU located in Germany. Therefore it is chosen to have regional LCI input data from Spain, Germany and Europe. The battery is expected to have a lifetime of roughly 20 years with 300 charge-discharge cycles a year. This results in a total of 6000 charge-discharge cycles. Wherever possible, most recent data from the year 2022 is chosen.

3.1.3. Data acquisition and LCA software

Data has been acquired through communication with the research projects wherever possible. For some processes, data was not available and other literature has been used for the LCI data. The LCI input data for the LIB and the VRFB are taken from da Silva Lima et al. [2021]. For the LCA, the Activity Browser has been used as software. This is an open source GUI that builds upon the brightway2 LCA framework [Steubing et al., 2020]. As a background database, EcoInvent version 3.8 has been used.

3.1.4. Functional unit

The function of the battery is to store electricity and return this electricity back to the grid. The function of the battery is furthermore extended with the different recommendations from Dieterle et al. [2022]. This leads to the following functional unit for the ORFB:

1 kWh of the total energy provided delivered back to the grid by the ORFB which has a total energy capacity of 200 kWh, a power capacity of 100 kW, a round trip efficiency of 65%, a Depth of Discharge of 80 %, and a total of 6000 cycles in 20 years of operation.

This procedure is also conducted for the LIB and the VRFB. The power capacity of the batteries are unknown. This lead to the following functional units:

1 kWh of the total energy provided delivered back to the grid by the LIB which has a total energy capacity of 1300 kWh, a round trip efficiency of 90%, a Depth of Discharge of 85 %, and a total of 3000 cycles in 10 years of operation.

1 kWh of the total energy provided delivered back to the grid by the Vanadium Redox Flow Battery which has a total energy capacity of 37.5 kWh, a round trip efficiency of 83%, a Depth of Discharge of 100 %, and a total of 6000 cycles in 20 years of operation.

3.2. Life Cycle Inventory

In this section it is described how the inputs for the LCI are obtained and modelled. The LCA model of the ORFB can be subdivided into three different phases; 1) Production phase of the ORFB battery, 2) Use phase of the battery, and 3) Decommissioning/End-of-Life phase of the battery. A global flowchart of these three stages can be found in figure 3.1. An exact overview of the LCI data for the ORFB can be found in the appendix. The LCI data for the LIB and the VRFB can be found in the paper from da Silva Lima et al. [2021].

3.2.1. Production phase: Electrolytes

As described in the introduction, the ORFB from baliht stores the energy in water based electrolyte solutions with an iron complex in the posolyte and DHPS in the negolyte as storage materials. The storage materials cannot be directly connected to the external database EcoInvent and therefore several chemical processes have to be modelled in the foreground system. In order to calculate the LCI inputs of these processes the framework from Piccinno et al. [2016] is used. In this paper, they describe how to obtain inputs for the production of chemicals with no current process data or only lab scale data available. Using this framework a laboratory scale reaction procedure can be converted into a larger scale chemical process. In this thesis, patents that describe the lab scale production of chemicals for the electrolytes have been used where possible. First a small overview of the framework is given. After that it is described how this is implemented to obtain the LCI data for the posolyte and negolyte solutions.

In the framework, the chemical production process is subdivided into two steps: 1)The reaction step, and 2)Processing, purification, and isolation steps. For each step in the chemical production process, the (main) material and energy inputs/outputs are calculated. A schematic overview of this can be found in figure 3.2.

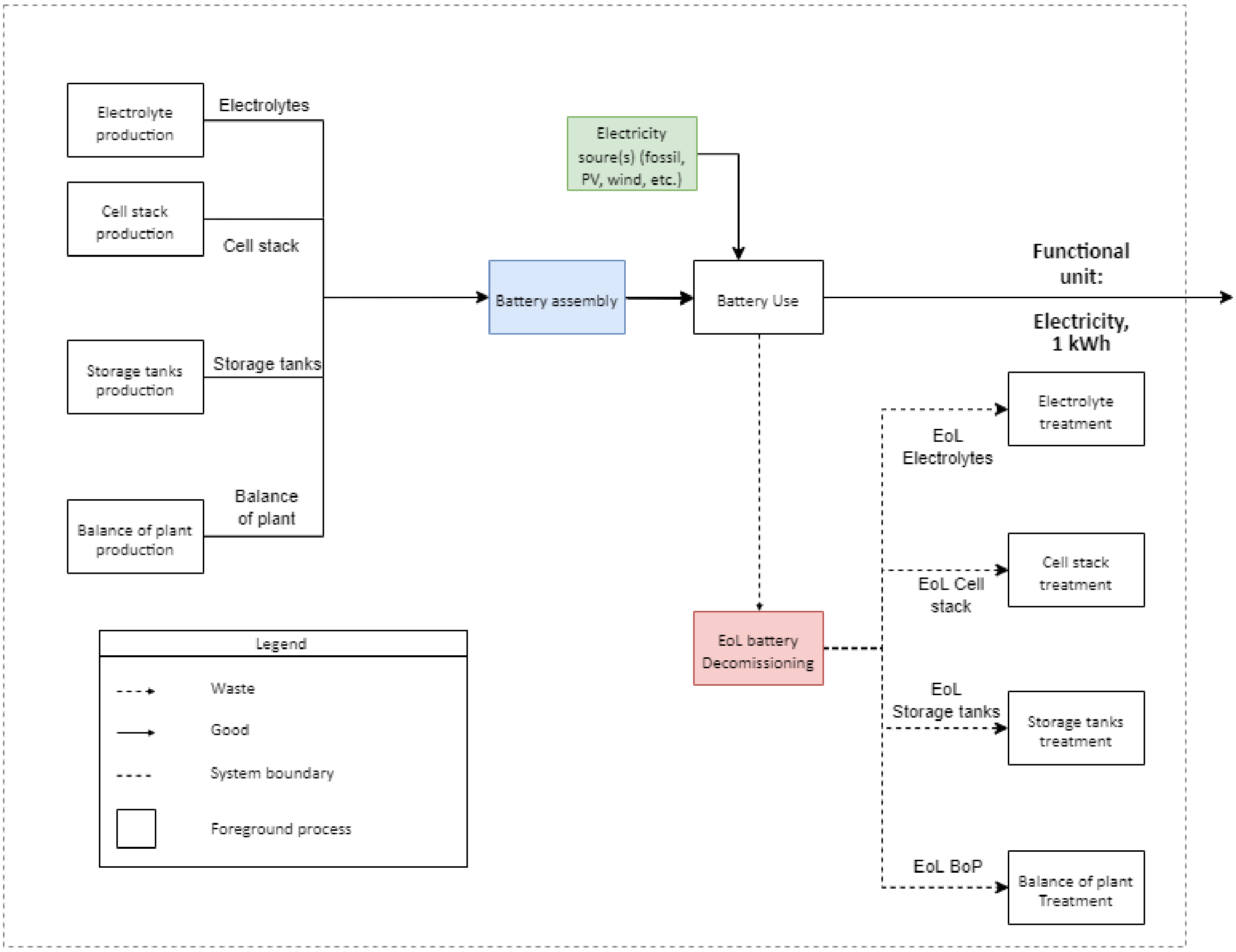

Figure 3.1: Global overview for the production of the battery (BoP = Balance of Plant, EoL = End of Life).

1) Reaction step:

The inputs for the reactants and solvents used for each process are derived from the laboratory scale reaction procedure. The first step to calculate these is to find the scaling factor for the solvent. In this LCA, a 100 L batch stirred tank reactor is used for the large scale chemical production process. The scaling factor for the solvent can then be derived by dividing 100 L by the volume of the solvent in the laboratory scale procedure. The amount of reactants can be calculated next by multiplying the laboratory scale reactant inputs with the scaling factor. In the scaling up of the process, it is assumed that 20% less solvent is used. In this LCA, there is not enough information available to calculate the inputs for catalysts for the different processes. It is assumed that catalyst for the different reactions can be reused, and the material inputs for these catalysts is therefore negligible small

Next to material inputs, energy inputs are another important aspect in the reaction process. In order to calculate these, a complete reactor design would be needed. This information is not available and getting this information would go beyond the scope of this study. In order to still get valuable inputs for the energy consumption a few assumptions are made. For the reaction step there are three main energy contributors. These are (1) heating up the reaction mixture to the reaction temperature Q_{heat}, (2) keeping the reaction mixture at the reaction temperature for the reaction duration Q_{loss}, and (3) stirring the reaction mixture E_{stirr}. For all these inputs there are equations which can be found below. For these energy inputs, (1) and (2) are considered heating inputs, where (3) is considered an electricity input. The total energy requirements for the reaction can be calculated through adding Q_{heat} and Q_{loss} and dividing it with an efficiency factor η_{heat} (see eq. 3.1).

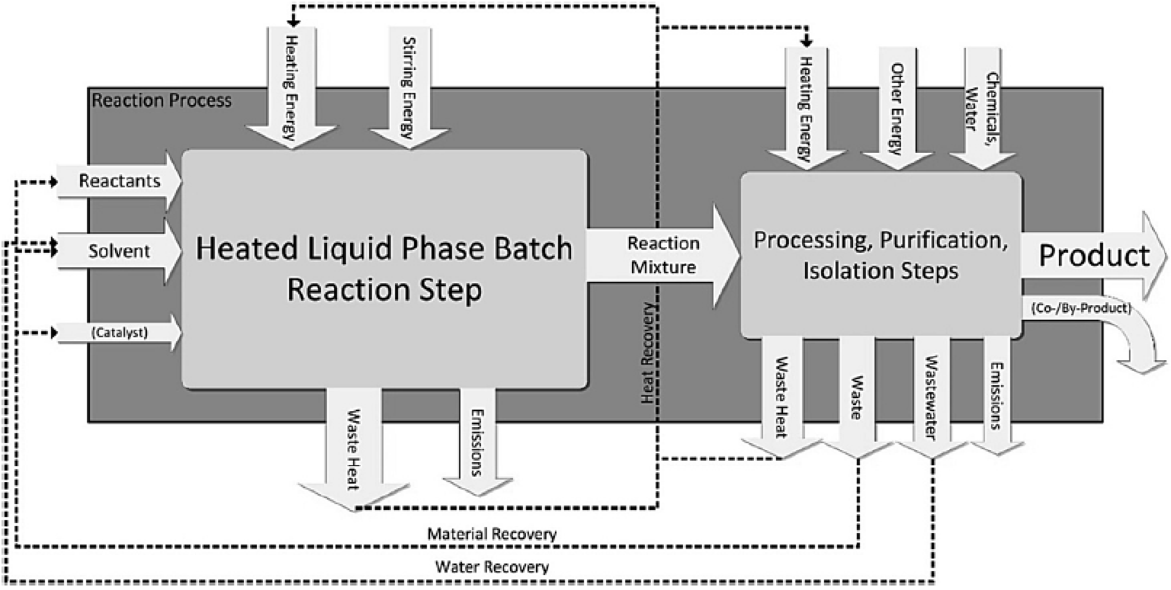

Figure 3.2: Schematic overview of the framework from piccinno et al. Piccinno et al. [2016]

.

$$Q_{reaction} = \frac{Q_{heat} + Q_{loss}}{\eta_{heat}} \tag{3.1}$$

Q_{heat} can be calculated through multiplying the specific heat capacity of the solvent (C_p) with the total mass of the reaction mixture and the total temperature difference ($T_r - T_{out}$). The equation can be found in eq. 3.2. The amount of energy needed to keep the reaction mixture at a specific temperature is equal to the amount of energy that is "escaping" the reaction vessel. The amount of energy escaping the reaction vessel is dependent on the total surface area of the reaction vessel (A), the insulation material (k_a), the thickness of insulation (s), the difference in temperature between the reaction vessel (T_r) and the outside temperature (T_{out}), and the reaction time (t). Combining these factors results into eq. 3.3. In the paper standardized values have been given for the different parameters in the equation. These values are used for the calculations in this LCA.

$$Q_{heat} = C_p \cdot m \cdot (T_r - T_{out}) \tag{3.2}$$

$$Q_{loss} = A \cdot \frac{k_a}{s} \cdot (T_r - T_{out}) \cdot t \tag{3.3}$$

The electricity needed to stir the reaction can be calculated through equation 3.4. The stirring energy is dependent on the power number (N_p), an impeller dependent number, the diameter (d) and the rotational stirring velocity (N) of the of the impeller. Next to these impeller dependent variables it is also dependent on the density of the mixture ρ_{mix}, reaction time t and the efficiency of stirring η_{stir}. The impeller dependent variables are taken from average values found in industry. See Piccinno et al. [2016] for more details about these.

$$E_{stir} = \frac{N_p \cdot \rho_{mix} \cdot N^3 \cdot d^5 \cdot t}{\eta_{stir}} \tag{3.4}$$

2)Processing, purification, isolation steps:

In the framework Piccinno et al. [2016] there are multiple processing, purification and isolation processes given. For this LCA only the procedures for filtration and drying are needed. It is assumed that these processes only need energy inputs and no extra material inputs. A description of these processes is given below. The electricity required to filtrate a certain amount of material is between 1-10 kWh per ton of dry material. To account for a worst case scenario, 10 kWh per ton of dry material is taken. The heating energy needed to dry a certain product can be calculated through equation 3.6. This is dependent on the energy needed to heat the solvent to its boiling point (equal as heating reaction mixture in eq. 3.2) and the enthalpy of evaporation ΔH^0_{vap}.

$$E_{filtr} = m_{dry} \cdot 10\ \mathrm{kWh/kg} \tag{3.5}$$

$$E_{stir} = C_p \cdot m \cdot (T_r - T_{out}) + \Delta H^0_{vap} \cdot m \tag{3.6}$$

The last important energy input for the LCI is the electricity required to pump the liquids through the whole system. It is assumed that this is equal to 55 joule per kg of pumped material. This value is derived from equation 3.7 using an average height difference of 4.2 meter and a pumping efficiency of 75%.

$$E_{stir} = \frac{m \cdot g \cdot \Delta h}{\eta_{pump}} = m \cdot 55\ \mathrm{J/kg} \tag{3.7}$$

LCI inputs for the negolyte:

The negolyte is an aqueous solution with 7,8-dihydroxyphenazine-5-sulfide (DHPS) as the active redox material in which the energy is stored. Next to the DHPS, there are some other compounds in the negolyte to stabilize the solution and improve the activity of the total negolyte solution. An overview of the LCI inputs for the final negolyte solution can be found in the appendix table A.8.

In the final negolyte solutions, all the components can be connected to the EcoInvent database except for the DHPS. The DHPS LCI inputs are therefore calculated using the method described above. In principle it is possible to produce the DHPS from waste lignin from the paper industry. This production step is however still in development and it is impossible to find reaction parameters. Therefore it is decided to model this from fossil based resources. The reaction steps are taken from several patents Rauchschwalbe et al. [2004], Saito et al. [1990], Wei et al. [2019]. The DHPS is synthesised through a multi step synthesis from hydroquinone and ortho phenylenediamine. The hydroquinone is first converted into 2,5-dihydroxybenzoquinone. In a parallel synthesis step, the ortho phenylenediamine is sulfonated to 2,4-diaminobenzenesulfonic acid. Finally, the 2,5-dihydroxybenzoquinone reacts with 2,4-diaminobenzenesulfonic acid to produce the DHPS. An overview of the reaction synthesis can be found in figure 3.3.

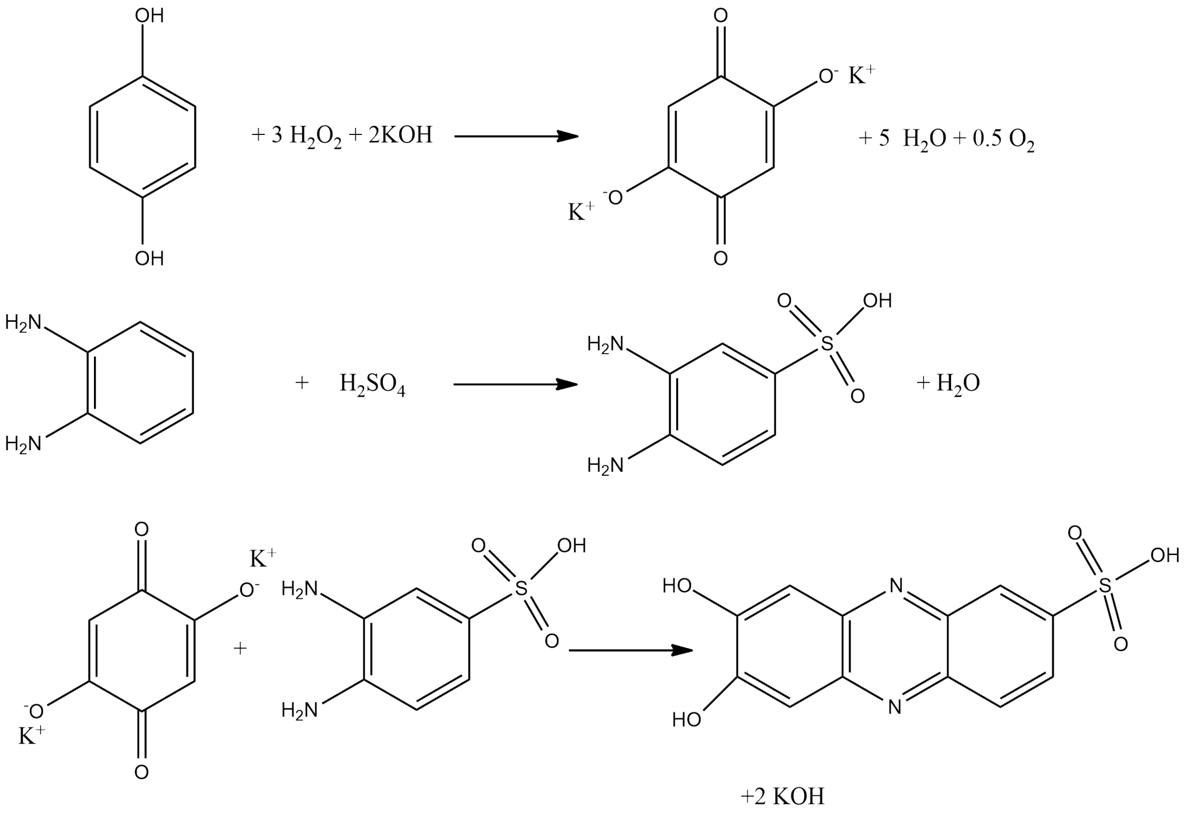

Figure 3.3: Reaction steps for the production of DHPS

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LCI inputs for the posolyte:

The posolyte is, similar as the negolyte, an aqueous solution with storage material and multiple other additives solved in it. A composition of the final posolyte solution can be found in table A.4. The storage component in the negolyte is the iron complex potassium ferrocyanide (K4[Fe(CN)6]). The production process for the potassium ferrocyanide is taken from Ullman's encyclopedia of industrial chemistry [Gail et al. [2000]]. A schematic overview of the production of the potassium ferrocyanide can be found in the flowchart. Unfortunately there is only a patent with reaction procedures available for the first steps of the ferrocyanide production chain; the production of the calciumferrocyanide complex. There is unfortunately little information available on the conversion of the calciumferrocyanide towards the potassiumferrocyanide. LCI inputs of these steps are based upon stochiometry and assumptions based upon the LCI inputs of the production of the calciumferrocyanide.

3.2.2. Production phase: Cell stack

The next part of the LCI of the battery production consists of the construction of the cell stacks. The cell stack consists of multiple individual cells who are stacked upon each other with at the end of each stack a current collector, an isolation plate and an end plate. Each of the individual cells consist of two bipolar plates with an electrode layer. Between each bipolar plate there is a membrane separating the two. The membrane is made out of sulfonated poly(ether-ether-ketone) (sPEEK). Each cell has a cell frame surrounding the different cells to protect the cell stack and give it mechanical strength. The different components and the amount of each component in the battery stack can be found in table 3.1. A detailed overview of the LCI inputs of each component can be found in the appendix.

In the next step the material inputs to produce one of each component are calculated. The material requirements

Table 3.1: Stack components and their dimensions. *Bipolar plate consists of bipolar plate with electrode layer. For a full overview of components in the bipolar plate see appendix table: A.12 to A.17

Cell Component	Amount per stack	Material	Mass [kg]
Bipolar plate	55	Graphite based*	0,5
Membrane	54	sPEEK Fumatech	0,01
Current collector	2	Copper	2,7
Isolation plate	2	PETG	0,4
End plate	2	Wood	7,5

for each components have been given by the stack producer. For the bipolar plate and the membranes, the LCI inputs to produce 1 kg of the component have to be calculated first. The inputs for the bipolar plate are derived from communication with project partners from the Baliht project. For the sPEEK membrane the inputs are taken from literature Di Florio et al. [2022], Weber et al. [2018]. An overview of the LCI inputs to produce 1 kg of the electrode and membrane material can be found in the appendix (see table A.12 and A.19) The current collectors, end plates and isolation plates all consist of one material. These components could directly be connected with the EcoInvent database.

Once the individual components are produced, they need to be attached to each-other in order to produce the cell stack. In a first step, the bipolar plates and membranes are attached to a frame. This gives the component some mechanical strength and shields it from external factors that could potentially harm the component. In the second step, the components attached to the cell frame can be attached to each other forming the cell stack. In this process there is a small loss of components of 3%. In order to produce one cell stack there is therefore 3% more components needed than the amounts given in 3.1. The lost components will directly go to the different End of Life options which will be discussed in section 3.3.

3.2.3. Production phase: Storage tanks

The electrolytes are stored externally in storage tanks. The total volume of the storage tanks equals 110% of the volume for each electrolyte and has the shape of a cube. The ORFB has a total of 12 storage tanks for each electrolyte. The material input is calculated via the density and the volume of the storage tanks. The specifications for the storage tanks can be found in table 3.2.

Table 3.2: Specifications for the Storage tanks

	Posolyte tank	Negolyte tank
Volume 1 Tank [L]	130	200
Material	Polyester mesh with alcryn	Polyester mesh with alcryn
Thickness [mm]	1	1
mass tank [kg]	1,06	1,41
Total number of tanks	12	12

3.2.4. Production phase: Balance of plants (BOP)

Next to the electrolytes, battery stacks and the storage tanks there is a balance of plant consisting of several peripheral components to support a good and safe operation of the battery. The peripheral components in the BoP of the ORFB are an energy management system, a battery management system, pipes, pumps, an inverter and multiple electronics. An overview of the components for each peripheral system can be found in the appendix.

3.2.5. Battery Assembly

Once all the individual components are produced they need to be transported and installed at the battery site. An overview of the different LCI inputs for the battery assembly can be found in table 3.3.

Table 3.3: Components needed to produce one battery

Input	Amount	Unit
Anolyte solution	862,5	kg
Posolyte solution	1725	kg
Battery segments	12	#
Posolyte tank	12	#
Negolyte tank	12	#
Balance of plant	1	#

3.2.6. Use phase of the ORFB

The use phase process is the central process in the LCA model and it produces the functional unit of the LCA model. In this process electricity and an ORFB battery are the inputs and the functional unit (1 kWh of electricity returned to the grid) and an EoL battery (waste) are outputs of the model. To calculate the amount of battery needed to return 1 kWh of electricity to the grid, it is necessary to first calculate the total amount of electricity returned back to the grid over the entire life cycle of the battery (E_{tot}). This can be calculated by summing up the energy delivered back to the grid of each individual cycle (see eq.3.8). This is dependent on the capacity of each cycle (C_i), the depth of discharge of each cycle (DOD) and the total number of cycles of the battery (n_{tot}). This equation can however be simplified by assuming linear degradation of the capacity of each battery and a fixed number for the depth of discharge. By assuming linear degradation of the battery, an average number for the capacity can be taken. It is assumed that the battery start at 100% capacity and reaches its end of life at 80% of its max capacity. The average capacity in each cycle is therefore 90% of the maximum capacity. Using this, eq. 3.8 can be simplified to eq. 3.9.

$$E_{tot} = \sum_{n_i=1}^{n_{tot}} C_i \cdot DoD_i \tag{3.8}$$

$$E_{tot} = n_{tot} \cdot 0.9 \cdot C_{max} \cdot DoD_{avg} \tag{3.9}$$

The total amount of electricity returned to the grid can be calculated using the battery specification given in 3.4. Once this number is calculated, the amount of battery needed to deliver 1 kWh of electricity can be calculated by taking the inverse of E_{total}.

Table 3.4: Battery specifications for the ORFB battery.

Parameter	amount	unit
Capacity	200	kWh
Depth of Discharge	80	%
Number of cycles	6000	cycles
E_total	864000	kWh
Round trip efficiency	65	%

Due to inefficiency of the battery, extra electricity is needed to deliver the electricity back to the grid. The ORFB battery has a total efficiency (η_{tot} of 65% due to losses of the charge-discharge reactions and extra electricity needed due to pumping of the electrolytes, losses at the inverter etc. The total amount of electricity needed to deliver 1 kwh of electricity to the grid can be calculated by eq. (3.10. In the LCA model, only the extra electricity needed due to inefficiencies is accounted to get a better insight in the impacts of the ORFB. The inputs for the use phase process can be found in table A.31.

$$E_{bat-loss} = \frac{1\,\mathrm{kWh}}{\eta_{tot}} - 1\,\mathrm{kWh} \tag{3.10}$$

There are many options for the source of electricity for the battery. For this LCA it is chosen to have electricity from photovoltaic panels as electricity source. Since the photovoltaic electricity inventories from EcoInvent are quite outdated (from 2012) and photovoltaic electricity has improved a lot over the last decade [Müller et al., 2021], it is chosen for a different inventory made by the IEA from the year 2020. A sensitivity analysis on the effect of different electricity sources on the total output of the battery has been conducted to verify how this changes total results.

3.3. End-of-life phase of the ORFB

At the end of life phase of the battery, the components are disassembled and send to corresponding EoL treatment options. The EoL strategy of the ORFB is currently still under development and LCI inputs are mostly based upon literature or connected to EcoInvent processes corresponding with the material used (eg. Current collector is made out of copper and sent to market for scrap copper). The details for the LCI inputs for the different components can be found in the appendix.

3.3.1. Negolyte:

The EoL treatment strategy for the DHPS is to incinerate it and capture the heat. It is assumed that upon incineration it is fully converted into carbon dioxide, nitrogen, sulfur dioxide and water according to the chemical reaction equation below (R1). Using stochiometric calculations results in the outputs depicted in table 3.5

$$C_{12}H_8O_5N_2S + 12.5\,O_2 \longrightarrow 12\,CO_2 + 4\,H_2O + N_2 + SO_2 \tag{R1}$$

Table 3.5: In- and outputs for the combustion of 1 kg of DHPS. *Enthalpy of formation for phenazine used as proxy for DHPS.

Item	Amount [kg]	Enthalpy of formation [kJ/mol]
Inputs		
$C_{12}H_8O_5N_2S$	1	237*
O2	1.37	0
Outputs		
CO2	1.81	-393,5
H2O	0.25	-285,8
N2	0,096	0
SO2	0,22	-296,84
Heat	21,9 MJ	

3.3.2. Posolyte:

In the posolyte, the potassium ferrocyanide is the most important component to dispose due to the toxicity of the cyanide [Gail et al., 2000, Gijzen et al., 2000, Kulig and Ballantyne, 1991, Nelson, 2006]. Ferrocyanide is considered to be less dangerous than hydrogen cyanide because the cyanide is bound to the iron atom. If the ferrocyanide is exposed to UV radiation, this bond can be broken and the toxic cyanide could be released into the environment. It is therefore still important to dispose the ferrocyanide [Kuhn and Young, 2005] into less harmfull substances.

There are multiple methods to dispose ferrocyanide. In this LCA it is assumed that the disposal of ferrocyanide is similar to the disposal of free cyanide or hydrogen cyanide. Due to a lack of data, the LCI inputs are based upon stochiometric calculations of the different EOL options. Energy and other inputs have been neglected.

The most utilized EoL option for cyanide is chlorination [Gail et al., 2000]. In this process, the cyanide is treated in an alkaline solution with chlorine. Using this treatment option, the cyanide is converted into cyanate (see reaction R2 and R3.
Chlorination:

$$\mathrm{Cl_2 + CN^- \longrightarrow CNCl + Cl^-} \quad \text{(R2)}$$

$$\mathrm{ClCN^- + H_2O \longrightarrow OCN^- + Cl^- + 2\,H^+} \quad \text{(R3)}$$

3.3.3. EoL Stack

There are still a lot of uncertainties regarding the EoL phase of the battery stack. In this LCA model it is assumed that the battery stack can be fully dismantled. In a next step, it is analysed which materials are in the stack component and a corresponding EoL option is taken. The main component in the cell frame is polypropylene reinforced with some glass fibers in it. These components are both send to corresponding incineration processes. There are multiple options to process the EoL bipolar plates [Rey et al., 2021]. In their analysis they concluded that a fenton reaction in combination with pyrolysis is the most environmentally friendly treatment option. This process has also been chosen in this LCA. For the sPEEK membrane, Polyethylene terephthalate incineration is taken because of the similarities in chemical structure. The current collector, mainly made out of copper is sent to scrap copper treatment, the end plate to waste wood and the isolation plate is also send to polyethylene therephtalate incineration.

3.3.4. Storage tanks and BoP

The storage tanks are made out of polyester and are sent to waste incineration of PET. The end of life for the balance of plant is not included due to a lack of available data. In future research it is suggested to look further into the EoL options for this.

3.4. Maintenance modelling of the ORFB

In the previous section of the LCA, it is assumed that the battery fulfills its function over its lifetime and at the end of its lifetime the battery gets completely decommissioned. This neglects an important feature of the ORFB, namely that of targeted maintenance of specific components of the battery to increase the total lifetime of the battery. In this chapter the effect of maintenance on the environmental performance of the battery is analysed. In order to analyse this, a simplified use phase model is constructed which generates inputs for an LCA model. A scematic overview of how the models are connected can be found in figure 3.4.

It has to be mentioned that the maintenance strategy for the battery is still under construction and there are still a lot of uncertainties. Due to this lack of data and to simplify the process, only the effect of the electrolytes are analysed in this analysis. For simplicity it is assumed that the electrolyte degradation only effects the capacity of the battery and the amount of cycles the battery can operate. The battery stack and other battery components are taken out of the analysis. The goal of this section is to set up an initial model and to show how a combination of use phase modelling with an LCA model can help in the decision making process. Instead of using fixed values for specific model inputs, a range of values for the inputs is specified. For the analysis a multitude of scenarios is created where random values for the inputs and treatment options are assigned (see section 2.2.2).

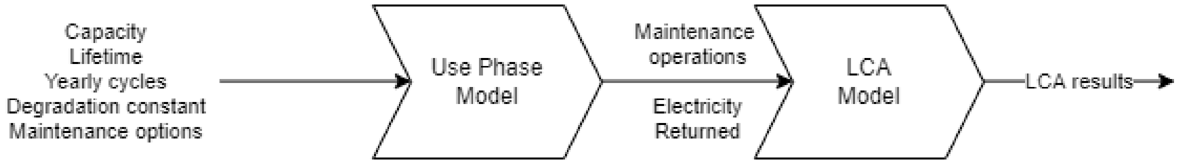

Figure 3.4: Schematic overview of how the Use Phase model and the LCA model are connected

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3.4.1. Battery use phase modelling including maintenance

There are multiple approaches on how to model the use phase of a battery. Some of these are very detailed in which day ahead data for the electricity marked are used to calculate the amount of electricity returned to the grid. In this research a more simplified model is used. In the model, the battery delivers a certain amount of electricity back to the grid during each cycle. This is dependent on the capacity during the cycle and the DoD during that cycle. To calculate the total amount of electricity returned to the grid, the sum of electricity of each individual cycle is taken. This can be described via equation 3.8 (see equation below).

$$E_{tot} = \sum_{n_i=1}^{n_{tot}} C_i \cdot DoD_i$$

In order to calculate the Electricity delivered every cycle, the capacity and DoD of every cycle has to be calculated. The capacity of the battery is dependent on the current state of health of the battery. The battery loses capacity during its lifetime due to battery degradation. In order to assess how the battery loses capacity during its lifetime there are multiple modelling approaches. In this research, a simplified approach is taken where the battery linearly loses some capacity each cycle. The capacity of an individual cycle can be calculated by subtracting a degradation constant (C_{deg}) from the capacity of the previous cycle (see eq. 3.11), the first cycle starts at the batteries max capacity.

$$C_i = C_{i-1} - c_{deg} \tag{3.11}$$

After a certain amount of cycles, the battery has lost so much of its capacity that it cannot fulfill its function properly anymore and a maintenance procedure is needed to regain some capacity. As already mentioned, this model only looks at the electrolytes. For the electrolytes the two main degradation mechanics are side reactions (HER/OER) and active material decomposition. Since the unbalance created by oxygen (OER) and hydrogen (HER) can be counteracted relatively easily, it is assumed that this does not effect battery degradation and is therefore neglected. In the model it is assumed that the battery degradation comes solely from active material decomposition. As discussed in section 2.5.3 there are three general procedures for electrolyte maintenance: 1) fully replace the electrolyte, 2) separate inert material and replace it with new active material, and 3) separate inert material and chemically reactivate it.

The way this is modelled is by introducing two variables called the "point of maintenance" and the "Capacity after maintenance". The point of maintenance is the value that indicates at which point a maintenance procedure is conducted. In other words, if the capacity of a certain cycle gets lower than the "point of maintenance" (e.g. 80% of max capacity), a maintenance operation is introduced. The "capacity after maintenance" is a variable that indicates the amount of capacity the battery has after a maintenance operation is conducted. This value is different depending on which maintenance operation is conducted. For a full replacement of the battery, this value is highest and it is assumed that the recovery point is equal to 100% of its max capacity. For the other two options a value lower than 100% is assumed, with the value for separate and replace inert active material higher compared to the chemical treatment option (explained in section 2.5.3). An example of how the energy output of the battery changes over the different battery cycles can be found in figure 3.5. In the figure the energy returned to the grid over the lifetime of the battery is depicted with the three different maintenance operations.

In summary, the model uses a list of variables and calculates the total amount of electricity and the total amount of maintenance procedures over the batteries life cycle. In table 3.6 an overview of the model inputs and outputs is given. Instead of a fixed deterministic approach a probabilistic approach is taken to assess how maintenance impacts and certain related parameters impact the total results of the LCA (see section 2.2.2). Therefore not a single value, but a range for each parameter is given and multiple scenarios are created. Each scenario with their corresponding outputs is then connected to the LCA model and the effect of certain input parameters on the environmental performance of the battery can be analysed. For simplicity, it is assumed that battery maintenance is performed to both of the electrolytes at the same time with the same treatment method. In reality it might be

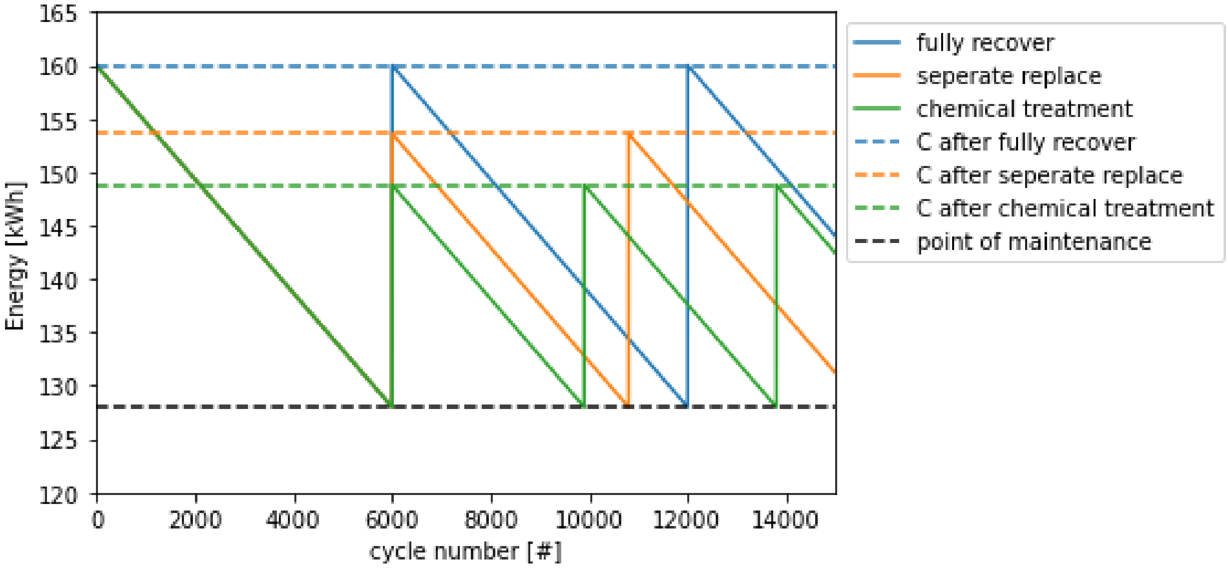


Figure 3.5: Overview of how electricity returned to the grid changes over cycles of battery. At the beginning all options behave the same, the blue and orange line are behind the green line.

Table 3.6: Inputs used for the Use Phase Model.

Variable	**Range**	**Unit**
Capacity	200-200	kWh
DoD	0.8-0.8	[ ]
Lifetime	30-50	years
Yearly cyles	200-400	cycles/year
Degradation constant	0.00542-0.00813	kWh/cycle
Point of maintenance	0.75-0.85	[ ]
C after maintenance (full Rep.)	1.00-1.00	[ ]
C after maintenance (Sep. Rep.)	0.93-0.99	[ ]
C after maintenance (Chem.)	0.88-0.96	[ ]

possible that only maintenance on one of the two electrolytes is conducted when one electrolyte degrades faster than the other.

3.5. LCA model including battery maintenance

The LCA model for the Baliht battery including maintenance is in principle the same as the base LCA model. The functional unit, the production phase, and the End of Life phase of the battery are identical to the base LCA. The use phase of the LCA model is however slightly different. It still has a battery, an EoL battery, electricity to count for energy losses , and the functional unit as inputs, but an extra flow called "maintenance" is added. This maintenance flow, just like the battery and EoL battery input, is normalized over the total electricity returned back to the grid by the battery. An overview of the flowchart for the maintenance part of the model can be found in figure x.

The maintenance input is connected to the three different maintenance options. With three different maintenance procedures for the two electrolytes, this results in a total of six processes. The LCI inputs for these processes can be found in the appendix. In the case of a full replacement of the electrolytes, the same inputs as in the battery productions are used. Next to this, electricity is needed to pump the electrolyte solution out and back into the storage tank. Equation 3.7 has been used to calculate the electricity consumption.

For the other two options the calculation of the LCI inputs is a bit more sophisticated. For both options it is assumed that the inert material can be filtrated and equation 3.5 has been used to calculate the energy required for the filtration. The mass of the inert material has been calculated by multiplying the total amount of active material with the percentage of capacity loss at the point of recovery (100% - point of recovery). This mass has also been taken for the amount of new active material added to the electrolyte solution.

For each of the electrolytes, a chemical reaction has been identified in order to recover the activity of the active material. For the posolyte, it is assumed that the inert active material only consists of ferrous hydroxide. This can be converted back into the ferrocyanide through a reaction with hydrogen cyanide. For the negolyte it is assumed that the hydrogenation reaction is reversible through the addition of oxygen (see figure 2.8, reverse reaction from MHPS-4 to MHPS). The solubility and the electrochemical activity of the MHPS is however lower compared to the activity of the DHPS. This is the main reason why the regained capacity is lowest using the chemical reactivation maintenance option.

4

Results

In this chapter the results from the LCA are analysed and discussed. The different modelling decisions are scrutinized and it is assessed how certain input parameters affect the total results of the LCA. In this section not only the total environmental burdens of the ORFB are analysed, but also a contribution analysis is conducted to assess which factors and flows contribute most to the total environmental burdens of the battery, and the performance of the battery is compared to the environmental performance of a LIB and a VRFB. This information can be used as guideline for the further development of the battery. After this, the results from the maintenance procedures are analysed.

4.1. Life Cycle Impact Assessment

For this LCA, the PEF (Product Environmental Footprint) impact family from the European platform on Life Cycle Assessment is chosen to convert the LCI outputs into different impact categories (European Commission. Joint Research Centre 2010; European Commission. Joint Research Centre. 2011). The PEF impact family is chosen because it is a harmonised European Method to calculate the environmental footprint of a product system. The PEF impact family is a multi criteria measure that has sophisticated models developed by experts to analyse the environmental burdens in 16 different impact categories [Manfredi et al., 2012]. These impact categories can be grouped into the following four categories: 1)Climate change, 2) Ecosystem quality, 3) Human health, 4) Resources. The results from the LCIA can be found in table 4.1.

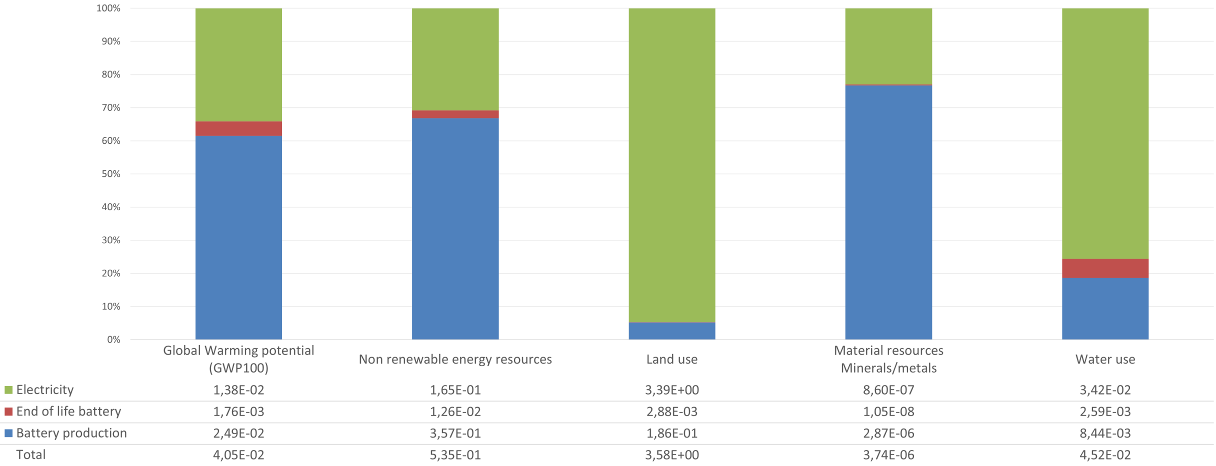
Table 4.1: LCIA results for the ORFB.

Impact group	Impact category	Impact	Unit	Norm. results
Climate change	Global Warming potential (GWP100)	4,05E-02	kg CO2-eq.	6,99E-16
Ecosystem quality	Acidification	3,34E-04	mol H+-eq.	8,71E-16
	Ecotoxicity, freshwater	3,00E+00	CTUe	3,68E-14
	Eutrophication, freshwater	3,01E-05	kg PO4-eq.	5,96E-15
	Eutrophication, marine	1,34E-04	kg N-eq.	6,88E-16
	Eutrophication, terrestrial	4,48E-04	mol N-eq.	3,67E-16
Human health	Human toxicity, Carcinogenic	8,05E-11	CTUh	3,03E-16
	Human toxicity, Non-carcinogenic	2,53E-09	CTUh	7,73E-16
	Particulate matter formation	2,68E-09	kg CFC-11 eq	5,41E-16
	Photochemical ozone formation	1,45E-04	disease incidence	5,17E-16
	Ozone depletion	1,13E-08	kg NMVOC-eq.	7,00E-17
	Ionising radiation	4,39E-03	kBq U235-eq.	1,51E-16
Resources	Non renewable energy resources	5,35E-01	MJ	1,19E-15
	Land use	3,58E+00	[ ]	3,71E-16
	Material resources Minerals/metals	3,74E-06	kg Sb-eq.	8,53E-15
	Water use	4,52E-02	m^3 world eq. Depr.	5,71E-16

4.2. Baliht battery use phase analysis

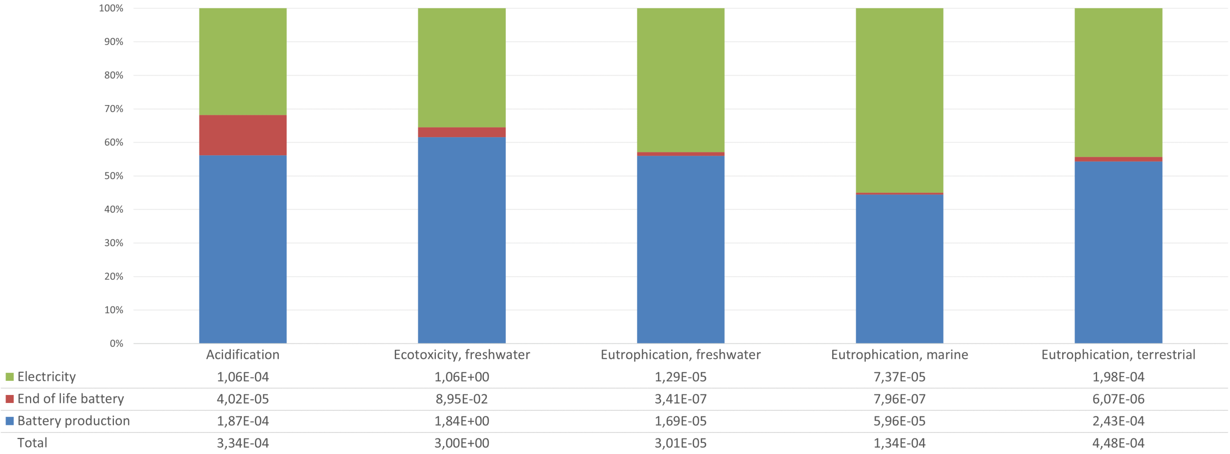
In figures 4.1, 4.2 and 4.3 the main results for the BALIHT battery can be found. In general the largest contribution for the total impact comes from the production of the battery (blue) as well as the electricity losses due to the inefficiency of the battery (green). The EoL stage (red) of the battery only has a minor contribution to the total results.

Improving the efficiency of the battery or reducing the environmental impacts of the production of the electricity could therefore significantly improve the battery performance. First, an analysis of which environmental flows and which individual processes have a large contribution towards the total environmental burdens of the battery. Afterwards, several aspects of the electricity input are discussed. Then A more in depth analysis of the environmental impacts in the battery production phase will be given in section 4.3 and after that the EoL section is further analysed..



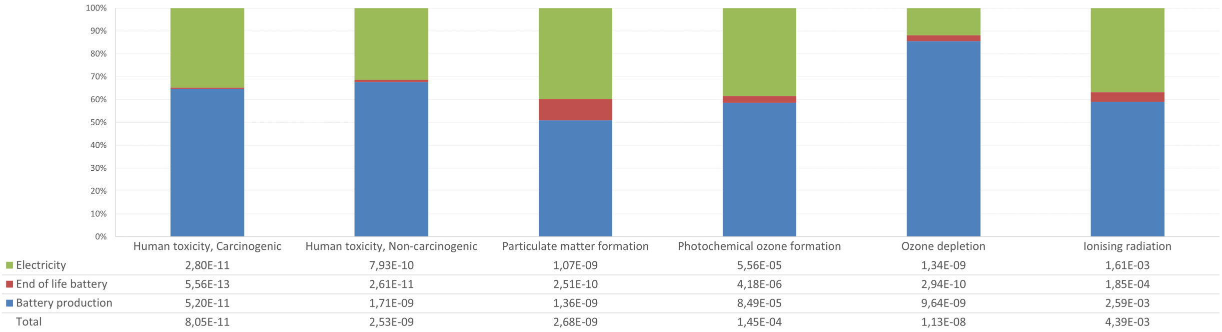
	Global Warming potential (GWP100)	Non renewable energy resources	Land use	Material resources Minerals/metals	Water use
🟩 Electricity	1,38E-02	1,65E-01	3,39E+00	8,60E-07	3,42E-02
🟥 End of life battery	1,76E-03	1,26E-02	2,88E-03	1,05E-08	2,59E-03
🟦 Battery production	2,49E-02	3,57E-01	1,86E-01	2,87E-06	8,44E-03
Total	4,05E-02	5,35E-01	3,58E+00	3,74E-06	4,52E-02

Figure 4.1: Climate change and resources impact categories (numbers for each impact category have the same unit as depicted in table 4.1).



	Acidification	Ecotoxicity, freshwater	Eutrophication, freshwater	Eutrophication, marine	Eutrophication, terrestrial
🟩 Electricity	1,06E-04	1,06E+00	1,29E-05	7,37E-05	1,98E-04
🟥 End of life battery	4,02E-05	8,95E-02	3,41E-07	7,96E-07	6,07E-06
🟦 Battery production	1,87E-04	1,84E+00	1,69E-05	5,96E-05	2,43E-04
Total	3,34E-04	3,00E+00	3,01E-05	1,34E-04	4,48E-04

Figure 4.2: Ecosytem quality categories (numbers for each impact category have the same unit as depicted in table 4.1).



	Human toxicity, Carcinogenic	Human toxicity, Non-carcinogenic	Particulate matter formation	Photochemical ozone formation	Ozone depletion	Ionising radiation
🟩 Electricity	2,80E-11	7,93E-10	1,07E-09	5,56E-05	1,34E-09	1,61E-03
🟥 End of life battery	5,56E-13	2,61E-11	2,51E-10	4,18E-06	2,94E-10	1,85E-04
🟦 Battery production	5,20E-11	1,71E-09	1,36E-09	8,49E-05	9,64E-09	2,59E-03
Total	8,05E-11	2,53E-09	2,68E-09	1,45E-04	1,13E-08	4,39E-03

Figure 4.3: Human health impact categories (numbers for each impact category have the same unit as depicted in table 4.1).

4.2.1. Elemtary flows and Process flows analysis

In table 4.2 the results from the process and elementary flows are given. In the table the most contributing process and elementary flows in each impact category are listed. These flows are not related to each other, meaning that the given elementary flow does not necessarily have to be produced at the corresponding process.

It is interesting to see that most of the listed processes are related to either electricity production from hard coal or specific mining operations. Some of these mining operations are also related to the coal production chain (lignite mining, coking). The copper value chain also has a large impact in some of the impact categories due to blasting operations as well as treatment of copper slag and sulfidic tailings.

For the elementary flows, an interesting contributor is the tetrachloromethane in the ozone depletion category. This flow is correlated to the electrode spray production which contains chlorodifluoromethane. It could be interested to look at other alternatives to reduce the impact in this impact category. Another interesting flow is the flow of Lead (Pb) and Arsenic (As) in the non carcinogenic human toxicity impact category. These flows are produced at the treatment of copper slag and a reduction of these flows should be a priority.

Table 4.2: Most important Process flows and Elementary flows.

Impact category	**Process**	**Elemtary flow**
Global Warming potential (GWP100)	Electricity production, hard coal	CO2
Acidification	Smelting of copper concentrate	SO2
Ecotoxicity, freshwater	Blasting	Al
Eutrophication, freshwater	Treatment of sulfidic tailings and spoil from lignite mining	P
Eutrophication, marine	Treatment wasterwater PV cell production	NO3
Eutrophication, terrestrial	Blasting	NOx
Human toxicity, Carcinogenic	Coking	Benzo(a)pyrene and Cr(VI)
Human toxicity, Non-carcinogenic	Treatment of copper slag	Pb and As
Particulate matter formation	Electricity production, hard coal	Particulates <2,5 micrometer
Photochemical ozone formation	Electricity produciton hard coal and blasting	NOx
Ozone depletion	Chlorodifluoromethane production	Tetrachloromethane
Ionising radiation	Treatment of tailing uranium milling	Radon-222
Non renewable energy resources	Hard coal mining	Oil. Crude in ground
Land use	Open ground construction PV	Transformation to urban
Material resources Minerals/metals	silver-gold mine operation	Tellurium
Water use	Multi-Si wafer production	Water

4.2.2. Electricity input

For the extra photovoltaic electricity that is needed due to battery inefficiencies, the production of the PV-panel has the biggest contribution in the total impact of the battery. In the PV panel production chain, the production of the silicon wafer for the pv panels is having the largest contribution. These impacts either come from mining operations for the silicium or wastewater flows in the wafer production. Since an "open ground installation" is used, the production of aluminium for the mount also has a significant contribution to the total environmental impact. This is also the reason for the high impact in the land use category, since large amounts of lands has to be cleared for the PV panel installation.

To assess the impact of how different electricity sources impact the total results, a sensitiviy analysis is conducted where the battery is connected to four different inputs: 1) solar pv-electricity from the IEA database, 2) solar pv-electricity from the EcoInvent database, 3) Wind electricity from EcoInvent database, and 4) The Spanish electricity mix from the EcoInvent database. The results from this analysis are depicted in figure 4.4.

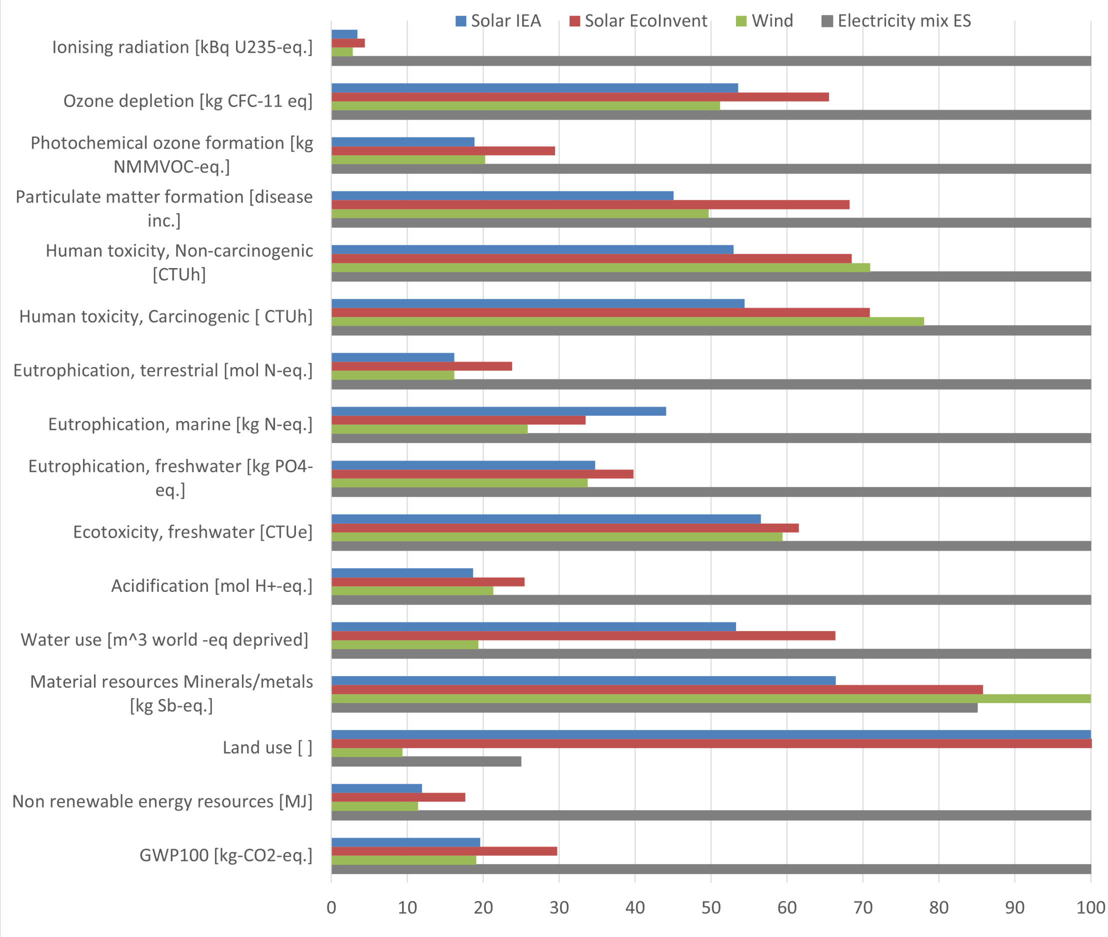


Figure 4.4: Change in impact with different Electricity inputs.

From the results it is concluded that the input for electricity in the battery has a large impact on the total performance of the battery. If the battery is connected to the Spanish electricity mix, the battery has the highest impact in all impact categories except for *mineral use* (wind electricity) and *land use* (solar electricity, EcoInvent database). Luckily, it is expected that the electricity mix in Spain will get cleaner over the years and the battery will most of the times be charged using renewable energy in the first place. The difference in outcomes in the different impact categories when the battery is connected to the EcoInvent solar power background system compared to the IEA background system is also significant. Changing towards a wind based electricity input also lowers the impact in most of the impact categories compared to the EcoInvent database.

4.2.3. Effect of round trip efficiency:

The effect of an increase in round trip efficiency can be seen in figure 4.5. In the figure the relative impact in each impact category is normalized over the impact of the base scenario which uses a round trip efficiency of 65%. The round trip efficiency and the total impact of the battery have a negative correlation (see eq. 3.10). The decrease of impact in the different impact categories is larger in impact categories in which the contribution of electricity is higher. With an increase of battery efficiency from 65% towards 80%, the total impacts of the battery can be lowered from 6% for *ozone depletion* all the way up to 53% for *land use*. On average the total impacts can be decreased by 20% to 30% for most of the impact categories.

From the different analyses it can be concluded that the electricity input is a very important factor for the total performance of the battery. The total life cycle impact of the battery can therefore be reduced significantly if the total electricity input is lowered and/or the environmental burdens of the electricity value chain are reduced. A promising aspect is the trend that the (environmental) performance of renewable energy sources is increasing over the last couple of years and will increase further and further, which will benefit the performance of the Baliht battery as well.

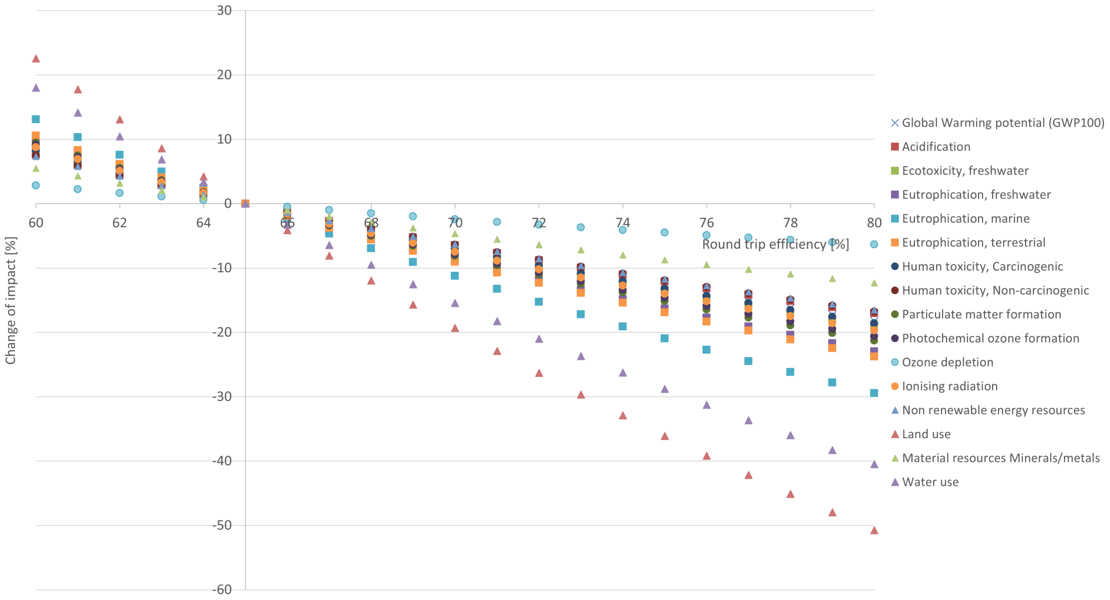


Figure 4.5: Change in impact with different values for the round trip efficiency to the base case of 65% efficiency.

4.2.4. Impact of the total amount of electricity returned to the grid

Another parameter that could have an important influence on the environmental impact of the battery is the total amount of electricity the battery returns back to grid over its entire life cycle. From eq. 3.9 it can be seen that this is dependent on the total capacity, the cycle life, and the DoD during each cycle. The total amount of electricity returned back to the grid has an inverse relationship with the battery production and battery EoL input. A higher maximum capacity, cycle life and DoD should in theory also lower the impact of the battery production and battery EoL stage of the battery and thus also lower the total impact of the battery. Unfortunately, reality is not as simple as this due to correlations between different variables in the battery; e.g. the DoD has an impact on the cycle life; higher DoD in general results in more battery degradation and thus a lower cycle life. Next to this, the battery capacity is a result of the total amount of active material in the electrolyte solutions. An increase of capacity is therefore directly correlated to the amount of electrolyte and the size of the storage tanks.

Detailed use phase modelling has to be conducted in order to fully grasp the impact of these parameters. In this research a simplified analysis is conducted in which the DoD is kept constant, but different values for cycle life/battery degradation and maximum capacity are analysed.

4.2.5. Cycle life/battery degradation

During each charge-discharge cycle, the battery loses a small fraction of its capacity. Once the battery reaches 80% of its maximum capacity, batteries are considered non-functional and they reach their End of Life stage. If the battery remains more of its total capacity after every cycle (there is less battery degradation), the battery can perform more cycles before it reaches the End of Life stage, which results in an increase of total amount of electricity returned to the grid. Minimizing degradation can therefore lower the environmental burdens of the battery. In this sensitivity analysis it is analysed how a change in the total number of cycles can effect the environmental performance of the battery by ranging the cycle life from 4000 to 8000 cycles.

From the results depicted in figure 4.6, it can be concluded that the cycle life is indeed an important parameter for the total environmental performance of the battery. Lowering degradation and increasing the total amount of cycles the battery performs can be a valuable strategy in order to lower the environmental performance since it lowers the amount of "battery" and "EoL battery" in the LCA model.

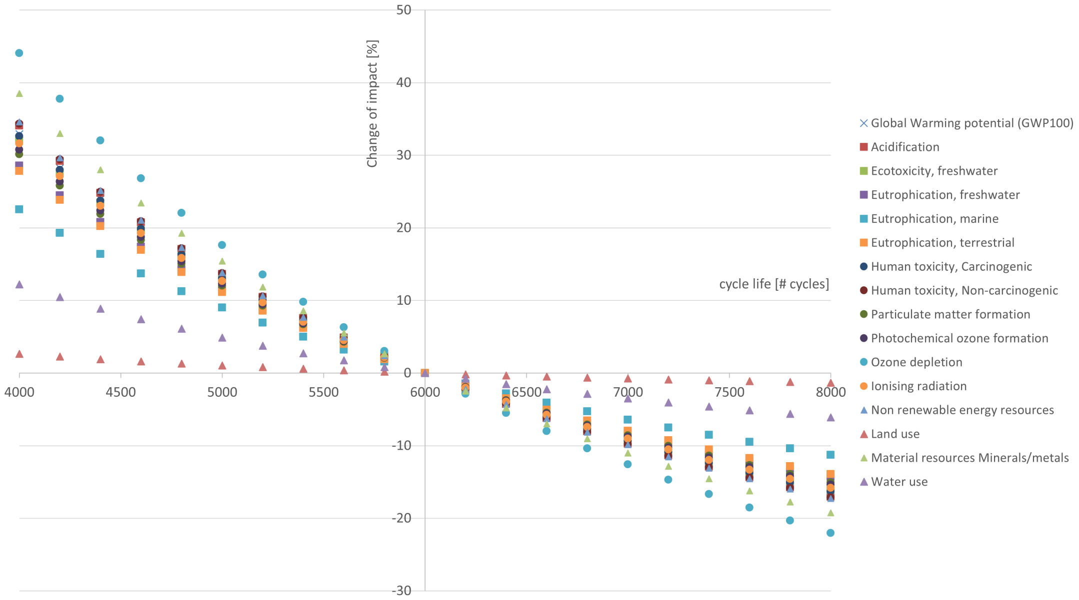


Figure 4.6: Change in impact with different cycle lifes of the battery to the base case of 12500 cycles. Low cycle life = high degradation = less electricity delivered back to grid, high cycle life = low degradation = more electricity delivered back to grid.

4.2.6. Different max capacities and E/P values

One of the big advantages of a flow battery compared to a LIB is its modular design. In a flow battery the battery stack, electrolytes and the other materials can be scaled independently from each other. In this section, the effect of an increase in total storage capacity over the total environmental impacts are researched. This will be done by parameterizing the total storage capacity of the model. Some of the battery components will scale up with increasing battery capacity while other components remain constant. The first step is to analyse which battery components are dependent on the total battery capacity and which components are independent (see table 4.3).

Table 4.3: Scaling dependency of components. *Tanks don't scale linearly but for simplicity it is assumed they do.

Component	Scales
Battery	Inverse relationship
EoL Battery	Inverse relationship
Posolyte	Increases linearly
Negolyte	Increases linearly
Battery stack	constant
Posolyte tanks	Increases linearly*
Negolyte tanks	Increases linearly*
BoP	constant

In the next step the capacity dependent components are parameterised in the model so that they also change with changing max capacities. The battery and battery end of life input in the use phase are calculated by equation 3.9. For the other variables with a linear relationship(P), the base value of the parameter (P_0) is multiplied with the ratio of the battery capacity of the scenario (C_i) over the base value of the battery capacity (C_0 = 200 kWh) (see eq 4.1).

$$P = P_0 \cdot \frac{C_i}{C_0} \tag{4.1}$$

The results for global warming can be found in figure 4.7, while the relative change in all impact categories can be found in figure 4.8. In the figure the total (black line) is the sum of the three underlying graphs (battery production, battery EoL, and electricity losses). With a lower capacity, the impact of the battery production and EoL stage gets more and more significant. This is because the impact of non-scaling components (battery stack and BoP) remains constant, but the total amount of electricity returned to the grid gets smaller. With an increase of battery capacity the battery production and EoL inputs gets less and less significant and it reaches an asymptote.

The effect for the other impact categories is similar to the global warming impact category. The change of impact is again higher in impact categories with a higher total contribution of the battery production phase.

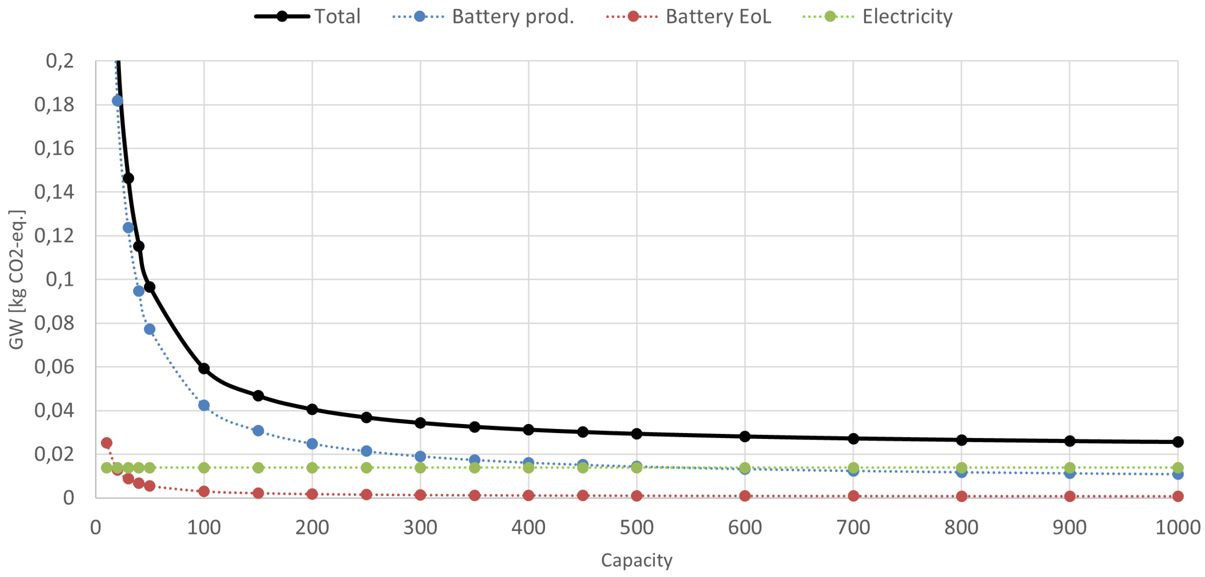


Figure 4.7: Effect of different battery capacities on global warming impact.

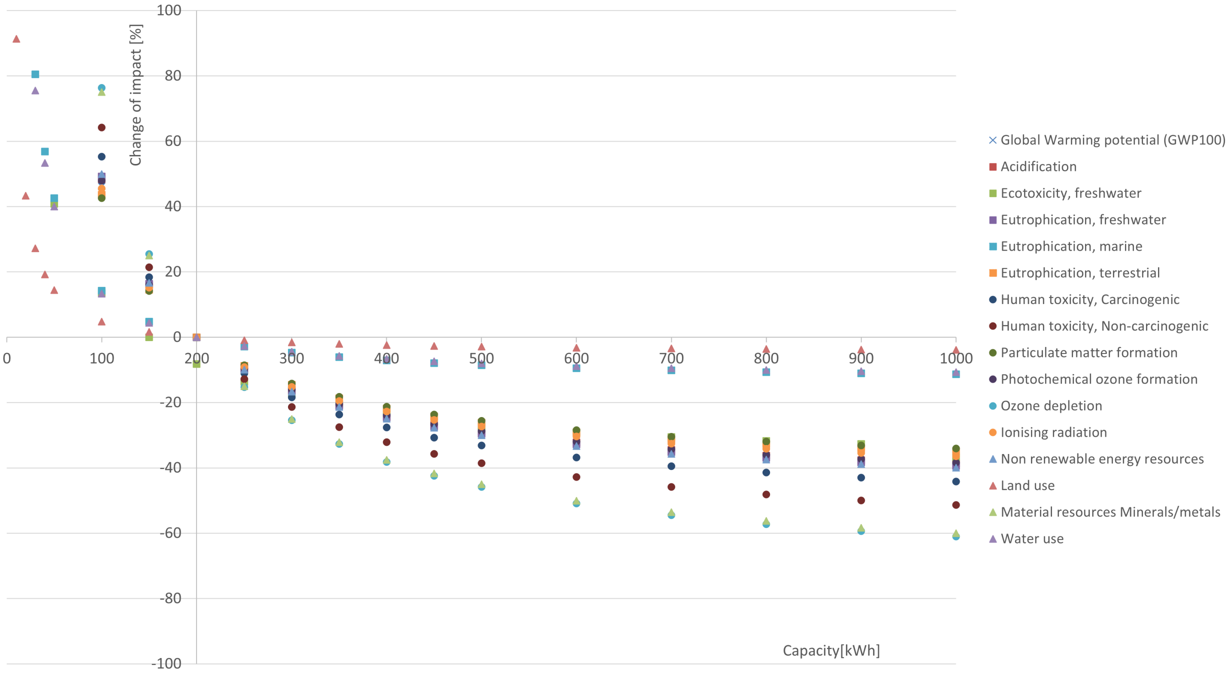


Figure 4.8: Change of impact of different battery capacities in the different impact categories.

4.3. Production phase of the Battery

The results for the different impacts of the different battery components can be found in figure 4.9. In the global warming impact category and the resource impact categories, the battery stack has the largest contribution. The BoP, negolyte and posolyte all have a smaller contribution. In the ecosystem quality impact categories, the battery stack as well as the BOP have a large contribution to the total impact of the battery. These two battery inputs have the largest impact except for the marine eutrophication category where the negolyte has the largest contribution. In the human health impact categories, the battery stack and the BoP also have a large impact to the total results. Especially the contribution of the battery stack in the ozone depletion impact category is large.

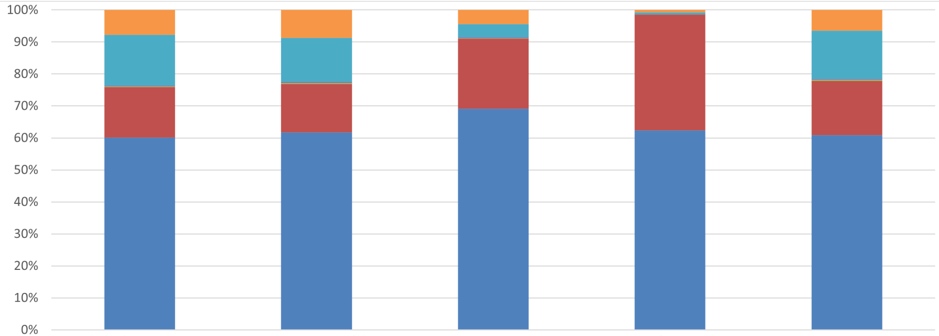
An overview of the most contributing products and processes in the production chain of the different battery components can be found in table B.1. For the battery stack the highest contributors are the copper production for the current collector, and the graphene production and electricity consumption in the bipolar plates production chain (see figure 4.10). In these processes, especially the mining of the copper has a large impact on the total environmental performance. The membrane has some impact to the total contribution in the global warming impact category while it only has a small contribution in the other impact categories. The end plate has a large contribution in the land use category because of the amount of land needed for the trees to produce the wood. The isolation plate has almost no contribution to the total results.

Since there are a lot of environmental burdens coming from the production chain of the bipolar plates and the the current collectors, a good strategy would be to re-use these components as much as possible. It would furthermore benefit if a more circular economy would be created surrounding the copper and graphene. It is therefore advised to already produce a sustainable EoL strategy for these two products.

For the posolyte, the total environmental impact is relatively low. The highest contributors vary per impact category. The most important ones are the electricity for the potassium ferrocyanide production, the hydrogen cyanide, the potassium carbonate and the potassium chlorite production chain.

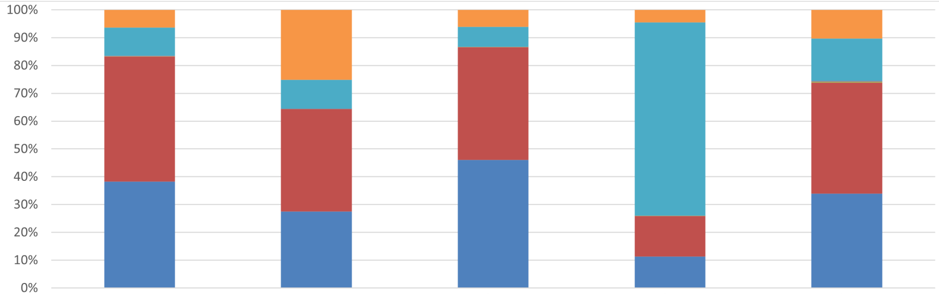
For the negolyte the biggest contributor in most of the impact categories is the production of the ortho-phenylenediamide production in the DHPS production chain. One important aspect here is that the current model has the environmental impacts of the negolyte from the fossil fuel based organic starting materials. These impacts can change if the DHPS is produced from lginin.

The environmental impacts in the Balance of Plant mostly come from the copper for the inverter. Similar to the current collector in the stack, the environmental impacts here are a result of the environmental burdens coming from the mining operations of the copper.



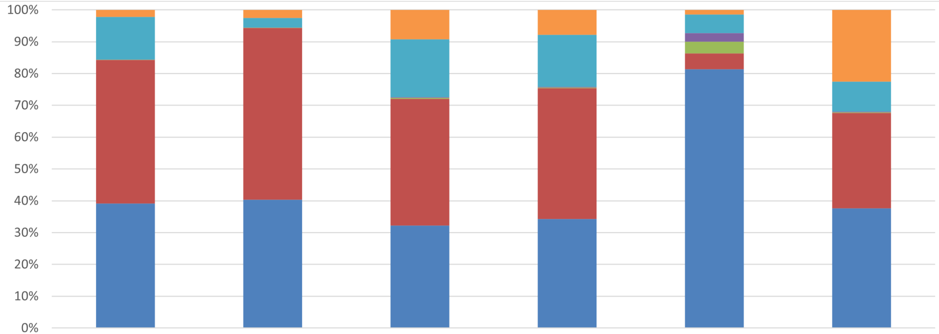
	Global Warming potential (GWP100)	Non renewable energy resources	Land use	Material resources Minerals/metals	Water use
🟧 Posolyte	2,39E-03	3,72E-02	7,76E-03	3,42E-08	8,47E-04
🟦 Negolyte	4,94E-03	5,88E-02	7,30E-03	3,09E-08	1,99E-03
🟪 Negolyte tank	5,28E-05	1,14E-03	2,19E-04	5,58E-10	3,55E-05
🟩 Posolyte tank	7,04E-05	1,52E-03	2,91E-04	7,44E-10	4,73E-05
🟥 BoP	4,88E-03	6,49E-02	3,81E-02	1,65E-06	2,22E-03
🟦 Battery Stack	1,86E-02	2,64E-01	1,20E-01	2,85E-06	8,01E-03
Battery total	1,86E-02	2,64E-01	1,20E-01	2,85E-06	8,01E-03

(a) Climate change and resources impact categories.



	Acidification	Ecotoxicity, freshwater	Eutrophication, freshwater	Eutrophication, marine	Eutrophication, terrestrial
🟧 Posolyte	1,06E-05	4,44E-01	1,01E-06	2,53E-06	2,04E-05
🟦 Negolyte	1,69E-05	1,84E-01	1,16E-06	3,85E-05	3,00E-05
🟪 Negolyte tank	2,28E-07	7,51E-04	1,28E-08	4,30E-08	4,31E-07
🟩 Posolyte tank	3,03E-07	1,00E-03	1,70E-08	5,73E-08	5,74E-07
🟥 BoP	7,53E-05	6,50E-01	6,69E-06	8,10E-06	7,90E-05
🟦 Battery Stack	6,39E-05	4,86E-01	7,58E-06	6,24E-06	6,69E-05
Battery total	1,67E-04	1,77E+00	1,65E-05	5,54E-05	1,97E-04

(b) Ecosytem quality categories.



	Human toxicity, Carcinogenic	Human toxicity, Non-carcinogenic	Particulate matter formation	Photochemical ozone formation	Ozone depletion	Ionising radiation
🟧 Posolyte	9,65E-07	4,17E-11	7,97E-11	5,34E-06	1,17E-10	4,74E-04
🟦 Negolyte	5,72E-06	4,88E-11	1,56E-10	1,11E-05	4,81E-10	1,99E-04
🟪 Negolyte tank	2,96E-08	5,94E-13	2,16E-12	1,55E-07	2,25E-10	3,92E-06
🟩 Posolyte tank	3,94E-08	7,91E-13	2,88E-12	2,06E-07	3,00E-10	5,22E-06
🟥 BoP	1,93E-05	8,83E-10	3,43E-10	2,80E-05	4,09E-10	6,29E-04
🟦 Battery Stack	1,68E-05	6,59E-10	2,77E-10	2,33E-05	6,66E-09	7,92E-04
Battery total	4,96E-11	1,63E-09	8,62E-10	6,82E-05	8,19E-09	2,10E-03

(c) Human health impact categories.

Figure 4.9: Contribution analysis of the production phase of the Baliht battery in the different impact categories.

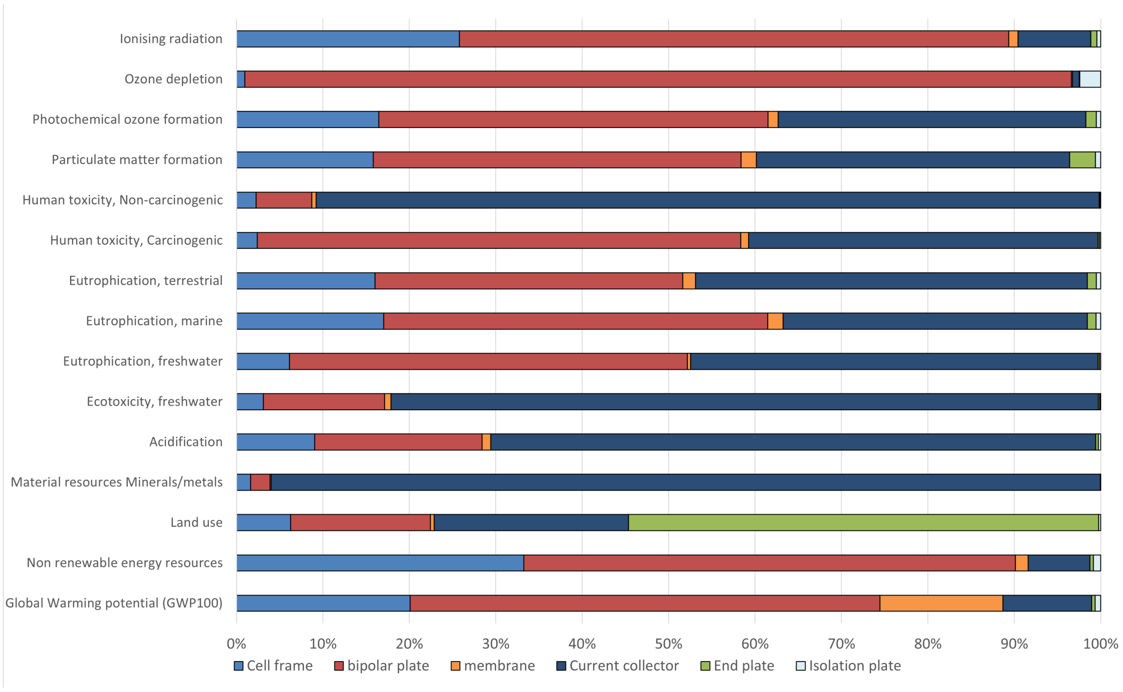


Figure 4.10: Contributions of the battery stack in the different impact categories.

4.4. End of Life phase analysis

The end of life stage of the battery only contributes to a minor degree to the total environmental impact of the battery. This is the results of two main reasons. The first one is the lack of information on the EoL strategy for the Baliht battery. Because of this, the EoL part of the model is very simplified and therefore certain inputs are potentially not included in the model. An example of this is in the battery stack. Currently it is assumed that the battery stack can be easily dismantled and the specific components are all sent to specific EoL treatment options. In reality, energy and chemicals might be needed to clean and dismantle the cell stack. Another factor that reduces the environmental impact of the EoL stage is the way the EcoInvent database deals with the different waste flows. In the EcoInvent database, the waste flows are treated and upon treatment (partially) converted into goods, e.g. PET is combusted to produce electricity/heat. Consequently, the substitution methods is used and the environmental impact to produce the good in the first place are subtracted from the end total. In principle, this is not a wrong method to deal with the conversion of the battery waste into new products. This method assumes however that it is possible to convert the waste streams of the battery the same way as any other waste streams of the material. In reality this might not be the case due to for instance the way the component is arranged in the battery (for instance in the cell stack) or regulations in regard to contamination with the different chemicals in the battery. A more thorough strategy on the EoL stage of the battery could give a better insight in the environmental inputs of the EoL stage of the battery.

4.5. Summary of base LCA for the ORFB

Now that the results from the base LCA model are analysed, sub-research question 3 can be answered:

What are important aspects contributing to the environmental performance of the battery?

From the results it is concluded that the production of the battery and the extra electricity inputs due to battery inefficiencies have the largest contribution towards the total environmental burdens of the battery.

For the battery production, a large part of its total environmental impact comes from the electrodes and copper collectors in the battery stack as well as the inverter in the BoP. The impacts from the electrolytes is relatively low, although it does have quite a large impact in the marine eutrophication impact category. The impacts of the battery production can be lowered by increasing the total amount of electricity the battery produces over its lifetime. This can be done by increasing the number of cycles the battery conducts over its lifetime as well as increasing the capacity of the battery. It is furthermore recommended to reuse some of the high impact components like the current collector, inverter and electrodes.

The environmental impacts from the electricity production are coming from the high impact of the silicon in the pv panels. A good strategy to lower these impacts is to increase the overall round trip efficiency of the battery.

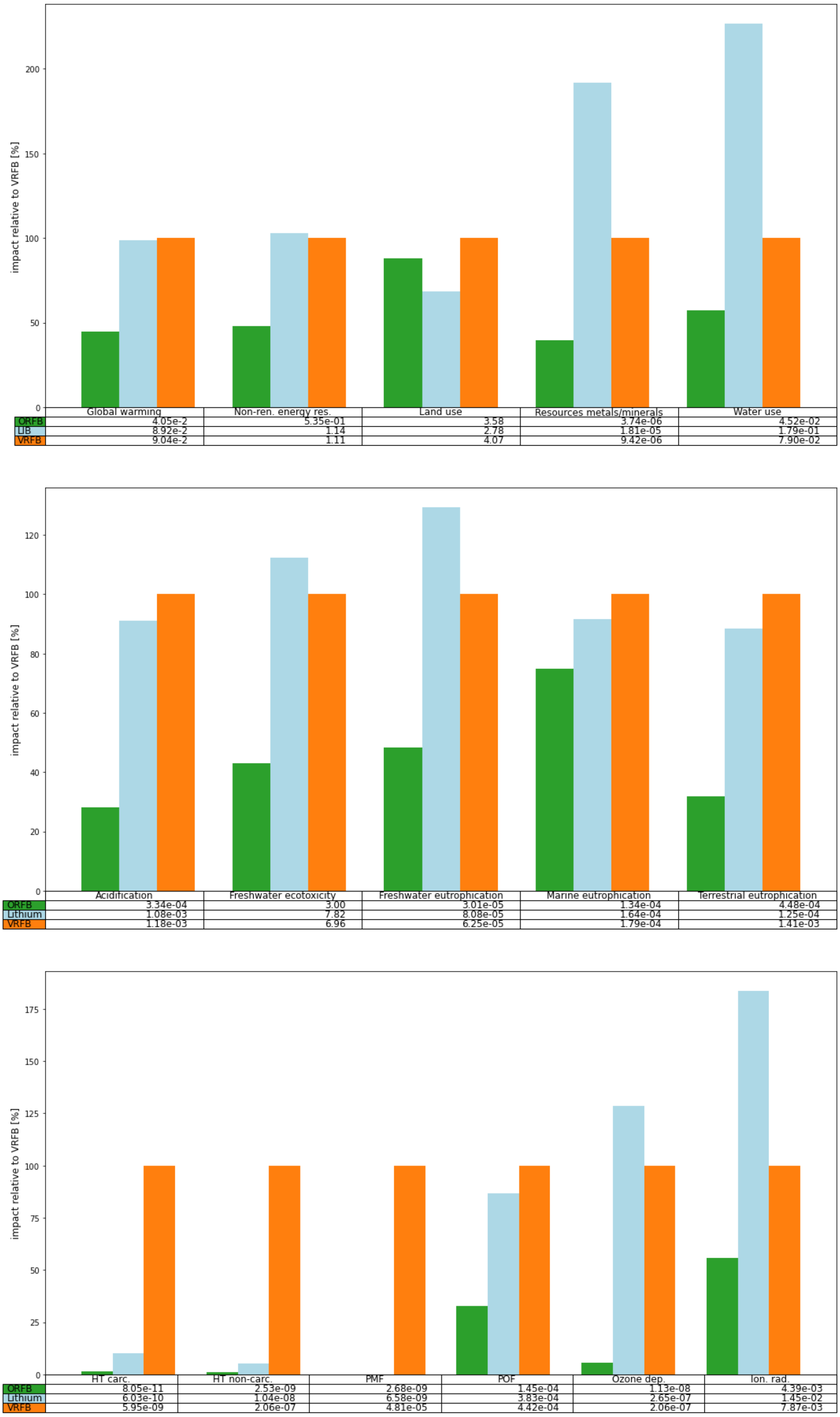
4.6. Comparison with LIB and VRFB

To assess how well the ORFB performs compared to similar type of batteries, the results are compared with a LIB and a VRFB. This is also sub research question 4.

How does the environmental performance of an ORFB compare to other types of batteries with similar functions?

From the results it is concluded that the ORFB scores better compared to the two other batteries in practically all impact categories (see figure 4.11). As discussed in the introduction (chapter 1) it is claimed that LIB and especially VRFBs have issues regarding material use and effects on human health. What is especially interested to see is how much lower the impact in the human health categories is. These high impacts on human health are mainly related due to the mining of the materials in the battery (cobalt for LIB and Vanadium for VRFB). Since the ORFB uses organic materials as storage materials, the impacts on human health is a lot lower.

It has to be mentioned that the LCI inputs of the LIB and VRFB come from a different research paper. It is well possible that several modelling decisions in the LCI model of these batteries are resulting in the difference in environmental impact. Next to this, the battery specifications are also different compared to the ORFB, which makes a comparison more difficult. Seeing that lots of the impacts in the value chain of the other batteries come from materials, which are not present in the ORFB (lithium, cobalt, vanadium), is however a promising prospect for the environmental performance of the ORFB.



	Global warming	Non-ren. energy res.	Land use	Resources metals/minerals	Water use
ORFB	4.05e-2	5.35e-01	3.58	3.74e-06	4.52e-02
LIB	8.92e-2	1.14	2.78	1.81e-05	1.79e-01
VRFB	9.04e-2	1.11	4.07	9.42e-06	7.90e-02

	Acidification	Freshwater ecotoxicity	Freshwater eutrophication	Marine eutrophication	Terrestrial eutrophication
ORFB	3.34e-04	3.00	3.01e-05	1.34e-04	4.48e-04
Lithium	1.08e-03	7.82	8.08e-05	1.64e-04	1.25e-04
VRFB	1.18e-03	6.96	6.25e-05	1.79e-04	1.41e-03

	HT carc.	HT non-carc.	PMF	POF	Ozone dep.	Ion. rad.
ORFB	8.05e-11	2.53e-09	2.68e-09	1.45e-04	1.13e-08	4.39e-03
Lithium	6.03e-10	1.04e-08	6.58e-09	3.83e-04	2.65e-07	1.45e-02
VRFB	5.95e-09	2.06e-07	4.81e-05	4.42e-04	2.06e-07	7.87e-03

Figure 4.11: Impact of the different battery types (ORFB = green, LIB = blue, VRFB = orange) scaled to the impact of the VRFB (set too 100%). (The values in the tables below the graphs use the same units as in table 4.1.

4.7. Maintenance of the battery

For the maintenance it has been chosen to only focus on the global warming impact category. The reason for this is that the main goal of this section is how a combination of use phase modelling with LCA can be a very strong tool. The same procedure can be done to all the other impact categories to obtain a full assessment. Unfortunately the inputs for the use phase model as well as the LCA are very uncertain and no real conclusions can be drawn yet. This aspect of the battery needs further research. The results for all the different scenarios in the global warming impact category can be seen in figure 4.13 and 4.12. From the histogram it is concluded that, using the current information, chemical treatment in general has the lowest impact in the global warming impact category over all the different scenarios. After that the partially replacement option is a good strategy and lastly the full replacement strategy scores the worst.

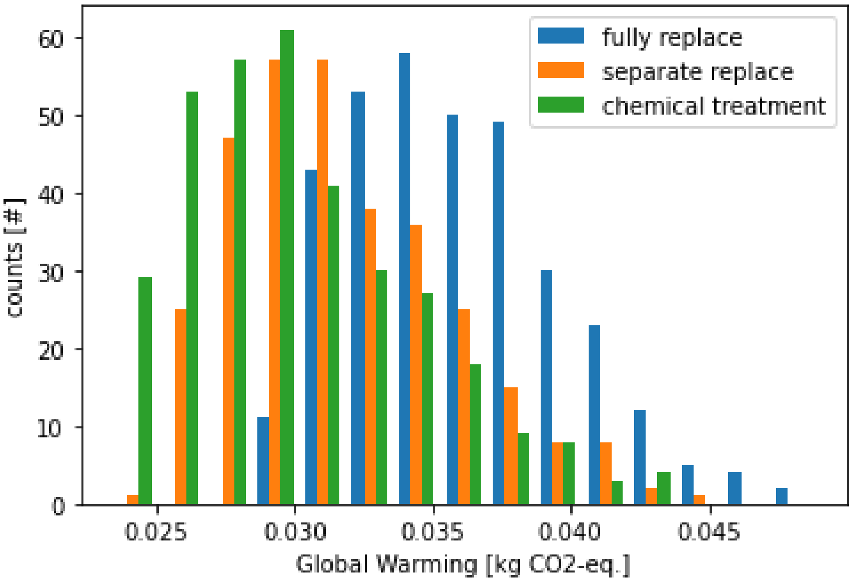


Figure 4.12: Histogram results for the maintenance modelling

In figure 4.13 the global warming impact has been plotted vs the different inputs from the use phase model. In the graphs the total amount of electricity returned to the grid is color coded. The clearest trend can be observed from the yearly amount of cycles and the global warming impact. More yearly cycles results in more electricity returned to the grid. Since the battery input, the EoL battery and the maintenance input for the use phase are inverse related to the total amount of electricity returned to the grid, the total impact of the battery is also getting smaller with more yearly cycles. The same trend can be observed with the total lifetime in years vs the global warming impact and can be explained in the same way.

With a lower degradation factor the total impact in global warming is getting lower. Lower degradation results in fewer maintenance operations and thus lower environmental burdens. The impact of the point of recovery seems to be negligible. For the recovery point at first glance a not expected trend can be seen. With a lower recovery point, it seems that the impact on global warming is lower. This is counter-intuitive since a higher recovery point means a "better" maintenance operation. This however can be explained because the recovery point is a direct result of the maintenance method chosen. Chemical treatment has a lower recovery point compared to the separate and replace option and the fully replace option has the highest one (fixed to 1.00). From the graph in the middle right, it can be observed that in general the impact from the chemical replacement option are lower than the results from the separate replacement option, with the highest impact in the fully replacement option.

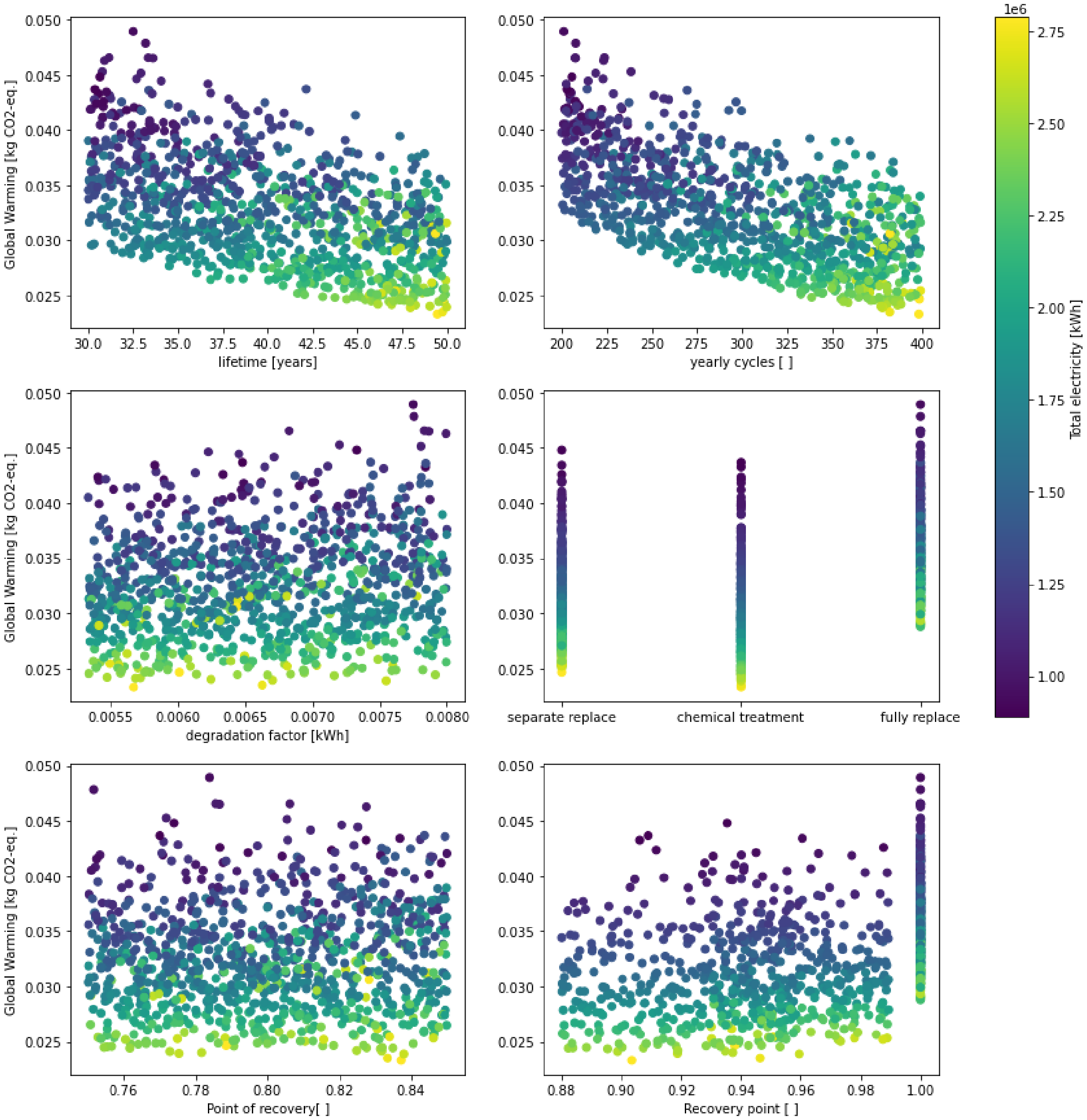


Figure 4.13: Global warming impact vs different use phase parameters.

To further analyse the effect of the maintenance impact of the battery, a second run of scenarios has been conducted where the lifetime, anf yearly cycles has been kept fixed (40 years, 300 cycles/year respectively). The results can be found in figure 4.15 and 4.14. With these results it is again concluded that the chemical treatment option for maintenance is the best option if it comes to the global warming category. Although there is more electricity delivered back to the grid if the fully replacement maintenance option is conducted, the relative large impact in the global warming category from fully replacing the electrolytes compared to the chemical treatment option counteracts this and results in a total net increase of impact.

Using the model it has been showed that chemical treatment would be the best option for the lowest environmental impact. It has to be mentioned though that this is a very basic model using a lot of simplifications and

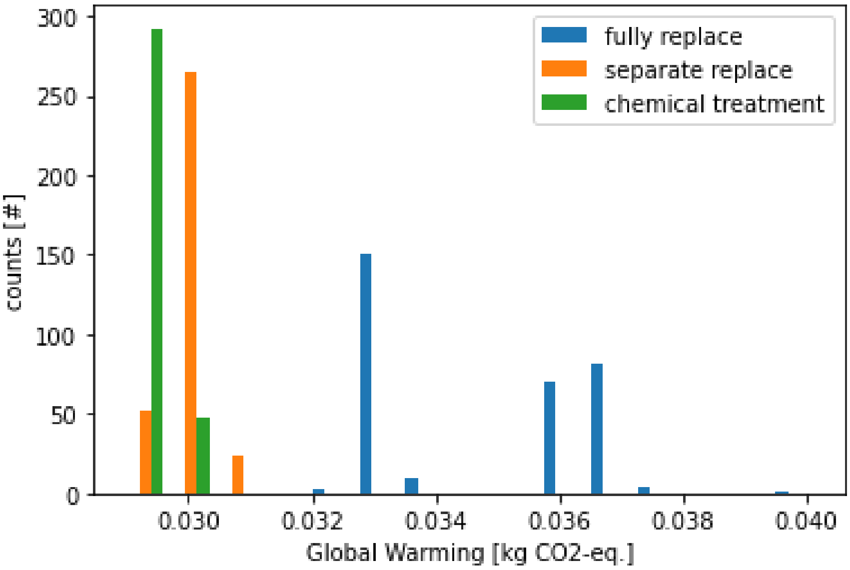


Figure 4.14: histograms with fixed values.

assumptions. In order to fully grasp the environmental impact of the different maintenance procedures a more detailed model is needed. The modelling of the electrolyte degradation is done in a very basic way. Next to this, the use phase model currently only looks at degradation of the electrolytes, where degradation from for instance the cell stack can also have a major impact. Further development of the use phase model could give a more accurate insight in what the best maintenance strategy is.

Next to this there are a lot of uncertainties about the use phase of the battery and the potential maintenance options itself. There is still a lot of research going on, on how and how fast certain components of the battery degrade and what their effect on the overall battery performance is. Next to this, the maintenance procedures themselves are also a big unknown. Due to these uncertainties in regard to the maintenance options of the electrolytes, the LCA model itself also has a lot of uncertainties. It might be possible that different chemical treatment options are needed or that due to inefficiencies of the chemical treatment reactions, more energy or materials are needed for the reactivation reaction. This could drastically increase the environmental impacts of the chemical treatment option. Further advancements in the battery research are needed to improve the results of this analysis.

Due to the large uncertainties one could argue that the results from this LCA are not that useful, but inherently all LCAs suffer from this. Using this approach does however show the power of using a probabilistic approach in LCAs. By applying a large set of scenarios, one can get a lot of valuable information on which parameters have the largest impact on the total results. This information can be very valuable for policy makers or product developers and the LCA practitioner itself. For policy makers a more statistically sound decision can be made. For product developers a better insight is given on which parameters are important to further develop and improve their product to lower the products' environmental impact. The LCA practitioner can use the results to get a better insight in the model itself to see which aspects might need more focus or need to be more detailed.

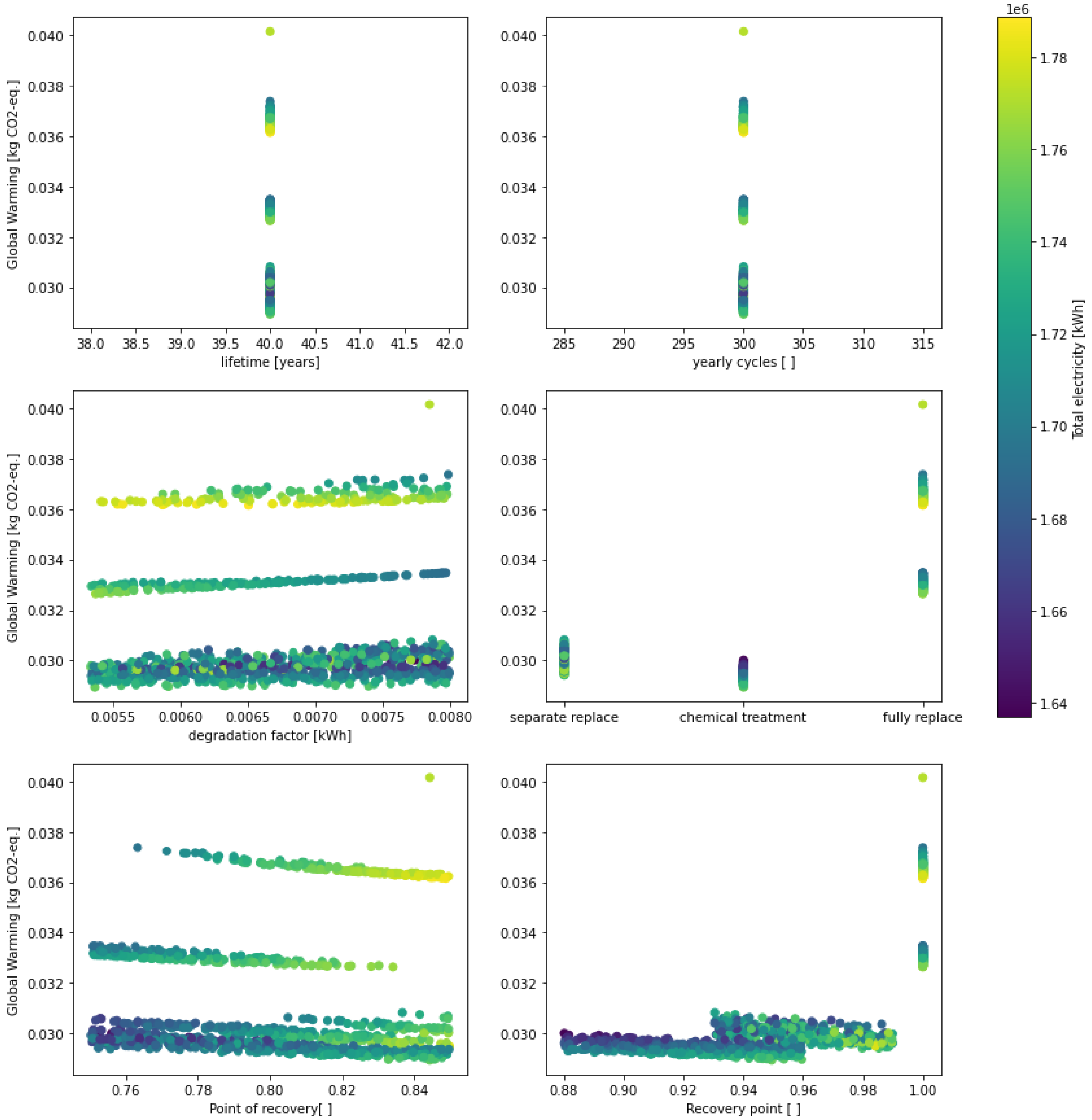


Figure 4.15: Results for maintenance modelling with fixed values.

Now sub-research question four can be answered:

How can maintenance operations improve the environmental performance of the battery
In general, the environmental impact of the battery is lower compared to a battery without maintenance operations. Maintenance can therefore be a good option to further improve the environmental sustainability of the battery. Some limitations of this study however is the large amount of inaccuracy of the input data. For a proper analysis further research needs to be conducted on this aspect.

5

Discussion

5.1. Limitations of the study

In this study the environmental performance of the battery is assessed, compared to LIBs and VRFBs and the effect of maintenance operations is analysed. There are however some limitations because of the lack of data and uncertainty of the LCI inputs of the battery. For the electrolytes the framework from Piccinno et al. [2016] is used. Using the framework a lot of estimations are made for the energy and material consumption to produce the chemicals. There are therefore quite some limitations regarding the LCA results of the electrolytes. Next to that, the production of DHPS is modelled from fossil fuel based hydroquinone. In an ideal scenario the DHPS is produced from lignin. Unfortunately there was no process data available for this. The LCI inputs for the stack are luckily well defined and a proper estimation of the results could be made here. For the storage tanks and BOP this is also true. The biggest current data gap is in the EoL stage of the battery. Unfortunately not a lot of conclusions can be drawn on the EoL stage because of this.

Since the battery is still in development, some of the battery parameters are also quite uncertain. This problem has been tackled by showing how the results of the LCA change when different values are used for these parameters. Next to this, current parameters of the battery are expected to improve and the environmental performance is expected to improve also.

In the comparison of results of the ORFB with the LIB and the VRFB, it is problematic that the LCI inputs of these batteries come from a different study. Several modelling decisions in the LCI model of these batteries could lead to a difference in environmental impact of the batteries. Next to this, the battery specifications of the LIB and VRFB are different compared to the ORFB, which makes a comparison more difficult.

The results for the maintenance model have the largest inaccuracy. This is a results the simplifications in the use phase model and the large uncertainties of the maintenance operations. The main goal of this section is to set up an initial model to show how a combination of use phase modelling with LCA can be very powerful. Further research is needed for a proper estimation on what the best maintenance operation is.

5.2. Future LCAs on batteries

Finally the last sub-research can be answered:

How can the environmental assessment for batteries, energy storage systems and in general be further improved?

From the conducted LCAs a few conclusions can be drawn for further recommendations for the LCA of batteries and for the methodology as a whole. One important aspect is that comparing different Energy Storage Systems is not always easy since the function of different ESSs can vary. Therefore it is important to properly document various key parameters like total capacity, total power, round trip efficiency, DoD, total cycle life and years of operation. As can be seen from the various sensitivity analysis, the effect of these parameters can greatly impact the total results of the LCA.

Because the results of the LCA are so dependent on these parameters, it is recommended to parameterize the LCA model with the key parameters mentioned above. It is furthermore recommended to extend the parameterization of the model to other processes as well (eg. make inflows dependent on efficiency of a process). By doing this a lot of information can be gained via a sensitivity analysis to find out which key parameters are important contributors to the total environmental impacts of the battery.

Parametrization of (key) processes in the LCA model is a practice that is recommended not only in LCA on batteries, but on all LCAs. Parameterizing the LCI inputs has multiple benefits: (1) it gives the LCA practitioner and reader of the LCA a better overview on how certain LCI inputs are calculated. (2) A sensitivity analysis can be conducted on the parameters which can give valuable information on the product system. As already discussed, this can give valuable information for future research strategies for emerging technologies (3) It is easier and more transparent to create future scenarios when parameters are introduced (eg. it is a lot more intuitive to increase the efficiency of a certain process than to change the input/output values of that process). This makes the creating of future scenarios a lot easier. It can furthermore be combined with a Global Sensitivity Analysis to make a better estimation on how probable one technology performs better compared to a different technology. (4) Parametrization gives the option to connect the LCA with "more sophisticated" models via the introduced parameter. LCAs are simplified models that use a linear approach to calculate environmental burdens of a product system. For some cases this is enough to get an "proper estimation" on the environmental impacts of a product system. For some product system, especially for emerging technologies with a lot of uncertainty, this linearization is not a good representation of reality. This linear behaviour can be changed by connecting it with a "more sophisticated" non-linear model (e.g. systems dynamics or agent base model). The results from this combination of modelling can greatly enhance the information gained from the LCA model and thus improve the decision making process. A disadvantage of this method is that it requires more data, it takes more time and increases the modelling knowledge requirements of the researcher.

6

Conclusion and recommendations

In this thesis the environmental impacts of an organic redox flow battery have been researched. There already have been quite a large amount of LCAs on batteries produced. Comparing different results from different studies is however difficult due to different modelling decisions as well as different functions of the battery system. Therefore guidelines from Dieterle et al. [2022] have been followed. In this thesis, a proper specification of the functional unit, a cradle to grave approach as well as a detailed LCI has been conducted.

In the thesis the following main research question was constructed:

What are the environmental impacts of an Organic Redox Flow Battery over its entire life cycle?

From the results of the LCA it can be concluded that the most important aspects for the environmental performance of the Baliht battery are the electricity needed due to inefficiencies in the battery and the production of the battery. In the battery production, the Battery stack and the inverter have the highest impact in most of the impact categories. a large contributor in most impact categories is the production chain of copper for the current collector and inverter. Creating options to reuse the copper or the battery stack/inverter can be good strategies to reduce the environmental impact of the battery. A strategy to decrease the environmental impacts of the battery is to increase the total amount of electricity the battery returns to the grid over its entire life cycle. This can be done by increasing the total amount of cycles or increasing the total capacity of the battery. The environmental impact of the battery can be reduced significantly if the round trip efficiency is increased from 65% to 80%. This can lead to environmental impact reduction of up to 53% depending on the impact category. Another focus points for the battery development should therefore be to increase the total round trip efficiency of the battery. Due to this low round trip efficiency it is also important to connect the battery with electricity from sustainable energy sources. Connecting it to the current energy grid results in a massive increase of environmental burdens.

Compared to similar type of batteries, the ORFB scores really well in all impact categories. A main reason for this is the relatively low environmental impacts of the storage materials (electrolytes) compared to the LIB and the VRFB. These other types of batteries have large environmental impacts related to the mining operations and the further treatment of the associated minerals. These mining operations are not needed for the production of the electrolytes of the ORFB.

The base LCA model has been further developed and connected with a simplified use phase model to analyse the effect of maintenance procedures on the environmental performance of the ORFB. Three different maintenance procedures have been identified for the electrolytes: 1)fully replace the electrolyte, 2)separate inert active material and replace it with new active material and 3) separate inert active material and chemically reactivate it. In this section a probabilistic approach was taken in order to identify which maintenance procedure showed the best environmental results and to find out which parameters are most important. From the results it is concluded that the impact on global warming can be reduced if maintenance operations are conducted on the battery. From the three different maintenance operations, (3) chemical reactivation of inert material shows the most promising results. In order to make a better conclusion on this, more research is needed however.

6.1. Future research

There are still a lot of uncertainties in regard to the use phase model and the maintenance procedure. Further analysis on the important battery specification have to be conducted in order to get a better insight of how battery maintenance can impact the total results. Next to that the End of Life strategy has to be further improved in order to get a better insight in the environmental performance of the battery.

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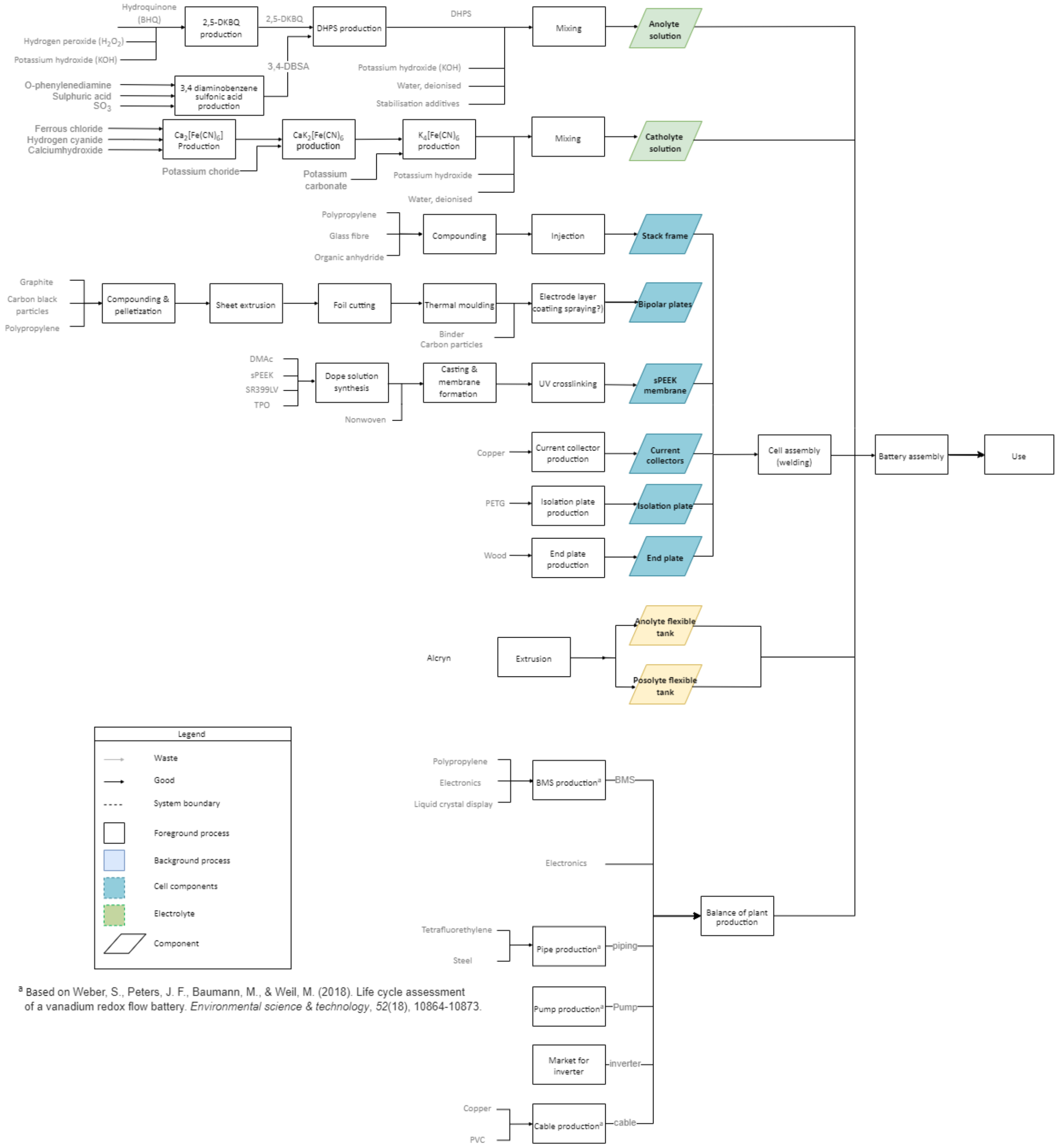
A

LCI of the ORFB

In this chapter of the appendix, the LCI inputs for the different processes have been presented starting with the production phase, then the use phase and in the end the EoL phase.

A.1. Production phase



[a] Based on Weber, S., Peters, J. F., Baumann, M., & Weil, M. (2018). Life cycle assessment of a vanadium redox flow battery. *Environmental science & technology*, 52(18), 10864-10873.

Figure A.1: Flowchart for the production of the battery. (nicer flowchart will be added later)

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A.2. Electrolytes

In the following tables the LCI inputs for the production of the electrolytes are given. First the production route of the active material is given and afterwards the final mixing of the components of the final posolyte is given. After that the LCI for the production of the negolyte is given. First the production of the DHPS and in the end the final mixing of the negolyte solution.

A.2.1. Posolyte:

Table A.1: LCI for the production of $Ca_2[Fe(CN)_6] \cdot 12\,H_2O$

Flow	amount	unit
Inputs		
chemical factory, organics	4E-10	unit
heat, district or industrial, natural gas	0,216	megajoule
hydrogen cyanide	0,326	kg
iron(II) chloride	0,177	kg
lime, hydrated, loose weight	0,47	kg
water, deionised	0,6	kg
electricity, low voltage	0,00023	kilowatt hour
Outflows		
$Ca_2[Fe(CN)_6] \cdot 12\,H_2O$	1	kg

Table A.2: LCI for the production of $CaK_2[Fe(CN)_6]$

Flow	amount	unit
Inputs		
Ca[Fe(CN)6_12H2O	1,539	kg
chemical factory, organics	4E-10	unit
heat, district or industrial, natural gas	0,78	megajoule
potassium chloride	0,4515	kg
water, deionised	0,6	kg
electricity, low voltage	0,0002	kilowatt hour
Outflows		
$CaK_2[Fe(CN)_6]$	1	kg

Table A.3: LCI for the production of $K_4[Fe(CN)_6] \cdot 3\,H_2O$

Flow	amount	unit
Inputs		
CaK2[Fe(CN)6	0,781802	kg
chemical factory, organics	4E-10	unit
heat, district or industrial, natural gas	0,78	megajoule
potassium carbonate	0,3272	kg
water, deionised	0,6	kg
electricity, low voltage	0,000237	kilowatt hour
Outflows		
$K_4[Fe(CN)_6] \cdot 3\,H_2O$	1	kg

Table A.4: LCI for the production of the final posolyte solution

Flow	**amount**	**unit**
Inputs		
K4[Fe(CN)6]_x_3H2O	0,211	kg
potassium sulfate	0,001	kg
sodium hydroxide, without water, in 50% solution state	0,005611	kg
sodium sulfate, anhydrite	0,001	kg
sulfuric acid	0,001	kg
water, deionised	0,913	kg
electricity, low voltage	1	kilowatt hour
potassium hydroxide	0,005611	kg
Outflows		
posolyte solution	1,138222	kg

A.2.2. Negolyte

Table A.5: LCI for the production of $C_6K_2H_2O_4$

Flow	amount	unit
Inputs		
chemical factory, organics	4E-10	unit
hydroquinone	0,766	kg
heat, district or industrial, natural gas	0,1162	megajoule
hydrogen peroxide, without water, in 50% solution state	0,71	kg
water, deionised	0,32	kg
electricity, low voltage	0,0107	kilowatt hour
Outflows		
$C_6K_2H_2O_4$	1	kg
hazardous waste, for incineration	0,3889	kg

Table A.6: LCI for the production of 3,4-diaminobenzene sulfonic acid

Flow	amount	unit
Inputs		
chemical factory, organics	4E-10	unit
heat, district or industrial, natural gas	0,984	megajoule
ortho-phenylene diamine	1,01937	kg
sulfur trioxide	0,0017	kg
sulfuric acid	1,684	kg
water, deionised	1,076	kg
electricity, low voltage	0,0971	kilowatt hour
Outflows		
3,4-diaminobenzene sulfonic acid	1	kg
hazardous waste, for incineration	2,767	kg

Table A.7: LCI for the production of DHPS

Flow	amount	unit
Inputs		
C6K2H2O4	0,8804	kg
3,4-diaminobenzene sulfonic acid	0,7662	kg
chemical factory, organics	4E-10	unit
acetone, liquid	2,135	kg
heat, district or industrial, natural gas	4,51	megajoule
water, deionised	2,723	kg
electricity, low voltage	0,0173	kilowatt hour
Outflows		
DHPS	1	kg
hazardous waste, for incineration	5,065	kg

Table A.8: LCI for the production of final negolyte solution

Flow	**amount**	**unit**
Inputs		
DHPS	0,146	kg
potassium sulfate	0,001	kg
sodium hydroxide, without water, in 50% solution state	0,0056	kg
sodium sulfate, anhydrite	0,001	kg
sulfuric acid	0,001	kg
water, deionised	0,978	kg
potassium hydroxide	0,0056	kg
Outflows		
Final negolyte solution	1,1382	kg
hazardous waste, for incineration	5,065	kg

A.3. Stack production

A.3.1. Frame production

The stack is shielded by a stack frame made out of polypropylene and glass fibers. The LCI of the frame can be subdivided into two processes: 1) the production of the compound and 2) the injection moulding for either the frame for the bipolar plate or the membrane. In a later step these frames get attached to the bipolar plates or the membranes and afterwards they're attached together to form the cell stack.

Table A.9: LCI for the production of the polypropylene based compound for the frames

Flow	**amount**	**unit**
Inputs		
acetic anhydride	0,02	kg
glass fibre	0,1	kg
polypropylene, granulate	0,88	kg
tap water	0,001	kg
electricity, medium voltage	0,6	kilowatt hour
Outflows		
polypropylene based compound ready for injection	1	kg

Table A.10: LCI for the production of the frame for the bipolar plates

Flow	**amount**	**unit**
Inputs		
polypropylene based compound ready for injection	0,46	kg
injection moulding	0,46	kg
Outflows		
Cell frame for bipolar plate	1	unit

Table A.11: LCI for the production of the frame for the membranes

Flow	**amount**	**unit**
Inputs		
polypropylene based compound ready for injection	0,0000038	kg
injection moulding	0,0000038	kg
Outflows		
Cell frame for membrane	1	unit

A.3.2. Production of bipolar plate

The production of the bipolar plate consists of four steps. The first step is the production of the compound for the bipolar plate. After the compound production, the material goes through an extrusion process. In a next step the bipolar plate is cut to get the right dimensions, and afterwards an embossing process is implemented to produce the bipolar plate. In a last step the bipolar plate is sprayed with a small electrode layer. The inputs for the production of 1 bipolar plate can be found in tables the tables below. During the extrusion, cutting and embossing process there are no losses.

Table A.12: LCI for the production of the compound for the bipolar plates

Flow	**amount**	**unit**
Inputs		
heat, district or industrial, natural gas	1,62	megajoule
carbon black	0,07	kg
electricity, low voltage	1,32	kilowatt hour
graphite, battery grade	0,73	kg
phenolic resin	0,12	kg
polypropylene, granulate	0,08	kg
Outflows		
bipolar plates compound	1	kg

Table A.13: LCI for the sheet extrusion of the bipolar plates

Flow	**amount**	**unit**
Inputs		
electrode compound	1	kg
electricity, medium voltage	0,683974	kilowatt hour
Outflows		
foil for bipolar plate	1	kg

Table A.14: LCI for the cutting of the bipolar plates. No info on energy consumption available. All foil can be used in the cutting process, thus no waste.

Flow	**amount**	**unit**
Inputs		
foil for bipolar plate	1	kg
Outflows		
Cutted Foil for bipolar plate	1	kg

Table A.15: LCI for the embossing of the bipolar plates

Flow	**amount**	**unit**
Inputs		
Cutted Foil for bipolar plate	0,5	kg
electricity, low voltage	2,75	kilowatt hour
Outflows		
structured bipolar plate	1	unit

Table A.16: LCI for the production of the spray paint for the electrode layer

Flow	**amount**	**unit**
Inputs		
N-methyl-2-pyrrolidone	0,96	kg
carbon black	0,02	kg
tetrafluoroethylene	0,02	kg
Outflows		
Electrode spraying paint	1	kg

Table A.17: LCI for applying the spray paint to the bipolar plate and producing final bipolar plate with electrode layer.

Flow	**amount**	**unit**
Inputs		
structured bipolar plate	1	unit
Electrode spraying paint	0,12	kg
Outflows		
Structured bipolar plate with electrode layer	1	unit

A.4. Production of Membrane

Table A.18: LCI for the production of the sPEEK thin film.

Flow	amount	unit
Inputs		
aniline	0,7	kg
formaldehyde	0,11	kg
heat, district or industrial, natural gas	3,38	megajoule
hydrogen fluoride	0,71	kg
hydroquinone	0,32	kg
injection moulding	1	kg
soda ash, dense	0,31	kg
sodium nitrite	1,4	kg
sulfuric acid	0,2	kg
transport, freight train	0,75	ton kilometer
transport, freight, lorry, unspecified	0,37	ton kilometer
water, deionised	4,17	kg
Outflows		
sPEEK membrane film	1	kg
Environmental outflows	0,2	kg
Carbon dioxide, fossil	0,36	kg
Dinitrogen monoxide	0,61	kg
Fluoride	0,39	kg
Sodium, ion	0,00537	cubic meter
Water		

Table A.19: LCI of the sPEEK membrane.

Flow	amount	unit
Inputs		
sPEEK membrane film	0,01	kg
Outflows		
sPEEK Membrane for ORFB	1	unit

A.5. Current collector

Table A.20: LCI for the production of the current collector

Flow	amount	unit
Inputs		
copper collector foil, for Li-ion battery	2,7	kg
Outflows		
Current collector	1	unit

A.6. Isolation plate

Table A.21: LCI for the production of the isolation plate

Flow	amount	unit
Inputs		
extrusion, plastic film	2,7	kg
polyethylene terephthalate, granulate, amorphous	0,4	kg
Outflows		
Current collector	1	unit

A.7. End Plate

Table A.22: LCI for the production of the endplate

Flow	amount	unit
Inputs		
sawnwood, hardwood, dried (u=20%), planed	0,012176	cubic meter
Outflows		
End plate	1	unit

A.8. Final stack assembly

In the last step the individual components of the stack are attached together to form the battery stack. In a first step the stack frame are attached to the bipolar plates and membranes and next all components are attached together.

Table A.23: LCI for the attachment of the stack frame to the bipolar plates

Flow	**amount**	**unit**
Inputs		
Cell frame	1,03	unit
Structured bipolar plate with electrode layer	1,03	unit
9.1.2 Frame EoL treatment	0,03	unit
9.1.3 Bipolar plate EoL treatment	0,03	unit
electricity, low voltage	0,196	kilowatt hour
Outflows		
Frame attached to bipolar plate	1	unit

Table A.24: LCI for the attachment of the stack frame to the membranes

Flow	**amount**	**unit**
Inputs		
Cell frame for membrane	1,03	unit
sPEEK Membrane for ORFB		unit
9.1.2 Frame EoL treatment	0,03	unit
9.1.4 membrane EOL treatment	0,03	unit
electricity, low voltage	0,196	kilowatt hour
Outflows		
Frame attached to membrane	1	unit

Table A.25: LCI for the production of the battery stack

Flow	**amount**	**unit**
Inputs		
Current collector	2,06	unit
End plate	2,06	unit
Isolation plate	2,06	unit
Frame attached to bipolar plate	51	unit
Frame attached to membrane	50	unit
9.1.5 Current collector EoL treatment	0,06	unit
End plate EoL treatment	0,06	unit
9.1.6 Isolation plate EoL treatment	0,06	unit
electricity, low voltage	10	kilowatt hour
Outflows		
Battery Stack	1	unit

A.9. Storage tanks

Table A.26: LCI for the production of the negolyte tank

Flow	**amount**	**unit**
Inputs		
extrusion, plastic film	1,0645	kg
polyethylene terephthalate, granulate, amorphous	1,0645	kg
Outflows		
Negolyte tank	1	kg

Table A.27: LCI for the production of the posolyte tank

Flow	**amount**	**unit**
Inputs		
extrusion, plastic film	1,4182	kg
polyethylene terephthalate, granulate, amorphous	1,4182	kg
Outflows		
Posolyte tank	1	kg

A.10. Balance of Plant

Table A.28: LCI for the production of the BoP

Flow	**amount**	**unit**
Inputs		
piping	75	m
market for pump, 40W	24	unit
Battery management system	1	unit
inverter, 500kW	0,2	unit
electronics, for control units	13	kg
Outflows		
Balance of plant	1	unit

Table A.29: LCI for the production of 1 meter of piping

Flow	**amount**	**unit**
Inputs		
extrusion, plastic pipes	0,11	kg
market for polyvinylchloride, suspension polymerised	0,11	kg
Outflows		
piping	1	m

A.11. Final battery production

Table A.30: LCI for the final assembly of the battery

Flow	amount	unit
Inputs		
posolyte solution	1725	kg
Final negolyte solution	862,5	kg
coated Negolyte tank	12	unit
Coated posolyte tank	12	unit
5.1.1 Balance of plant	1	unit
Battery Stack	12	unit
transport, freight, lorry 16-32 metric ton, EURO6	32952	ton kilometer
transport, freight, sea, container ship	6753,6	ton kilometer
Outflows		
Battery	1	unit

A.12. Use phase of battery

Table A.31: LCI for the battery use phase

Flow	amount	unit
Inputs		
Electricity, PV, at 570 kWp open ground, multi-Si	0,538461538	kWh
Battery in port of Ibiza	5,55556E-07	unit
End of life battery	5,55556E-07	unit
Outflows		
Electricity delivered back to grid (FU)	1	kWh

A.13. End of Life

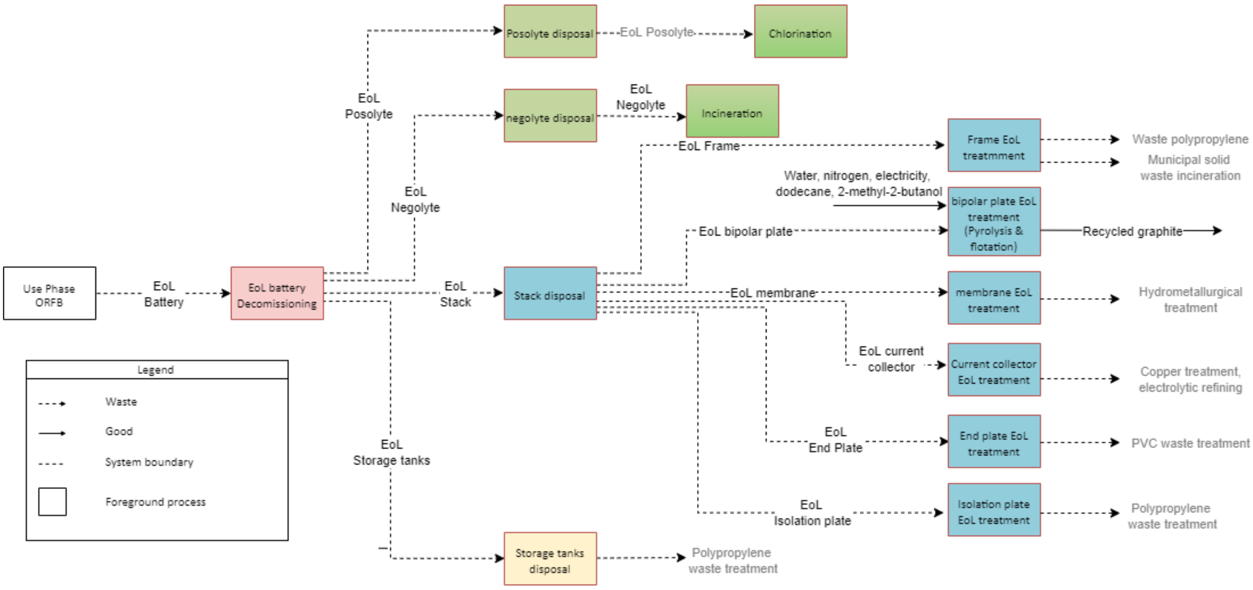

Figure A.2: Flowchart for the EoL phase of the battery. (nicer flowchart will be added later)

Table A.32: LCI for the battery disassembly

Flow	amount	unit
Inputs		
end of life battery	1	unit
Outflows		
End of life battery stack	12	unit
Posolyte waste	1725	kg
Negolyte waste	862,5	kg
End of life negolyte storage tanks	12	unit
End of life storage tank	12	unit

A.14. Posolyte EoL

Table A.33: LCI for the treatment of the posolyte solution

Flow	**amount**	**unit**
Inputs		
Posolyte waste	1,1382	kg
Outflows		
$K_4[Fe(CN)_6]$ for chlorination treatment	0,211	kg
Environmental outflows		
Hydroxide	0,004087	kg
Potassium, ion	0,07812	kg
Potassium, ion	0,005813	kg
Sodium, ion	0,00341	kg
Sulfate	0,001518	kg
Water	0,000913	cubic meter

Table A.34: LCI for the treatment of $K_4[Fe(CN)_6]$. Inputs calculated via stochiometric calculations.

Flow	**amount**	**unit**
Inputs		
$K_4[Fe(CN)_6]$ for chlorination treatment	1	kg
chlorine, gaseous	1,007215	kg
water, deionised	0,255902	kg
Environmental outflows		
Chloride, ion	1,007215	kg
Iron, ion	0,1322	kg
Potassium, ion	0,370259	kg
Thiocyanate, ion	0,59684	kg

A.15. Negolyte EoL

Table A.35: LCI for the treatment of the negolyte.

Flow	amount	unit
Inputs		
Negolyte waste	1,1382	kg
Outflows		
DHPS into combustion	0,146	kg
Environmental outflows		
Hydroxide	0,004078	kg
Potassium, ion	0,004352	kg
Sodium, ion	0,003543	kg
Sulfate	0,001228	kg
Sulfuric acid	0,001	kg
Water	0,000978	cubic meter

Table A.36: LCI for the incineration of waste DHPS.

Flow	amount	unit
Inputs		
DHPS into combustion	1	kg
Oxygen	1,36853	kg
Outflows		
heat, district or industrial, natural gas	15,323	MJ
Environmental outflows		
Carbon dioxide, fossil	0,004078	kg
Nitrogen	0,004352	kg
Oxygen	0,003543	kg
Sulfur dioxide	0,001228	kg
Water	0,001	kg

A.16. Battery stack EoL

Table A.37: LCI inputs for the EoL of the battery stack

Flow	**amount**	**unit**
Inputs		
End of life battery stack	1	unit
Outflows		
Frame EoL treatment	108	unit
Bipolar plate EoL treatment	55	unit
Membrane EOL treatment	54	unit
Current collector EoL treatment	2	unit
End plate EoL treatment	2	unit
Isolation plate EoL treatment	2	unit

Table A.38: LCI inputs for the EoL of the battery stack frames

Flow	**amount**	**unit**
Inputs		
Frame EoL treatment	1	unit
Outflows		
municipal solid waste	0,004381023	kg
waste polypropylene	0,405	kg

Table A.39: LCI inputs for the EoL of the bipolar plates, only the graphene in the bipolar plate has been accounted for.

Flow	**amount**	**unit**
Inputs		
Bipolar plate EoL treatment	1	unit
Outflows		
Graphene treatment, pyrolysis + flotation	0,365	kg

Table A.40: LCI inputs for the EoL of the treatment of graphene via flotation and pyrolysis

Flow	**amount**	**unit**
Inputs		
Graphene from bipolar plate	100	kg
2-methyl-2-butanol	13,2	kg
kerosene	26,4	kg
nitrogen, liquid	8,318	kg
water, deionised	2,2	kg
electricity, low voltage	102,95	kilowatt hour
Outflows		
Treated graphene	100	kg
Environmental outflows		
Nitrogen	12,848	kg
Water	2,2	cubic meter

Table A.41: LCI inputs for the EoL of the membranes

Flow	**amount**	**unit**
Inputs		
Membrane EoL	1	unit
Outflows		
treatment of waste polyethylene terephthalate, municipal incineration	0,01	kg

Table A.42: LCI inputs for the EoL of the current collectors

Flow	**amount**	**unit**
Inputs		
EoL current collector	1	unit
Outflows		
market for scrap copper	2,7	kg

Table A.43: LCI inputs for the EoL of the isolation plates

Flow	**amount**	**unit**
Inputs		
EoL Isolation plate	1	unit
Outflows		
treatment of waste polyethylene terephthalate, municipal incineration	0,4	kg

Table A.44: LCI inputs for the EoL of the endplates

Flow	**amount**	**unit**
Inputs		
EoL End plate	1	unit
Outflows		
market for waste wood, untreated	7,5	kg

A.17. Storage tanks EoL

Table A.45: LCI inputs for the EoL of the negolyte storage tanks

Flow	**amount**	**unit**
Inputs		
End of life negolyte storage tanks	1	unit
Outflows		
treatment of waste polyethylene terephthalate, municipal incineration	1,0645	kg

Table A.46: LCI inputs for the EoL of the posolyte storage tanks

Flow	**amount**	**unit**
Inputs		
End of life negolyte storage tanks	1	unit
Outflows		
treatment of waste polyethylene terephthalate, municipal incineration	1,41822	kg

A.18. LCI flows maintenance procedures

A.18.1. Posolyte

Table A.47: LCI inputs for the fully replace treatment of the posolyte.

Flow	**amount**	**unit**
Inputs		
posolyte solution	1725	kg
electricity, low voltage	0,0527	kilowatt hour
Outflows		
Fully replace treatment posolyte	1	unit
Posolyte waste	1725	kg

Table A.48: LCI inputs for the separate and replace treatment of the posolyte.

Flow	**amount**	**unit**	**Formula**
Inputs			
K4[Fe(CN)6	73,338	kg	(1-Maintenace_point)*366.69
electricity, low voltage	0,0527	kilowatt hour	
electricity, low voltage	0,73338	kilowatt hour	(1-Maintenance_point)*366.69*0.01
Outflows			
Separate replace treatment posolyte	1	unit	
Posolyte waste	73,338	kg	(1-Maintenance_point)*366.69

Table A.49: LCI inputs for the chemical treatment of the posolyte.

Flow	amount	unit	Formula
Inputs			
electricity, low voltage	kilowatt hour	unit	
electricity, low voltage	kilowatt hour	kilowatt hour	(1-Maintenance_point)*366.69*0.01
electricity, low voltage	kilowatt hour	kilowatt hour	
hydrogen cyanide	kilogram	kg	(1-Maintenance_point)*140.85
Outflows			
Chemical treatment posolyte	1	unit	

A.18.2. Negolyte maintenance

Table A.50: LCI inputs for the fully replacement treatment of the negolyte.

Flow	amount	unit
Inputs		
Final negolyte solution	862,5	kg
electricity, low voltage	0,0264	kilowatt hour
Outflows		
Fully replace treatment negolyte	1	unit
Negolyte waste	862,5	kg

Table A.51: LCI inputs for the separate replacement treatment of the negolyte.

Flow	amount	unit	Formula
Inputs			
DHPS	22,128	kg	(1-Maintenace_point)*110.64
electricity, low voltage	0,0264	kilowatt hour	
electricity, low voltage	0,22128	kilowatt hour	(1-Maintenance_point)*110.64*0.01
Outflows			
Separate replace treatment negolyte	1	unit	
DHPS combustion	22,128	kg	(1-Maintenance_point)*110.64

Table A.52: LCI inputs for the chemical treatment of the negolyte.

Flow	amount	unit	Formula
Inputs			
chemical factory	4E-10	kilogram	
electricity, low voltage	0,0264	kilowatt hour	
electricity, low voltage	0,22128	kilowatt hour	(1-Maintenance_point)*110.64*0.01
electricity, low voltage	1,38	kilowatt hour	
oxygen, liquid	2,422	kilogram	(1-Maintenance_point)*12.11
Outflows			
Chemical treatment negolyte	1	unit	

B

Appendix: Results

B.1. Contributors Battery production

Table B.1: Overview of most contributing factors for the battery stack, electrolytes and BoP.

Impact category/Battery component	**Battery stack**	**Posolyte**	**Negolyte**	**BoP**
Climate Change	Bipolar plate	HCN production Electricity for potassium ferrocyanide production	Hazardous waste incineration Ortho phenylenediamine production	Inverter production
Acidification	Copper for current collector	Electricity for potassium ferrocyanide production HCN production Potassium carbonate production	Ortho phenylenediamine production	Copper for inverter
Ecotoxicity	Copper for current collector	Potassium carbonate production Potassium chlorite production	Ortho phenylenediamine production Hazardous waste incineration	Copper for inverter
Freshwater Eutrophication	Copper for current collector Electricity for bipolar plate	Electricity for potassium ferrocyanide production	Hazardous waste incineration Ortho phenylenediamine production	Copper for inverter
Marine Eutrophication	Bipolar plate Copper for current collector	HCN production Electricity for potassium ferrocyanide production	Ortho phenylenediamine production	Copper for inverter LCD screen for BMS
Terrestrial Eutrophication	Bipolar plate Copper for current collector	HCN production Electricity for potassium ferrocyanide production	Ortho phenylenediamine production	Copper for inverter
Human toxicity carcinogenic	Coking for production of graphite in bipolar plate	Steel for chemical factory Electricity for potassium ferrocyanide production	Benzene chlorination for ortho phenylenediamine production	Steel and copper for inverter
Human toxicity non-carcinogenic	Copper for current collector	Electricity for potassium ferrocyanide production Potassium carbonate production	Ortho-phenylenediamine production	Copper for inverter
Particulate matter formation	Bipolar plate production Copper for current collector	Electricity for potassium ferrocyanide production HCN production Potassium carbonate production	Ortho phenylenediamine production Acetone production	Copper for inverter
Ozone depletion potential	Tetrafluorethyle for spraying	Electricity for potassium ferrocyanide production Potassium carbonate production Potassium chlorite production Lime production HCN production	2-nitroaline in ortho phenylenediamine production chain	Inverter production
Ionising radiation	Nuclear energy in electricity mixes	Nuclear energy in electricity mixes	Nuclear energy in electricity mixes	Nuclear energy in electricity mixes
Non renewable energy resources	Coal for electricity Polypropylene for frame	Electricity for potassium ferrocyanide production HCN production	Ortho phenylenediamine production Acetone production	Inverter production
Land use	Wood for endplate (forest)	Electricity for potassium ferrocyanide production Potassium carbonate production Potassium chlorite production	Ortho phenylenediamine production Hazardous waste incineration	Inverter production
Materials metals/minerals	Copper for current collector	Materials for chemical factory	Materials for chemical factory	Copper for inverter
Water usage	N-methyl-2-pyrrolidone for electrode spray	Electricity for potassium ferrocyanide production HCN production Potassium chlorite production	Ortho phenylenediamine production Hydrogen peroxide production Acetone production	Inverter production