MODELLING AND DESIGN OF STRUCUTRAL BATTERIES WITH LIFE CYCLE ASSESSMENT

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ABSTRACT

A multifunctional structural battery consisting of carbon fibers, lithium-electrode coatings and a structural battery electrolyte is investigated with an analytical bottom-up model. This model has a multiphysics approach, calculating both mechanical properties and electrical energy storage. The intention of the model is twofold; first, calculating the potential mass saving with using a structural battery instead of the combination of a monofunctional carbon fiber composite and a monofunctional lithium ion battery. Second, the model is used to investigate the behavior of the mass saving due to changing variables of the structural battery. This variable sensitivity analysis is made in order to understand the behavior of the structural battery and its sensitivity to the different construction variables. The results show that the structural battery can save up to 26% of mass compared to the monofunctional parts.

Next, the model of the structural battery is further utilized in a life cycle assessment, where the manufacturing, usage and recycling of the structural battery is investigated. The life cycle assessment examines the structural battery as the roof of an electric vehicle. This analysis is compared to the same assessment for a steel roof and standard lithium ion batteries, which shows that manufacturing the carbon fibers and structural battery with clean energy is most important for decreasing the emissions from manufacturing.

INTRODUCTION

Composite materials are a well-known solution to make lightweight and high-performance structures for the transport industry. But within electrification of vehicles composite materials will not be enough to reach a low enough total mass of the vehicle. This is due to the significant mass that is required for electrical energy storage. The mass of the structure and the mass of the energy storage are the largest contributors to the total mass of the vehicle.

One route to decrease the mass of an electric vehicle is to join these two functionalities, energy storage and structure, into one. This can be done by creating a material that is simultaneously performing both functions. This material is then referred to as a multifunctional material, and for the specific functions of structure and energy storage; a structural battery (SB).

Such SBs can be achieved by combining the technologies from composite materials with lithium ion batteries (LiBs). Carbon fibers are well known to be lightweight with high strength and stiffness. Furthermore, it is also known that carbon fibers intercalate lithium ions [1]. This lithium ion intercalation is a requirement for carbon fibers to be possible to use as a negative electrode in LiBs. Secondly, there needs to be a positive electrode. The positive electrode is made from an active material, e.g. $LiFePO_4$. This material is coated onto carbon fibers, where the carbon fibers act as reinforcement for the structure and as current collectors for the battery function [2]. Lastly, the lithium ions need to be transported between the electrodes to charge and discharge the battery. This is commonly made with liquid electrolytes. However, for this material to have any structural use, the fibers need to be included in a solid matrix material. These opposite properties are facilitated by a new structural battery electrolyte (SBE) [3], [4]. This SBE is a bi-continuous and phase-separated network of a structural polymer backbone percolated with a liquid electrolyte. Figure 1 shows the construction and buildup of such structural battery.

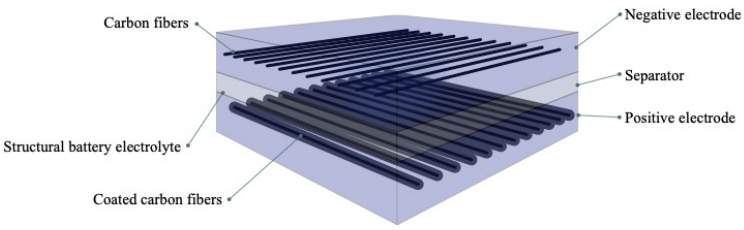

Figure 1: Schematic showing the basic construction of a structural battery cell.

To further understand, predict and design the properties of an SB, a modelling-analysis has been made. This model is made from an analytical bottom-up approach, analyzing all ingoing materials and parts from both a structural and electrochemical point of view. The comparison of a SB versus a conventional structure is made such that a plate of the SB has the same bending stiffness as a plate of conventional construction material. The mass of these are then known and they perform the same mechanical function. Additionally, the SB is storing electrical energy. This is then matched with a standard LiB such that both the SB and the LiB is storing the same amount of energy. Since mass saving is desired, the aim is for this SB to have a lower mass than the combined mass of the conventional structure and the standard LiB.

This model is then utilized to adjust design variables and study their effect on the mass saving of the SB. The desired outcome is to find which variables are the most important for making a high-performing SB and predict possible future mechanical and electrochemical properties of the SB. Furthermore, this model is used to make a life cycle assessment (LCA) for the use of SBs in an electric vehicle. All ingoing materials and processes are analyzed from a life cycle point of view, with regards to energy and materials consumed in the production phase, the usage phase and the recycling phase.

1 METHOD

The method consists of modelling two different competing systems. The first is a system containing monofunctional parts; one part that carries the load, i.e. a conventional composite structure, and another part that stores electrical energy, i.e. standard lithium ion battery. These monofunctional systems are separate and has their discrete masses. Both the monofunctional systems are then considered to be replaced by a single system, which is a multifunctional material that simultaneously can carry mechanical load and store electrical energy, see Figure 2. This multifunctional material is referred to as a structural battery and has its separate mass. The aim is for the multifunctional system to have a lower mass than the sum of the monofunctional systems as:

$$m_{SB} < m_{LiB} + m_{comp} \tag{1}$$

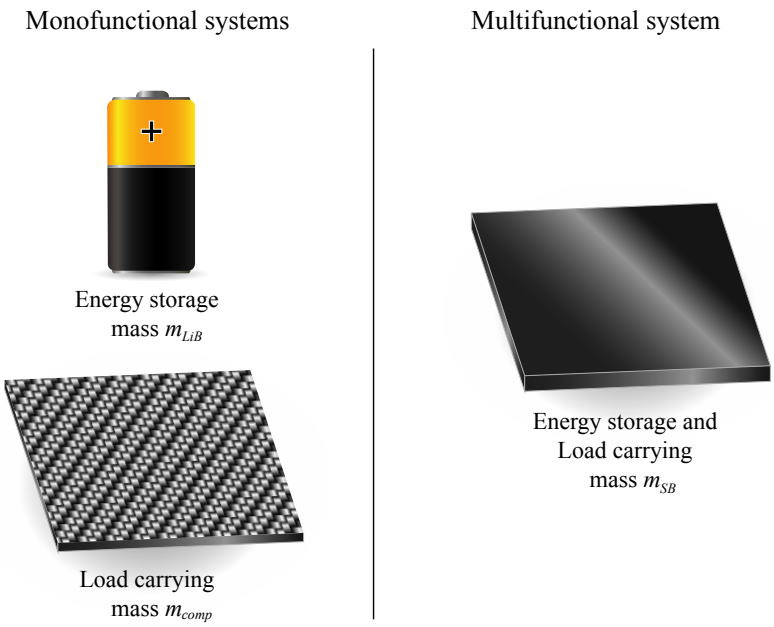

Figure 2: The monofunctional systems and multifunctional system it is compared to.

For this mass comparison to be fair, it naturally comes with some further constraints; namely that the total energy storage in the lithium ion battery is the same as the total energy storage in the structural battery and that the conventional composite structure and the structural battery perform the same mechanical function.

The energy in a battery is commonly measured in watt hours (Wh*)* and a state-of the-art lithium ion battery today has a cell-level energy density between 100–265 Wh/kg, in this work 175 Wh/kg is chosen as the energy density for the reference battery. The mass of lithium ion battery is then given from its energy density and matched to the total energy available in the multifunctional structural battery. For the mechanical part, it requires a little bit more consideration. There are many different metrics for a composite plate, in-plane stiffnesses, bending stiffnesses, shear properties, buckling behavior, vibrational behavior etc. For ease of calculations, one single metric is chosen, but any can be used in similar calculations, depending on the most crucial load case. The global plate bending stiffness, due to a uniform pressure P with simply supported boundary conditions is chosen herein, see Figure 3. There are some benefits with this; first is that it produces a single, well defined and simple metric for its stiffness, namely the midpoint deflection. Secondly, all calculations for this number are possible to calculate analytically. The plate has the width (w) 1 m and length (L) 1 m. Since the interest in this paper is to compare the monofunctional composite structure with the multifunctional structural battery, the distributed pressure is set to unity (1 N/m^2).

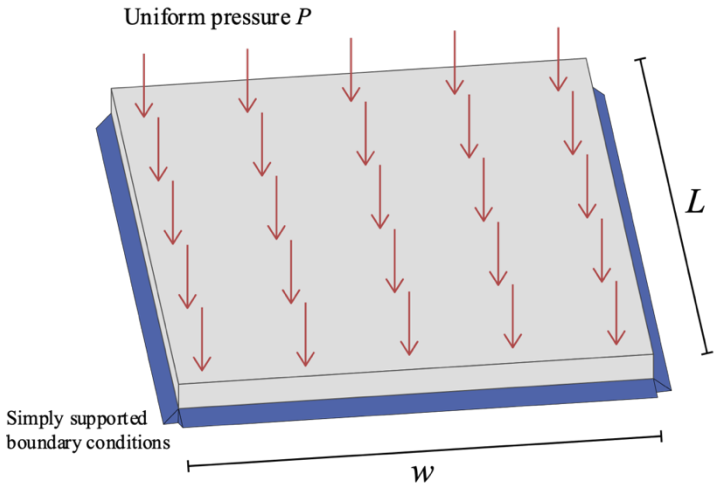

Figure 3: Load case is a uniform pressure on the plate with simply supported boundary conditions, the plate has the dimensions *w* and *L*.

Furthermore, the composite layup, fibers, matrix and manufacturing process all also has a great effect on the mechanical properties of the plate. The monofunctional composite structure is chosen as an aircraft-grade UD carbon fiber and epoxy system, with the lamina properties given in Table 1. The layup of both the monofunctional composite structure and the structural battery is chosen to a quasi-isotropic layup with symmetric and balanced 0°, 90°, 45° and -45° layers. The ply thickness of the monofunctional composite structure is chosen so that the midpoint deflection of the monofunctional plate is exactly the same as the multifunctional structural battery.

Table 1: Material properties of the monofunctional carbon fiber composite lamina.

Property	Value
E_1	147 GPa
E_2	9 GPa
G_{12}	3.3 GPa
ν_{12}	0.31
ρ	1610 kg/m^3

1.1 Construction and model of the structural battery

The model for the structural battery is a multi-physics analytical model, where all internal parameters for the structural battery design and construction are adjustable. This model calculates the mass of the structural battery, the energy content, and the midpoint deflection of the structural battery. All of these values are parametric and investigated with regards to different variables. Some of the most important variables are chosen to be separately investigated. Each of these variables for the structural battery is independently investigated in a sensitivity analysis, with regards to their contribution to the mass saving of using a multifunctional structural battery instead of monofunctional lithium ion battery and conventional composite structure. The value of the variable which maximize the mass saving of the structural battery is chosen as the constructing value in this analysis. Understandably, all variables are limited to what is practically achievable and manufacturable.

Figure 4 shows one unit-cell of the structural battery. It contains a negative electrode with carbon fibers impregnated with SBE, in the negative electrode the carbon fibers are both current collectors and the active electrode material by intercalation of lithium ions into the graphitic structure of the fiber [1], [5]. The variables for the negative electrode are the volume fraction of fibers in the electrode as well as the amount of fibers (ply area density). The positive electrode contains the same carbon fibers

and the same amount of fibers. In this case the carbon fibers are current collectors for the electrode and are coated with a positive electrode material ($LiFePO_4$), as well as binder and carbon black [2]. The volume fraction of fiber in the positive electrode is its only variable. The separator is modelled as a layer with the properties of the SBE, the addition of a separating cloth is not considered to add any stiffness. For the separator, its thickness is a variable. Furthermore, the SBE has two important properties; ion conduction and load carrying (elastic modulus), both of these metrics are also variables in this analysis. The analysis in this paper is made for a fixed charge and discharge time of 10 hours.

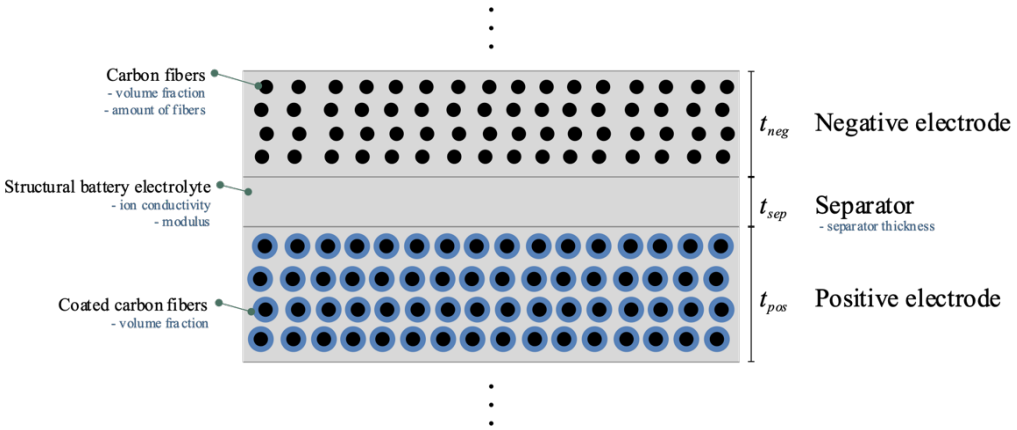

Figure 4: Internal structure of a unit-cell of structural battery. It consists of one layer of negative electrode, containing carbon fibers and SBE electrolyte/matrix. The positive electrode contains the same amount of carbon fibers with the same SBE, the fibers in the positive electrode are also coated with positive electrode active material. The two electrodes are separated by a separator made from randomly oriented glass fibers. The metrics that are considered variables in this analysis are marked.

1.2 Life cycle assessment

In order to assess the life cycle of a structural battery, a different comparison is made; instead of comparing the structural battery to a carbon fiber composite plate (and lithium battery), it is compared to a steel plate (and the same battery). All layups and definitions are the same, as well as the load case and boundary conditions. The steel plate is considered to have an elastic modulus of 200 GPa, Poisson's ratio of 0.25 and a density of 7800 kg/m^3, has a thickness of 0.8 mm and is 1.5 m wide and 2m long. These dimensions are selected in order to represent the roof of a large electric vehicle.

The life cycle assessment is made comparing two different designs of an electric vehicle; a monofunctional design with a steel roof and a lithium ion traction battery. And, a multifunctional design that replaces the steel roof and part of the original traction battery, see Figure 5. The amount of traction battery that is replaced is corresponding to the energy content of the structural battery roof. The life cycle assessment does only take these functional parts into account and compare them, it does not include the rest of the car. The metric used for this life cycle assessment is mass of CO_2-equivalent, which is a number for how much global warming potential a product has, by estimating its life cycle greenhouse gas emissions. The life cycle starts with the raw material extraction, both for steel and all constituents and materials for both the conventional lithium ion battery and the structural battery. Next, all sections of raw material refinement, manufacturing, coating and assembly are considered, including transport from the raw material extraction to the manufacturing plant and from the manufacturing plant to the user. Many of these operations need electricity, for which an electricity mix of about 45 g CO_2-equvalent/kWh is used, corresponding to the average Swedish electricity mix. The same electricity is used for propulsion of the vehicle. After use, material recycling is considered wherever possible, e.g. the carbon fiber is assumed to be recovered by pyrolysis.

The main objective with the structural battery is to reduce mass of the vehicle, compared to using a steel roof and lithium ion traction batteries. This is modelled through an energy reduction value according to worldwide harmonized light-duty vehicles (0.069 Wh/kg/km) [6].

The comparison has a large impact from the original lithium ion battery system, which herein is considered to be of NCA type (Panasonic NCR18650A). The battery is commonly used in electric vehicles and high performing [7]. Any battery management systems and casings/protections for the original battery are not considered, since they are equally needed of the structural battery.

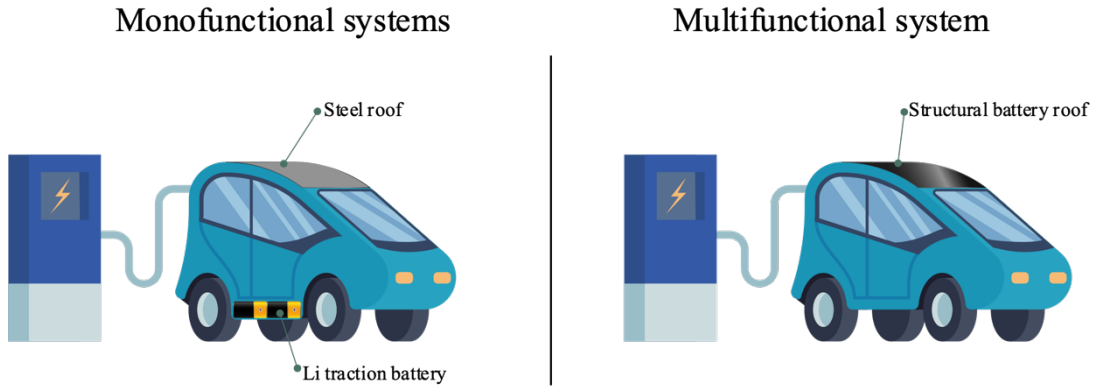

Figure 5: The two different design that are compared in the LCA; a monofunctional system containing a steel roof and conventional lithium ion traction batteries. And, a multifunctional system where both the steel roof and part of the traction battery is replaced with a structural battery.

2 RESULTS AND DISCUSSION

2.1 Structural battery – mass saving and variable sensitivity

A construction of a multifunctional structural battery plate is compared to a monofunctional carbon fiber composite plate and a monofunctional lithium ion battery. The structural battery plate is matched in mechanical performance to the composite plate by its midpoint deflection due to a uniform pressure (simply supported boundary conditions). And, the structural battery is matched in electrical performance by its total energy storage, such that the lithium ion battery stores the same amount of energy. The results show that the structural battery has a mass of 2.6 kg, the composite plate 1.9 kg and the lithium ion battery 1.7 kg. This means that the multifunctional structural battery would save about 26% of mass compared to the monofunctional components.

For the sensitivity analysis, each variable is varied separately and then plotted, providing its mass saving for the structural battery. Figure 6a shows a varying volume fraction of fibers in the negative electrode. A higher volume fraction of fibers will increase the mass saving of the structural battery, this is natural since it increases the overall stiffness of the material, while also decreasing internal distances in the cell with better electrical properties as a result. However, note that this value cannot be allowed to reach its physical maximum of packing, since the electrical storage require ion transport through the matrix to all fibers. This ion transport is an important property of any lithium ion battery and need to be further analyzed in detail for the structural battery in future research. Figure 6b also shows the volume fraction of fibers, but for the positive electrode. In this case, the upper limit of volume fraction of fibers is also limited by the positive electrode coating. The volume fraction of fibers in the positive electrode shows the same trend as for the negative electrode.

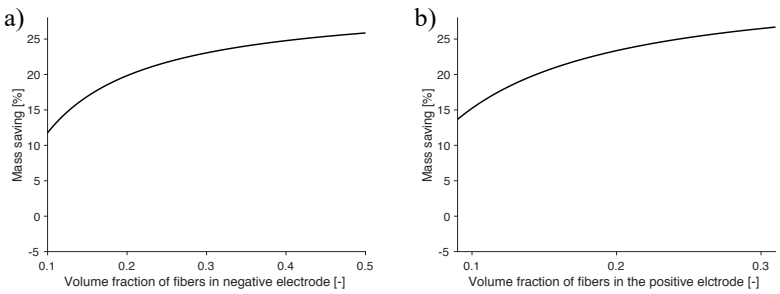

Figure 6: When replacing carbon fiber composite and lithium ion battery with structural battery, its a) mass saving as a function of the volume fraction of fibers in the negative electrode of the structural battery, b) mass saving as a function of the volume fraction of fibers in the positive electrode of the structural battery.

When changing the amount of carbon fibers in both electrodes (carbon fiber area density), the results behave as in Figure 7a. It shows that a higher area density increases the mass saving of the structural battery. This is because increasing the amount of carbon fibers will, in relation, decrease the percentage of separator, which means that the overall stiffness increases. Interestingly, this is opposite of what is expected for only increasing energy storage, where thin electrodes are desired. Furthermore, decreasing the thickness of the separator will increase the mass saving of the structural battery, as seen in Figure 7b. This is expected since a thinner separator will not only decrease low stiffness material in the laminate, providing better mechanical properties, but it will also reduce the electrode distance, with increased energy storage properties.

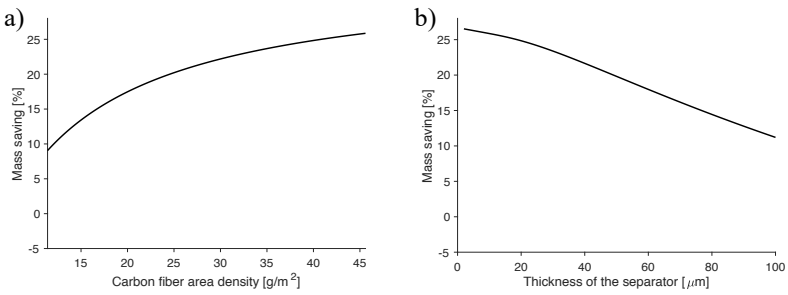

Figure 7: When replacing carbon fiber composite and lithium ion battery with structural battery, its a) mass saving as a function of the carbon fiber area density in both electrodes of the structural battery, b) mass saving as a function of the thickness of the separator in the structural battery.

The SBE also has some intrinsic properties, specifically its ion conduction and elastic modulus. These properties are generally conflicting, where a higher modulus generally decrease the ion conductivity, and vice versa. Figure 8a shows that an increased ion conductivity will drastically increase the mass saving of the structural battery up to a plateau occurring at about $1 \cdot 10^{-3}$ S/cm, since this is where the SBE's ion conductivity coincide with that of commercial liquid electrolytes. On the other hand, Figure 8b shows that an increased elastic modulus has very little impact on the mass saving of the structural battery. This means that for further research on structural batteries, increasing the conductivity of the SBE could be more rewarding from a mass saving perspective.

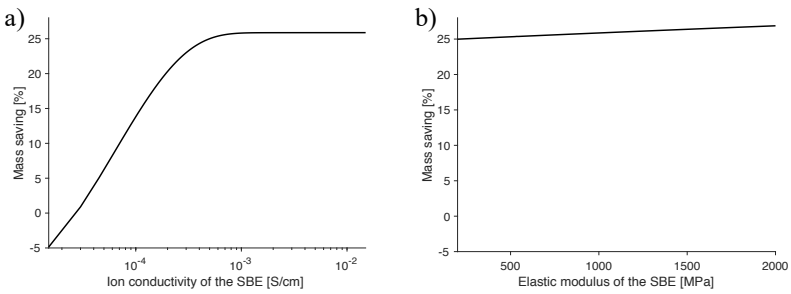

Figure 8: When replacing carbon fiber composite and lithium ion battery with structural battery, its a) mass saving as a function of the ion conduction in the SBE, b) mass saving as a function of the elastic modulus of the SBE.

2.2 Life cycle assessment

Results from the life cycle assessment are given as kg CO_2-equivalent and shown in Figure 9. The results are presented as net impact from replacing a steel roof and lithium ion battery with a structural battery. The steel roof and the structural battery has the same bending stiffness, and the replaced lithium ion battery stores the same amount of energy as the structural battery does. Negative numbers thus represent a decrease in global warming from using a structural battery. The production and recycling of the structural battery naturally do emit greenhouse gases, but this emission is counteracted by the avoided production and recycling of the steel roof and the original traction battery. This is further aided by the decreased mass of the vehicle, by decreasing the burdens in use. From these results can be seen that manufacturing the structural battery in Sweden would decrease the total greenhouse emissions from the structural battery compared to a steel roof and original traction batteries.

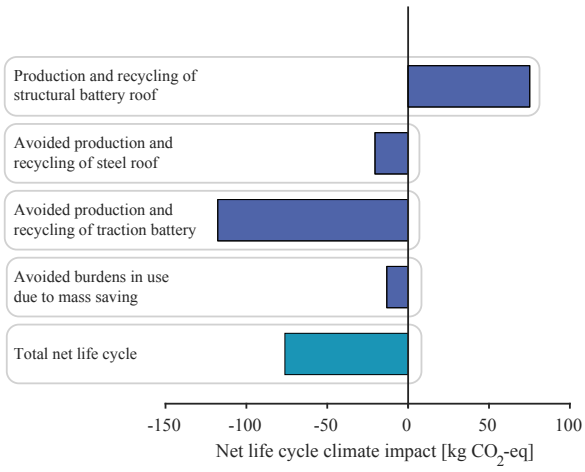

Figure 9: Life cycle climate impacts from the production and use of the structural battery, compared to the avoided production and recycling of the steel roof and original traction battery. A negative value represents a decrease in CO_2-equivalent emissions during the lifetime.

Looking at the production of the structural battery, the contribution from the different materials and parts of manufacturing and making the structural battery are presented in Figure 10. The values are given for a Swedish electricity mix. It can be noted that the production of carbon fibers and energy consumption during structural battery production are by far the largest contributors to greenhouse emissions. This means that producing carbon fibers and structural batteries with clean electricity will contribute to significantly decreased greenhouse emissions. The other materials in the structural battery all have a lower impact, with the $LiFePO_4$ in the positive electrode being the largest of them.

Bisphenol A dimethacrylate is the monomer used for the SBE. Notably, the transport of raw materials and structural batteries, has a small contribution to the greenhouse emissions.

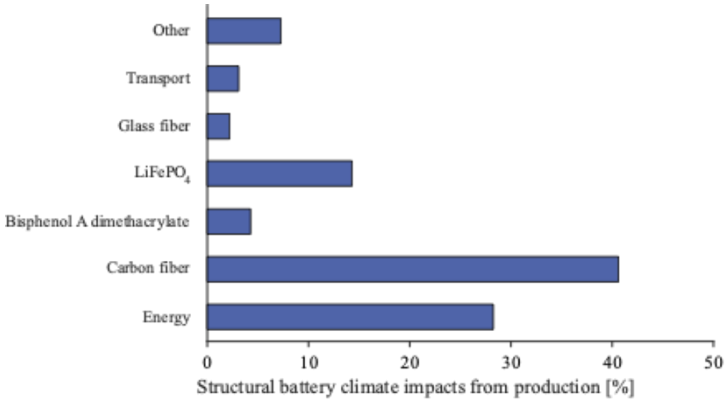

Figure 10: Distribution of climate impacts (CO_2-equivalent) during the production-phase for the structural battery, for Swedish electricity mix.

3 CONCLUSIONS

A plate of structural battery has a potential to save up to 26% of mass compared to the combined mass of a plate of carbon fiber composite and a standard lithium ion battery. Investigating the sensitivity of different variables for the structural battery shows a large significance for some, and very little for other, which makes the importance of further modelling and understanding of structural batteries apparent. There are many different parameters at play, and they come from very different fields of research. Understanding their behavior and interaction will be crucial for the success of multifunctional structural batteries in broad use.

The sensitivity analysis has produced some insights into structural batteries, such as improving the conductivity of the SBE has a larger impact on the mass saving of the structural battery than improving its stiffness. Such knowledge is important for focusing further research on properties which may have a large impact on the overall properties of the structural battery.

The ion transportation in an electrolyte of a lithium ion battery is a very important property, maybe even more so in an SBE. Considerations with regards to packing of carbon fibers and volume fractions are important in order to facilitate ion transport, but also internal characteristics of the SBE such as electrolyte/polymer content and tortuosity are important. These investigations require further modelling and understanding.

The life cycle assessment has produced further understanding into the manufacturing, use and recycling of structural batteries. Utilizing a structural battery in the roof of an electric vehicle can decrease greenhouse emissions compared to a steel roof and an original traction battery. The emissions in production of the structural battery mostly stem from carbon fiber production and general energy use, the other ingredients have a significantly smaller contribution, the same applies to transports in production.

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