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Life cycle analysis on phase change materials for thermal energy storage.

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Abstract

Sustainable energy sources and utilization is a large area of interest and the developments are moving fast. Recently, thermal energy storage in the form of phase change materials other than water have caught more interest and a need of analysis for the entire life cycle of the materials have appeared. Previous work in the area shows that health and safety aspects of the products' life cycle have been neglected and comparisons between different phase change materials other than water are sparsely researched. The objectives for this report are to compare three different phase change material intended for thermal energy storage in a life cycle analysis point of view with both environmental and health and safety aspects. A screening process of materials was subsequently performed in order to find suited materials given the objective (Octadecane, Xylitol and Manganese Nitrate Hexahydrate), taking into consideration the relevance in the scientific community amongst other criteria. The life cycle is in this work bounded from cradle to grave without recycling and for a thermal energy storage heating system operating in Scandinavian climates assuming 52 cycles per year. The results indicate that Octadecane are preferable in terms of global warming potential over 100 years (ca 4.5 kg CO_2/kg Octadecane produced) and Xylitol more preferable in terms of cumulative energy demand (ca 21.5 MJ per kg Xylitol produced) and energy payback time (1.17 years). The health and safety aspects are difficult to evaluate in terms of working conditions and ecotoxicity but a simple scale have been put to use to give an overview of the health risk associated with each material. In the health and safety aspects Xylitol also show the most promise but further development of a methodology for evaluating these terms are recommended.

Sammanfattning

Hållbar energiteknik är ett omtalat och snabbt utvecklande område där fasomvandlandematerial för termisk energiförvaring har dragit till sig uppmärksamhet. På grund av denna uppmärksamhet har behovet för en fullständig livscykelanalys för de relevanta materialen uppkommit. Föregående rapporter och journaler om ämnet har visat brister i fokus på hälso- och säkerhetsaspekter och i jämförelse med andra fasomvandlandematerial än paraffiner och vatten. Målet med denna rapport är att utföra och jämföra livscykelanalyser för tre olika fasomvandlandematerial med både miljöaspekter och hälso- och säkerhetsaspekter. En urvalsprocess av intressanta material har därmed genomförts för att hitta lämpliga kandidater att undersöka (Oktadekan, Xylitol och Mangan nitrat hexahydrat), med avseende på bl.a. hur mycket materialen studerats inom termisk energiförvaring. Livscykeln inom denna rapport är bunden från *Cradle-to-grave* utan återvinning av material och opererar under skandinaviska förhållanden med 52 värmecykler per år. Resultaten indikerar att Oktadekan är mest lämpad för globaluppvärmnings potential över 100 år (ca 4,5 kg CO_2/kg Oktadekan producerad) och Xylitol mest lämpad för kumulativt energikrav (ca 21,5 MJ per kg Xylitol producerad) samt återbetalningstid för energi (1,17 år). De hälso- och säkerhetsaspekterna är svåra att definiera inom arbetsförhållanden och ekotoxicitet men en enkel skala baserad på ’GHS hazard statements’ har etablerats för att få en överblick över materialens hälsorisk. Även här visade Xylitol vara mest lämpad men fortsatt utveckling av en metodik för att analysera dessa aspekter rekommenderas.

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Nomenclature

Abbreviation	Meaning	Unit
LCA	Life Cycle Analysis	-
PCM	Phase Change Material	-
TES	Thermic Energy Storage	-
LHS	Latent Heat Storage	-
SHS	Sensible Heat Storage	-
BIST	Building Integrated Solar Thermal	-
TCM	Thermochemical Materials	-
MOFs	Metal Organic Frameworks	-
EPBT	Energy Payback Time	Years
GWP_{100}	Global Warming Potential 100 years	$tonnes\ CO_{2,eq}$
CED	Cumulative Energy Demand	$\frac{MJ}{KG}$ PCM
EI99	Eco-Indicator 99	mPt
IPCC 2013	Intergovernmental panel on climate change standard 2013	-
ΔH_m	Enthalpy of fusion	$\frac{J}{g}$
C_p	Specific heat capacity	$\frac{J}{mol \cdot K}$
Wt.%	Weight percent	-
LCI	Life Cycle Inventory	-
LCIA	Life Cycle Inventory Analysis	-
Tm	Melting temperature	°C
BOD5	Biological Oxygen Demand	kg
COD	Chemical Oxygen Demand	kg
DOC	Dissolved Organic Carbon	kg
TOC	Total Organic Carbon	kg
E_{in}	Energy required to create a TES system	MJ
$E_{out.a}$	Annual energy output for a TES system	MJ
Q_{PCM}	Energy storage capacity of a PCM	$\frac{MJ}{KG}$
GHS	Globally harmonized system	-
CLP	Classification, labelling and packaging	-
$CO_{2,eq}$	Carbon dioxide equivalent (variable in calculating GWP)	t

1. Introduction

1.1 Life Cycle Analysis

Life cycle analysis, or LCA, is a method to evaluate materials and products effects on environment and social aspects. There are different types of LCAs depending on the stage in the product cycle, the most inclusive assessment is cradle to grave that analyses the material for its environmental and social aspects during its entire lifetime from extraction and production to usage and liquidation [1]. This is the scope that will be used in this report.

Different standards are in place to ensure continuity in different areas of LCAs, where, the most common ones are the ISO 14040:2006 which refers to the principles and framework of an LCA [2] and ISO 14044:2006 which refers to the requirements and guidelines [3]. These two standards will be referred to, in this project work and report.

1.2 Phase Change Materials

PCMs have been recognized as a potentially viable form of TES due to their thermodynamic properties. The PCMs that this report will evaluate include; salt hydrates, paraffins, fatty-acids and sugar alcohols.
Previously conducted LCAs on PCMs have the purpose to evaluate if a TES system with PCMs can be efficient enough in terms of energy efficiency to overcome the materials' environmental footprint or to compare different types of PCMs to water.

1.3 Thermal Energy Storage

Thermal energy storage (TES) is an advanced energy technology that usually involves temporary storage of high- or low temperature energy to be harvest later or at another location. Examples of when this technology are in use are solar energy for heat at night-time and ice for cooling during summer [4]. TES systems can use both latent heat [1] (LHS) storage and sensible heat[2] storage (SHS) [5] and often both from energy surplus from machines, environment and even the occupants in the area [4].
The general idea of using TES is to save energy and stabilize the on- and off- peaks in the power system and has therefore attracted large interest in a variety of sectors, for example industrial, commercial and residential sectors. The basic principles of TES process are the same for all TES systems and can be described by at least three stages of charging, storage and discharging. This process can be cyclic or linear [4]. Figure 1: Schematics over a thermal energy storage heating system, adapted from DN Tanks describes a simple schematic over a water-based TES system and the cycles of charging and discharging during on peak and off peak. The red arrows represent hot water flowing through the system that in turn powers the buildings heating system. The blue arrows represent the cold water flowing through the system to be stored in the Thermal energy storage. On the left-hand side an on-peak[3] in the power system is shown and the dotted lines means that the heaters in the system are turned

[1] Latent heat is the heat from the energy stored in the materials phase change [5].
[2] Sensible heat is the heat stored in the material without phase change [5].
[3] On-peak are here defined as the time when the TES system are required/active, for example at night time or winter time when the temperature drops.

off and thus the system saves energy. On the right- had side an off-peak[4] is represented and the heaters in the system are turned on to recharge the tank and to power the buildings heating system which is now in lower demand.

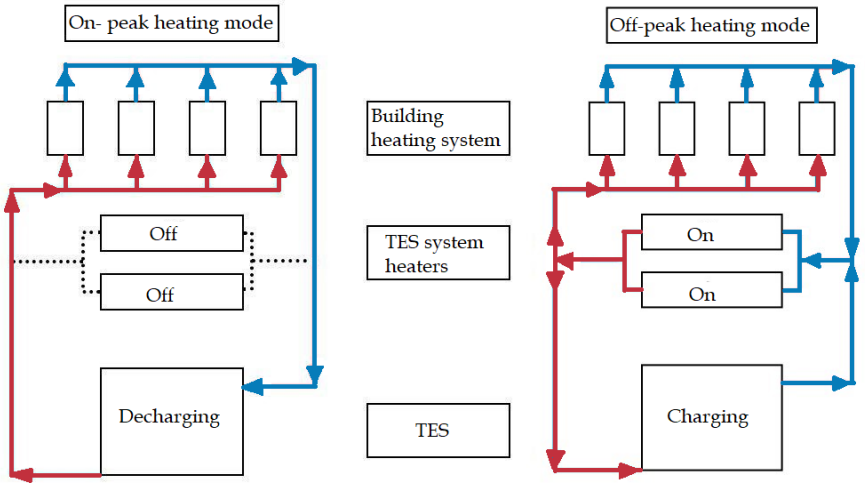

Figure 1: Schematics over a thermal energy storage heating system, adapted from DN Tanks [85]

1.4 Previous LCAs on PCMs for TES

The potential of energy storing with PCMs has lately attracted more interest and as an effect of that the research conducted on PCMs for TES with LCA objectives has increased. Most articles, books and papers are focused on either comparing organic and inorganic PCMs with water or to compare TES systems with or without PCMs in terms of energy efficiency and energy payback time (EPBT), i.e. the amount of time it takes before the invested energy into the production of a product is saved during the products usage (assuming the product improves the energy efficiency of a system). Three articles and one conference paper has been selected to represent the research field of LCA on PCM for TES.

In one article [6] representing the LCAs of building integrated TES systems, a building integrated solar thermal (BIST) systems with PCM (Myristic acid) and rock wool and a BIST system with only rock wool as isolation are compared in terms of EPBT[5], cumulative energy demand (CED)[6] and global warming potential for 100 years (GWP 100a)[7]. This article is conducted with IPCC 2013 methodology and under the assumption of Mediterranean climate (France), 25 years shelf life, and scenarios with and without recycling of the BIST system components. In the scenario without recycling the GWP and CED shows a slight advantage to the system without PCM, GWP 100a showed 0.67 MJ/kWh to 0.74 MJ/kWh and the CED showed 0.06 kg CO_2/kWh to 0.08 kg CO_2/ kWh. The EPBT on the other hand are very similar in both cases if auxiliary heating is not included, both are about 1.3 years. If the

[4] Off-peak are here defined as the time when the TES system are not required/active, for example at daytime or summertime when the temperature rises.
[5] Generally defined as the amount of years the unit have to operate in order to store/save as much energy as it took to produce it.
[6] The sum of the direct and indirect energy usage throughout the products life cycle
[7] A measurement of how much heat a greenhouse gas traps in the atmosphere relative to CO_2 over a period of 100 years. Measured in carbon dioxide equivalents, $CO_{2,eq}$

auxiliary heating is included the EPBT shows an advantage to the system with PCM. In the scenario with recycling the environmental profile improves considerably but have not been thoroughly examined [6]. Another article [7] with the focus on PCMs integrated in buildings but have the objective to research if the payback in energy can overcome the cost of energy during production and disposal of the PCM. This article is conducted with EI99 methodology and under assumptions of Mediterranean climate (Spain), approximated values of disposal of paraffins and three different comfort requirements during the year.[8] To create a baseline for energy consumption the author has set up tree cubicles with electric radiators and heat pumps that can be measured. Several hypothetical alternatives in the system design, PCMs (RT-27 paraffin and hydrated salt SP-25 A8) and weather conditions are discussed and the result shows that integrating PCMs in building does not save enough energy to overcome the cost at production and disposal in a normal building lifespan[9] in the three different climate conditions[8]. If the salvation of energy would come up a point where the buildings environmental impacts are reduced to 10 percent, the building should have a life span of 100 years and experience summer climate all year around. However, the report shows that the salt hydrate have a significant advantage over the paraffin in the production because it is not fossil based and are therefore a better choice to include in buildings to save energy [7].

Except for building cooling and heating applications PCMs on TES can be used in solar energy. An article [8] with the focus on different type of TES for a solar power plant, SHS with molten salt (60 wt.% $NaNO_3$ and 40 wt.% KNO_3) and high temperature concrete and LHS using a eutectic salt (54 wt.% KNO_3 46 wt.% $NaNO_3$). The method used is Eco-Indicator 99 (EI99) and the aim is to analyse if the energy savings are enough to overcome the environmental impacts from the production of the whole system. The results show that the TES using high temperature concrete are the most energy efficient per kWh stored of all three dues to the simple construction and the TES using molten salt (60 wt. % $NaNO_3$ and 40 wt. % KNO_3.) are the least energy efficient due to the complex structure of the product [8].

Most LCA on PCMs for TES has been for a specific application as seen above, therefore an article [9] on material and component level of the PCM was written. In this article they compare PCMs and thermochemical materials (TCM) with water to see the benefits of using innovative storage mediums in terms of global warming potential (GWP). The materials analysed where sensible water[10] as a benchmark, paraffins (PCM), salt hydrates (PCM), silica gel (TCM), a variations of zeolites (TCM) and a variation of metal organic frameworks (MOFs) (TCM). The international standards ISO14040 and 14044 was implemented together with the European standards EN15978 and 15804 for building applications. The conclusion was that in high temperature storage (heating applications and solar thermal storage) PCMs were not beneficial compared to water but in low temperature storage with small temperature gradients (cooling applications) the PCMs were beneficial [9].

1.5 Objectives

The interest in PCM for TES are building and have spiked the research on LCA on PCM for TES, even if the area has expanded there are gaps of focus and knowledge. The previous

[8] Summer period: four months with heat pump activated to set temperature to 24 Celsius in cubicle, Winter period: four months with electrical radiator to set temperature to 24 Celsius in cubicle and No controlled temperature: four months where temperature is not manually controlled [7].
[9] Normal lifespan of a building is calculated to be between 50 and 100 years, in this case 75 years are assumed to be a normal lifespan [7].
[10] Both as solid for cooling applications (ice) and liquid for heating applications (water)

work in the area reveals a gap of focus for the health and safety impacts and therefore this report will conduct a basic LCA on PCM for TES with both environmental and health and safety aspects to provide a template for further research. This report will also investigate the prospect of using alternative PCMs, aside from paraffins and water, to store thermal energy.

2. Background

2.1 Life cycle analysis

2.1.1 General methodology and standards

LCA is an internationally used method to determine the environmental and social impacts of a product, system or organization, during the different stages of its life cycle. The method has been used for decades by public and private entities, there are several standards to regulate the methodology of the LCA on both national, international and global levels [1].

Most projects require a life cycle assessment over a life cycle analysis. A life cycle analysis is an analysis of material, system or organizational data on a specific entity, for example an emission factor. To accomplish an assessment, the analysis from the data collected must be implemented on an environmental or social happening [1].

Alongside the ISO standards different methodologies on how to define environmental damage are in place, Eco-Indicator 99 (EI99) are one of them and defines environmental damage in three categories; Human health which includes diseases and death due to climate change, radiation and both repertory and carcinogenic effects , resources which includes the energy consumption to extract a minimizing resource in the future and quality of ecosystem which includes ecotoxicity, acidification, eutrophication and land-uses effect on biodiversity of all living organisms' [10]. Another standard on how an LCA should be conducted and calculated have been constructed by an intergovernmental panel on climate change (IPCC 2013) as an intergovernmental body of the United Nations. [11]. The methodology they established describes emissions factors to calculate the impact of greenhouse gases [12] from different sources, for example fertilizers or direct gas emissions from fumes [13].

2.2 Phase change materials

2.2.1 Definition and General knowledge

A phase change of an arbitrarily selected material is the induced transformation of the materials atomic structure. As energy is transferred in to, or out of the observed system (i.e. the observed material), the vibrations of the interatomic bonds will increase or decrease, affecting how stable the system is. If a certain level of energy in the system will be reached, a change of the subatomic structure will be more thermodynamically favorable, i.e. a change of state is likely to occur. The energy that is required for a phase change does not change the substance's temperature, and can therefore be classified as latent heat, as opposed to sensible heat. Latent heat goes towards increasing the energy of the atom constituents until an energy level is reached where a phase change is favorable, example being going from a solid structure to liquid. An increase of latent heat does not affect the temperature of the material, as it is held (nearly) constant throughout the process. An important property that the phase change process is quasi-

static, meaning that the process can be repeated by lowering and increasing the energy in the system [14], [15].

As the energy required to induce a phase change in material, and the temperature in which the desired phase change occurs, differs largely for all substances, some materials are more suitable for storing energy in practical applications. Considering this, materials with a phase change that is suitable for storing and releasing energy, i.e. possessing a high heat of fusion, are thus commonly referred to as *Phase Change Materials*, or PCMs for short. As the process of storing and releasing energy in a PCM is reversible, it is of interest to integrate PCMs in TES-systems, labeling the method as "latent heat energy storage", as opposed to sensible heat TES or chemical TES. Due to the properties of a PCM, latent heat TES systems can potentially store up to four times as much energy per volume compared to sensible heat TES systems under smaller increments of temperature. This property can be a compelling factor in a variety of applications [16].

PCMs can be divided into two general categories: Solid-solid and solid-liquid. Solid-Solid phase transitions are phase changes that occur within material as it stays in solid form, i.e. a rearrangement of atoms to a more thermodynamically favorable position within the lattice. An example of this would be a polymer transition from semi-crystalline to amorphous structure. Solid-solid phase transitions are advantageous in the sense that volume change through the phase transitions is of a lesser magnitude than solid-liquid transformation. They do, however, generally require less energy in order to complete the transition and has therefore a lower phase transition enthalpy, meaning that they can store less latent energy. Solid-liquid transformations generally have a larger phase transition enthalpy and can therefore store more latent energy. They do however experience change in volume on a larger scale which has to be accounted for when designing TES system. It can be noted that the liquid-vapor phase transition generally possesses a large phase transition enthalpy, but mainly due to the large increase in volume of a substance that undergoes this transition, they are not considered within the common definition of PCMs. To encapsulate; when discussing a PCM, it is commonly agreed upon that you refer to a material with a suitable solid-liquid phase change enthalpy, and in some cases a solid-solid transformation [14].

2.2.1.1 Requirements for PCM?

As stated in the previous section; for a material to be referred to as a PCM it needs to fulfill certain criteria, where a considerable enthalpy of fusion and a suitable phase change temperature are the most essential ones. There are however several other important aspects one must consider when selecting a PCM for application. These requirements are commonly divided into physical, technical and economical requirements.

The physical requirements include [14];

- *Suitable phase change temperature* for the application
- *Large phase change enthalpy* as this correlate to increased energy storage potential
- *Cycling stability*. For extended number of cycles, it is desired that the PCM does not drop significantly in performance
- Limited *supercooling*
- Good *thermal conductivity* as this reduces the time to store or release energy in a given volume of the PCM material

Supercooling is a phenomenon that occurs when undergoing the liquid-to-solid transformation that a temperature significantly below the melting point must be reached before the material begins solidification, and therefore release heat. What this implies is that a supercooled PCM will only store sensible heat until this point is reached. It is therefore advantageous for the temperature range for the supercooling effect to be as narrow as possible [14].

The technical and economic aspects affect the ease of construction and applications for the PCM, some of these requirements include [14]:

- *Low vapor pre*ssure as this reduces mechanical stress on the vessel containing the PCM
- *Small volume change* as this reduces mechanical requirements for the vessel
- *Compatibility* for the PCM with other materials, prolonging the life length of the vessel. An example of this is the corrosive properties of the PCM
- *Safety constraints*, as toxic and flammable material are non-desirable
- *Low cost* as this increases the viability for large-scale usage for the PCM
- *Good recyclability* as it is beneficial economically as well from an environmental perspective

2.2.2 Paraffins

'Paraffin' is an umbrella term commonly used for high-molecular weight alkane hydrocarbons and thus belong to the 'inorganic' category of PCM. Paraffins follow the general formula $C_n\ H_{2n+2}$. Paraffins are commonly divided into liquid paraffins and solid paraffins, based on their state at room temperature. Liquid paraffins consists of $C_{10}H_{22} - C_{18}H_{40}$ alkanes. Solid paraffins, otherwise known as paraffin wax consists of $C_{20}H_{42} - C_{40}H_{82}$ alkanes [17].

Alkanes vary from each alteration (i.e. varying the amount of carbon and hydrogen atoms in the molecule) regarding their thermodynamic properties but usually fall within certain boundaries. The melting temperature varies from -182.5 to 90 ℃, whereas paraffin wax lies above 36.4℃. The specific heat of paraffin wax is generally accepted to have a value of approximately 2.1 $\frac{kJ}{kg \cdot CK}$, and a heat of fusion of approximately 215-230 $\frac{kJ}{kg}$. Paraffins have a relatively low thermal conductivity [14] , [17].

2.2.3 Salt hydrates

Salt hydrates are inorganic compounds consisting of a distinct mixing ratio of salt and water molecules, forming a stable crystal structure. Salt hydrates have a high variety of melting points and thermal properties. There is a big variety of salt hydrates. They melt congruently, semi-congruently or incongruently, of which the salt hydrates of interest for TES purposes are the ones that melt congruently. These number of salt hydrates are more limited in number. The collected, most cited data shows that the thermodynamic properties for the congruently melting salt hydrates have a melting temperature that varies from 8.1 to 116.7 ℃. The heat of fusion varies from 116 to 296 $\frac{kJ}{kg \cdot CK}$. Supercooling is a common phenomenon in this material group. Salt hydrates have a relatively high thermal conductivity [14], [18], [15].

2.2.5 Fatty-acids

Fatty Acids are organic compounds characterized by the formula $CH_3(CH_2)_{2n}COOH$. Fatty acids have not been studied as extensively as salt hydrates or paraffins but there are some saturated fatty acids that are of interest for TES purposes. The collected data for the relevant fatty acids has shown that the melting temperature varies from 8 to 64 ℃, and that the enthalpy of fusion ranges from 149 to 222 $\frac{kJ}{kg \cdot CK}$. Fatty acids have a relatively low thermal conductivity [14], [19].

2.2.6 Sugar alcohols

Sugar alcohol is an organic compound, and is a somewhat new class of material, and has therefore little general available information. Sugar alcohol are a hydrogenated form of carbohydrate and its general chemical structure is $HOCH_2[CH(OH)]_nCH_2OH$, different forms are obtained through alterations of the general formula as well as the orientation of the OH-groups. It has high density, which results in a relatively high enthalpy of fusion. Studies has shown that the melting temperature (for the relevant sugar alcohols for TES purposes) ranges from 94 to 188 ℃, and the enthalpy of fusion ranges from 263 to 351 $\frac{kJ}{kg \cdot CK}$. Sugar alcohols have however shown to be prone to some supercooling [14].

3. Methodology

3.1 Methodology ISO 14040:2006/ ISO 14044:2006

The methodology of an LCA includes four stages and three phases that are guided by different standards. Here, a ‘stage’ is defined with time limitations, and a ‘phase’ is defined as an ongoing process during the progression of the LCA.

3.1.1 Goal and scope for ISO standards

The first stage of an LCA is to determine a goal and scope of the study [2]. This is the stage where the object or objects of the study should be clearly defined [3], the extent of the analysis is determined, the application of the LCA is considered and an outline of the results is designed [20].

The goal of the LCA may seem straightforward but can be difficult to determine [1]. The Goal should state the reason why the LCA is conducted [2], the intended purpose of the report and the type of report the results should be presented in, and the intended audience [3], [20].

The scope of an LCA can differ widely depending on what object is chosen to be analyzed and the goal of the report, it should therefore be determined in the beginning of the process before material data are collected [2].
The scope should outline the results by stating the impact categories that will be assessed and define a functional unit to be used for comparison of objects or relations to impact categories. Some typical environmental impacts are global warming and toxicity [21]. The functional unit is defined by the object’s performance characteristics which are often expressed in terms of the amount of material per use [20].

The quality of data required, assumptions and value choices that must be made in order to get through the process are also determined in this phase.
System boundaries should be stated and should contain the different stages and unit processes of the object’s life cycle, [3]. In Figure 2 and Figure 3 system boundaries are represented at two different levels on detail. In the first figure three different system boundaries are represented by arrows that reaches over the process steps chosen to analyze represented by the blocks. In the second figure the same system boundaries are represented by arrows reaching over the detailed process steps.

Value choices are the different priorities made during the first stages of an LCA. They are made to move the project forward, for example during object screening where a value choice could be to prioritize a mechanical property over another.

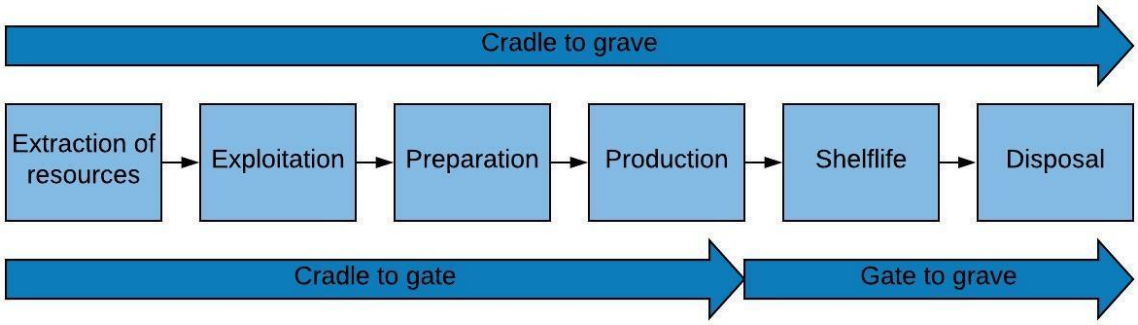

Figure 2: Explanation of different system boundaries for a standard process redrawn from Curran M.A 2016 [1]

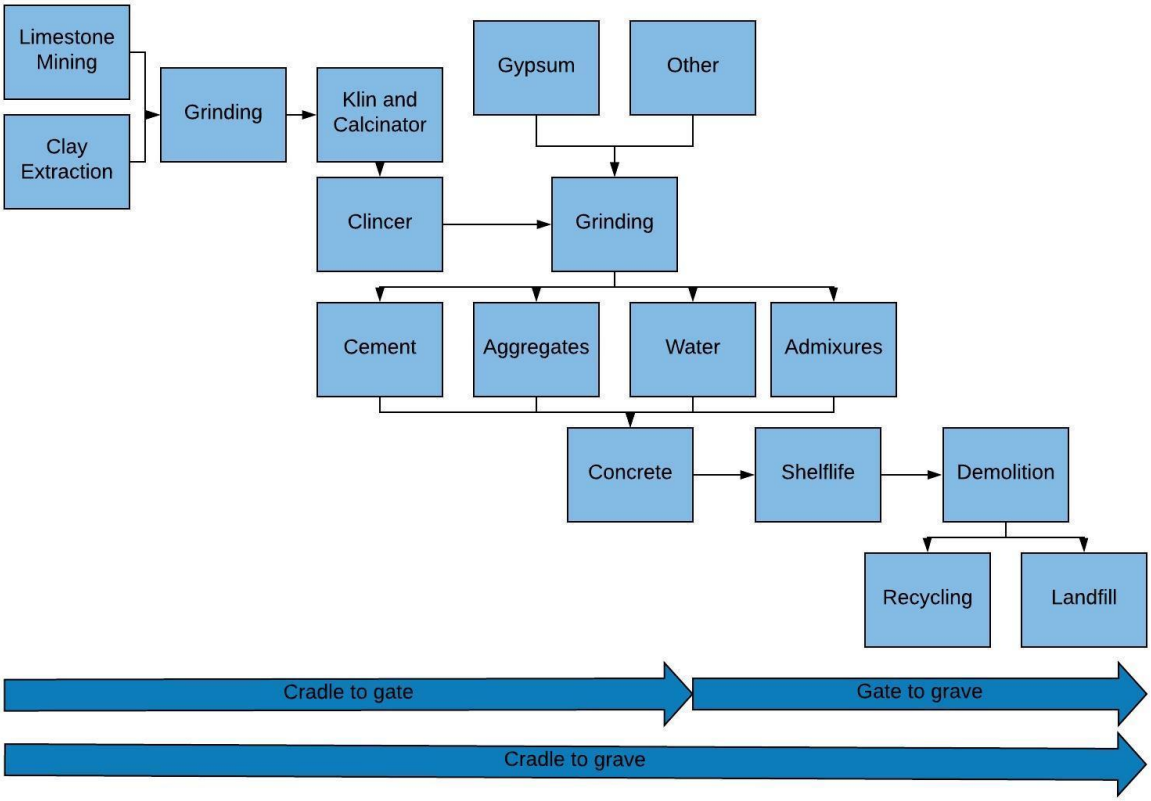

Figure 3: System boundaries for a detailed process of concrete redrawn from Sorensen B. 2011 [21]

Limitations of the required data must also be defined in the scope. They should contain the geographical and time limitations to be analyzed.

Lastly the format and type of the report and critical review should be determined before going to the next stage. It's important to have in mind that all boundaries, limitations, value choices and other assumptions will give reason to a relative analysis and not an absolute value to the object's emissions and impacts [2].

3.1.2 Life cycle inventory (LCI)

The second stage of an LCA is to create a life cycle inventory (LCI) by collecting material, process or organization data from the separate stages in the object's life cycle that are relevant to the chosen impact categories defined within the scope. While acquiring more data, new limitations and boundaries may be defined to reach the goal of the LCA, and if this is not possible, the goals can be revised [2]. When the data are collected, calculations to validate the relations to the unit process as well as the relations to the chosen functional unit are required [3], [20]. If a specific unit process in the production are chosen to be analyzed most often the data collecting shows numbers from the entire process and therefore some calculations of the amount contributed from the chosen unit process are required, perhaps in terms of percent. Another example of calculations made in this stage is the recalculations from the collecting unit, often in terms of kilograms or volumes, to the chosen functional unit stated in the scope, often in terms of volume per use or volume per efficiency.

3.1.3 Life cycle impact assessment (LCIA)

The third stage is to make a life cycle impact assessment (LCIA) where the data from the LCI is analyzed by its relevance to the system boundaries and sorted by the chosen impact categories and happenings stated in the goal and scope [20]. This is the stage where the LCA should get its system-wide perspective and should therefore be transparent to make a critical review easily conducted [22].

Here the data required in the LCI is assigned to one or more impact categories [2]. For each of these categories, an impact indicator are selected and the LCI results are calculated to an impact result by this indicator [22], an example of one of these indicators are the emissions causing the thinning Ozone layers' effect on global warming. These indicators can be viewed as a step between LCI and LCIA where the raw data from the LCI are being normalized and sorted into an impact category in the LCIA. In Figure 4 the two different stages are represented by the darker boxes and the indicators linking them together are represented by the lighter box together with some examples. The arrows in the bottom of Figure 4 represent the normalization of units conducted in order to evaluate the results. The collection of these impact results gives an overview of how the inputs and outputs of the objects' life cycle influences different environmental and social aspects [20]. Often, a grading system is needed to draw a conclusion if a comparison of objects is needed. However, there is no scientific basis to determine this grading system [3]. Therefore, the value choices are stated in the goal and scope stage and as a continuous phase to be improved during the project.

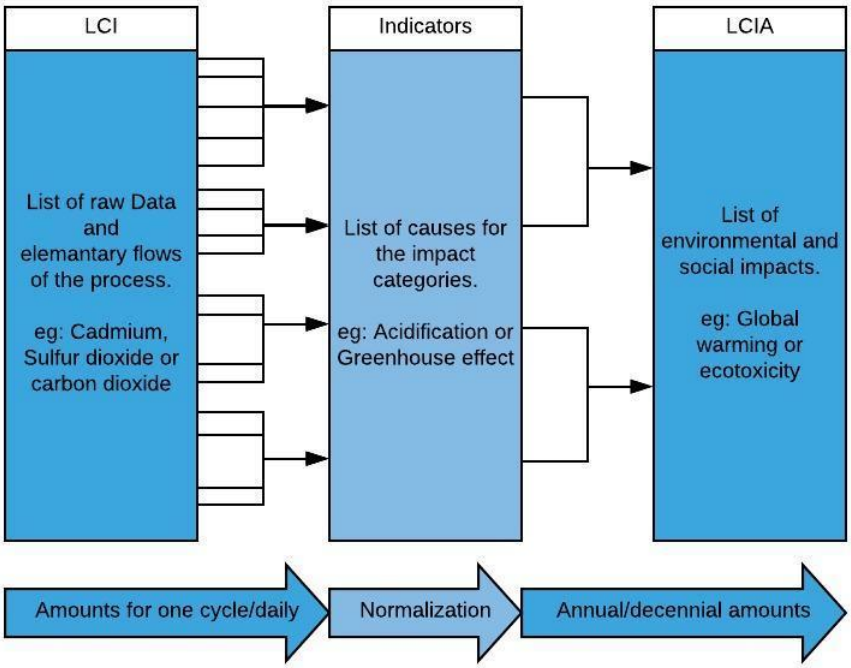

Figure 4: Flowchart of the methodology from LCI to LCIA, redrawn from Hauschild M, Huijbregts M. 2016 [23]

3.1.4 Life cycle interpretation

The last stage of an LCA is to interpret the results from the LCIA. This stage is a systematic procedure to identify, qualify, evaluate and present the results from the previous stages to make a conclusion based on the goal and scope of the LCA [2]. This interpretation also punctuates the strengths and weaknesses of this method compared to other techniques [3].

3.1.5 Report and critical review

The report and critical review phase should be considered during the entire process to ensure relevant results from the different stages. It should be defined within the goal and executed continuously during all the stages [1].

The purpose of the report is to deliver the information required to the intended audience in a clear and understandable manner. Therefore, the report should contain an explanation of the goal and scope from the first stage of LCA, the result and a quality analysis of the LCI, The models used to characterize the systems and the relations from data collected to the impact categories and lastly a conclusion and how it was drawn.
A sensitivity analysis of the relative nature of the LCIA due to the limitations and boundaries should also be conducted in order to increase its' credibility [3].

3.1.6 Limitations

The limitations should be stated within the goal and scope stage but due to the nature of the stages more limitations will be defined within the LCA investigation, and therefore defining the limitations is considered as an ongoing process and will change during the completion of the LCA [2].

3.1.7 Conditions of value choices and optional elements

This phase is defined within the goal and scope stage. However, due to the nature of the LCI which requires more information along the process, some choices must be reviewed and redefined to meet the goal and scope completely. Therefore, this phase is also an ongoing process within the LCA [2].

3.1.8 Relations between the stages

The methodology of an LCA constitutes of a process where the different stages are built by the results of the previous stage [2]. In Figure 5 the solid lines describe definite paths from one stage to another where major changes should not be conducted. The dashed lines describe paths where the changes should be constricted to and documented at.

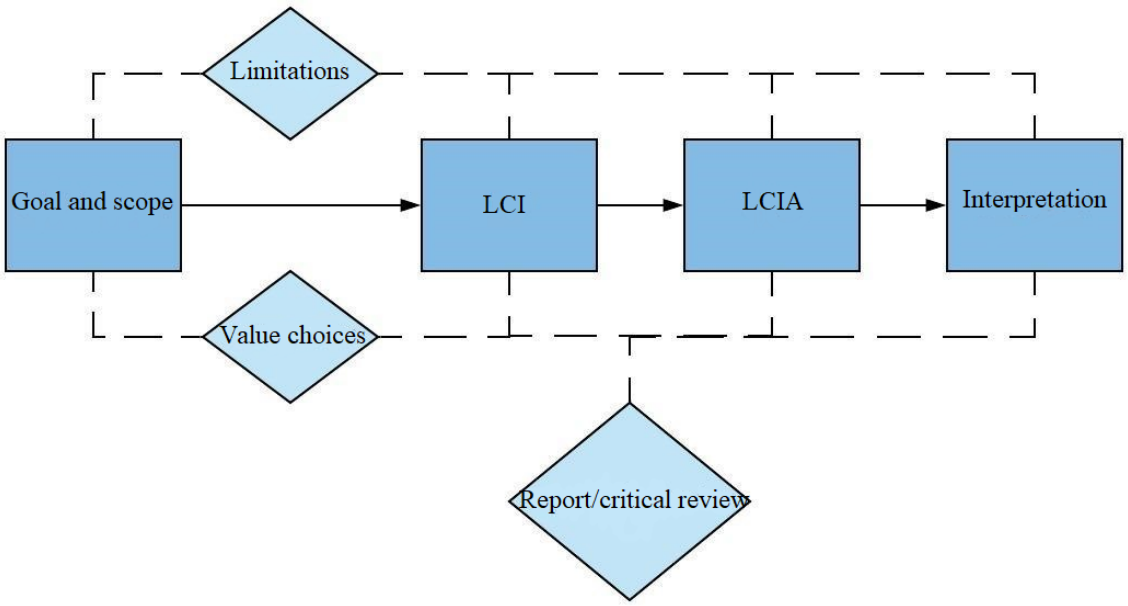

Figure 5: Flowchart of the relationship between stages and phases in an LCA, redrawn from M.A Curran [1]

3.2 Project Methodology

3.2.1 Screening of materials

For this project, a low number of PCMs were selected since the objective is to simply establish a framework from which further comparison of a higher number of PCMs can be accomplished. The PCMs where selected using a rough guideline in which the investigated materials would have roughly the same melting temperature and could therefore be used for the same sorts of application. The selected temperature range for this analysis were 0 to 100 °C, meaning that the investigated PCMs are viable for low temperature applications. Studies have shown that organic compounds and salt hydrates have shown to be promising for low temperature applications as opposed to eutectic compounds which have shown to be more promising for medium temperature applications (100 to 250 °C) [23]. Considering this, compounds such as fatty acids, paraffins, sugar alcohols and salt hydrates were of great interest for this articles purposes when selecting PCMs to investigate further.

After deciding on material groups to investigate for the LCA, further screening of materials was performed as each of these material groups has a large amount of diversity. Our most important criteria were that the material ought to have been studied extensively with TES applications as focus, implicating that the material has shown promise for practical usage along with having available LCI inventory data. Enthalpy of fusion, safety of usage and chemical stability were also considered for further screening of the materials. This process is illustrated in Figure 6 and in Figure 7. Material data for the selected material of interest is presented in Table 1: Material data for the inorganic PCMs and Table 2: Material data for the organic PCMs.

Considering these criteria, it was decided that the LCA was to be conducted on three materials from different material groups, these materials are *Manganese hexahydrate*, *Octadecane* and *Xylitol*, as Manganese nitrate hexahydrate and Octadecane has a somewhat similar melting temperature and due to lack of available data for other materials, Xylitol was selected as the third material of comparison.

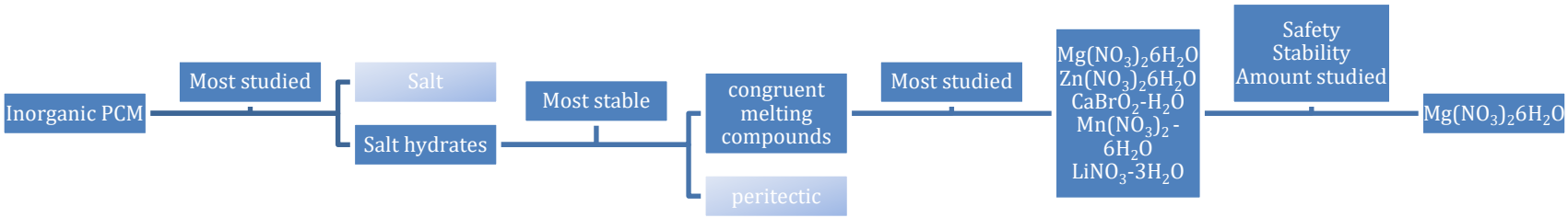

Figure 6: Flowchart of the screening process for inorganic PCMs

Table 1: Material data for the inorganic PCMs

Name	Chemical composition	T_m [°C]	ΔH_m [J/g]	C_p [J/mol*K]	Safety	Source
Magnesium nitrate hexahydrate	$Mg(NO_3)_2$ -$6H_2O$	90.0	160	*Solid:* 270 *Liquid:* 300	3	[24] [25], [26]
Zinc nitrate hexahydrate	$Zn(NO_3)_2$ -$6H_2O$	36.4	130	-	3	[24], [27]
Calcium Bromide hexahydrate	$CaBrO_2$-6H2O	34.3	116	-	-	[28]
Manganese nitrate hexahydrate	$Mn(NO_3)_2$ -$6H_2O$	26.0	140	-	3	[24], [29]
Lithium nitrate trihydrate	$LiNO_3$-$3H_2O$	30.0	125	-	-	[24]

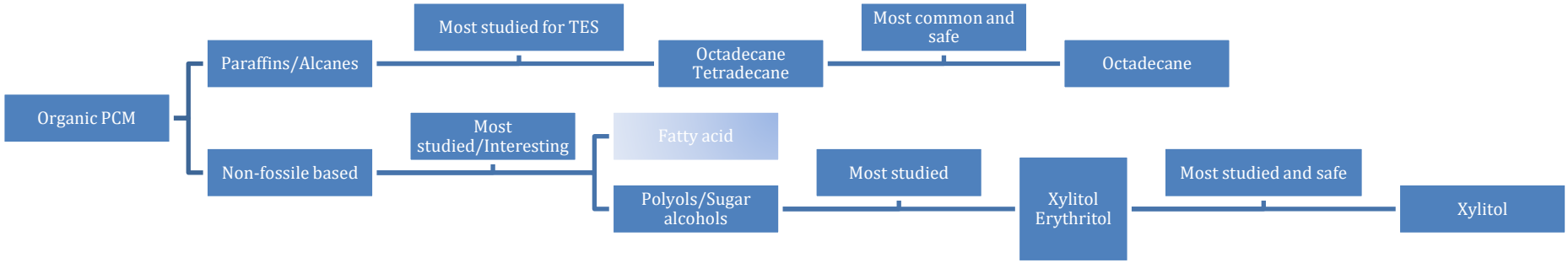

Figure 7: Flowchart of the screening process for organic PCMs

Table 2: Material data for the organic PCMs

Name	Chemical compound	T_m [°C]	ΔH_m [J/g]	C_p [J/mol·K]	Safety	Source
Octadecane	$C_{18}H_{38}$	28.0	244	*Solid:1800 Liquid:2300*	6	[30], [31], [17]
Tetradecane	$C_{14}H_{30}$	5.8	5.11	-	6	[32], [33], [34]
Capric acid	$CH_3(CH_2)_8COOH$	32.0	153	-	3	[14], [35]
Caprylic acid	$CH_3(CH_2)_6COOH$	16.0	149	-	4	[36]
Lauric acid	$CH_3(CH_2)_{10}COOH$	42-44	178	-	3	[37]
Myristic acid	$CH_3(CH_2)_{12}COOH$	58	186, 204	-	3	[38]
Palmitic acid	$CH_3(CH_2)_{14}COOH$	61, 64	185, 203	-	2	[39]
Xylitol	$C_5H_7(OH)_5$	94.0	263	*Solid: 323 Liquid:* 3146	2	[40], [41], [42]
Erythritol	$C_4H_6(OH)_4$	120.0	340	-	2	[43]
D-Mannitol	$C_6H_8(OH)_8$	167.0	316	-	1	[44]
Galactitol	$C_6H_8(OH)_6$	188.0	351	-	1	[45]

3.2.2 Safety Evaluation Parameters

Safety parameters of materials is a very broad category as materials can affect the human body in numerous ways, which can be very hard to quantify. When conducting an LCA it is of interest to quantify the results in order to ease comparison between different objects (materials or products), and we must therefore define a system which allows us to quantify the hazardous effects of different compounds to the human body in order to allow for a more general comparison. This system allows for a comparison between manufactured products, as it does not consider of the manufacturing process of the products.

There are several standards to use when classifying a compounds hazardous effects on human health and other aspects, such as environmental. One of the most widely used standards is the *EU CLP Regulation*, which came into use 2009, aligning existing EU legislation with the Globally Harmonized System (GHS). Using the CLP regulation as a basis for ranking the selected materials is therefore a logical choice as it can be expanded to most other materials for future work within this area [46].

For this report, we will adopt a simple, definitive, ranking system in order to easily categorize different PCMs according to different levels of risk. The system has six different categories, named 1,2,3,4,5 and 6, where a PCM that is harmless will place in at '1', and thereafter rise in placement as the levels of risk associated with the PCM increases. The levels of risks are consequently based on the GHS system and definitions. The placement will be based on the GHS hazard statements [47]. Our definition of each level is as follows:

1. Practically harmless
2. Causes temporary irritations and discomfort
3. May cause serious irritation and discomfort
4. Prolonged use may cause permanent damage
5. Causes permanent/and or serious damage
6. Interaction is fatal under GHS definition.

If a material has been allocated GHS hazard statements associated with different risk levels, the material will be ranked after the highest level of risk that the separate GHS hazard statements reach. The categorization of each level of risk can be observed in Table 3.

The levels of risk of an arbitrary chemical are based on their associated GHS hazard statements, which in themselves can at times be somewhat vague for the reader, as well as differ in allocated statements according to different sources. The established system is thus based on definitions that are subject to imbrication, which can be expected due to the difficulties of creating a simple quantifiable method of evaluating the associated health risks of chemicals. The system is however, for the scope of this report, suited for evaluation of a larger number of chemicals (i.e. screening processes) where a more in-depth analysis of the promising chemicals is to be recommended.

Table 3: Categorization and definition of the "level of risk" by GHS hazard statements

Level of Risk	Risk	GHS Hazard Statements[11]
1	Harmless	-
2	Mild	H315, H316, H320,
3	Moderate	H302, H303, H305, H312, H313, H317, H319, H332, H333, H335
4	Harmful	H301, H311, H314, H318, H331, H341, H360, H361, H361d, H362, H372, H373
5	Very harmful	H340, H350, H351, H370, H371,
6	Fatal	H300, H304, H310, H330,

[11] The GHZ Hazard Statements meaning can be found in appendix GHS hazard statements.

3.3 Goal and Scope of the conducted LCA

(Objective) The Goal of this LCA is to compare environmental, health and safety impacts of three different PCMs to find which option show the most potential as a PCM for heating applications in TES for future studies and use, and doing so, build upon the methodology framework when conducting LCAs within this area.

(Materials) The PCMs analysed are the organic fossil based Octadecane, organic non-fossil-based Xylitol and inorganic salt hydrate Manganese Nitrate Hexahydrate.

(System boundaries) The LCA will be conducted from cradle to grave. Figure 8: Simplified production chain from cradle to grave of paraffin wax with system flows shows the system boundaries chosen for Octadecane and are put together by previous LCIs [48], [49], [50], [51], various sources of the individual production steps [52], [51] and by estimation of usage and disposal. Figure 9 shows the system boundaries for Xylitol and are put together by previous LCIs [53], [54], [55], [56] as for Octadecane and by estimations of usage and disposal. Figure 10 shows the same for Manganese Nitrate Hexahydrate and are by the same means put together by previous LCIs and other sources [57], [58], [59], [60], [61], [62], [63], [64], [65], [66] and estimations of usage and disposal. The figures shows the basic production stages of each material and lifecycle phases with usage and disposal. All PCMs have been analysed under the same conditions under use (simple TES system from Figure 1), with the exception of disposal of the PCMs, where Octadecane and Xylitol has been assumed to be part of combustion and Manganese Nitrate Hexahydrate is assumed to be used for landfill, however, not data is available for the energy and emission of the landfill process, rendering the disposal of Manganese Nitrate Hexahydrate as *inconclusive*.

(System flows) Here system flows are defined as the energies, gases, solids and liquids that take a direct part of the products lifecycle by either being emitted or used in the process, the flows are represented in Figure 8, Figure 9 and Figure 10 by the arrows pointing in (substances being used) or out (substances being emitted) from the process block. The red arrows and blocks are representing hazardous substances, the green arrows and blocks are representing positive output, the blue are by/coproduct and the black are the process stages analysed. These system flows have been collected from previous LCI work for each material and screened by most impact or relevance to the chosen impact categories.

(Impact categories) In this LCA the impact categories chosen are GWP100, CED, EPBT, sustainability in use and Sustainability in production. The two categories last mentioned are combinations of how safe the material and its' process are in health and safety aspects during production and possible malfunction during use like leakage or fire. They are further defined by impact indicators described in chapter 3.4 Impact categories.

(Impact indicators) The indicators chosen to represent the main issues contributing to the chosen impact categories are greenhouse effect for GWP100 and energy efficiency for CED and EPT. More indicators are needed for the health, safety and sustainability aspects, those indicators are flammability, reaction to skin contact, inhalation, toxicity of vapour-, liquid- and solid phase[12] in both production and leakage in possible malfunction, acidification by emissions in both production and leakage in possible malfunction, recyclability and expected life time of the material.

[12] Reaction to skin contact, inhalation and toxicity of vapour-, liquid- and solid phase may be referred to human interaction safety as a collective term.

(The functional unit) of The LCI is 1 kg. The gathered data will therefore be recalculated to the values required in order to produce 1 kg of the selected PCM. The energy storage of the PCM will also therefore be based on 1 kg of the material.

(Assumptions) In order to include the transportations' impact in this LCA an assumption of similar transportation distances and methods for the materials are made in order to quantify a result. Because of difficulties finding data for the separation of the paraffin waxes and further processing to get Octadecane an assumption of ready product after filtering are taken.

(Value choices) During screening of PCMs materials with a high research rate was favoured in order to get good quality and quantity of data to the LCI. This may have led to a different material selection than the most energy efficient ones. Human interaction safety has also been given a high ranking in selection of material.

(Limitations) For Octadecane the production data are limited to the United States of America both onshore and offshore production of crude oil and wax. This is because the area has been studied more extensively there due to the oil boom during the early 2000s. Further no limitation has been considered due to difficulties to provide data.

(Report and critical review) This report is intended mainly for university students and researchers and are a part of the authors' bachelor theses. The report format will be as a technical report and the critical review will be conducted by students, postdoctoral researchers and professors as two oppositions, one halfway and one at the end, that will be documented but not published.

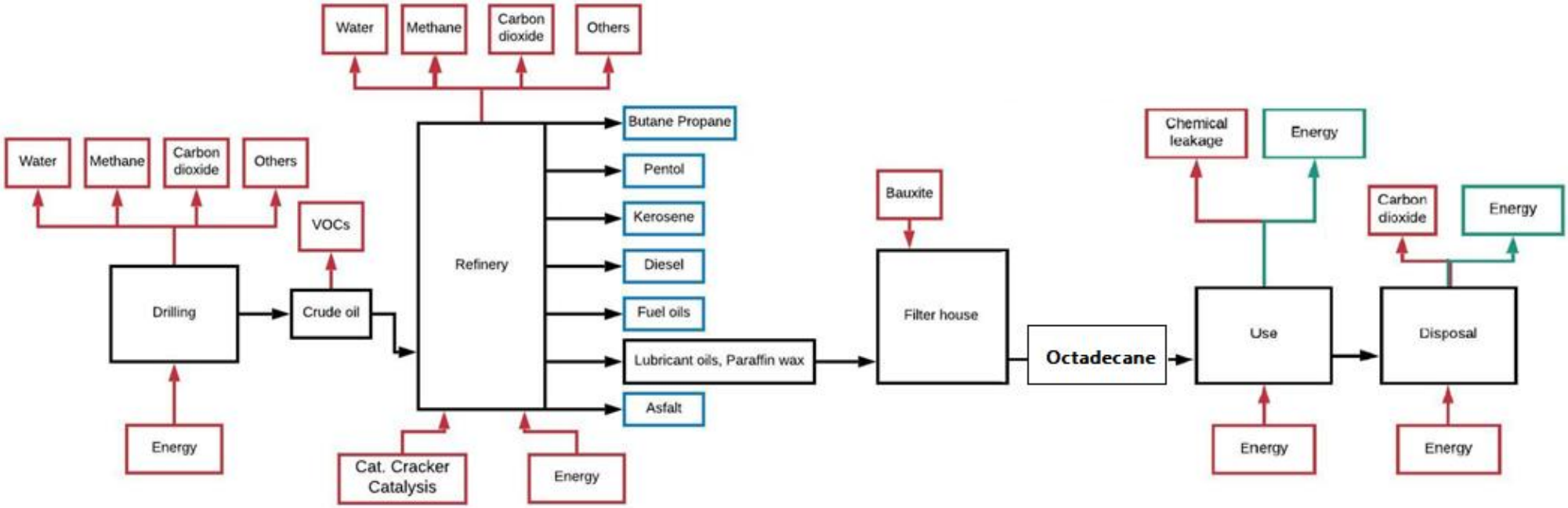

Figure 8: Simplified production chain from cradle to grave of paraffin wax with system flows

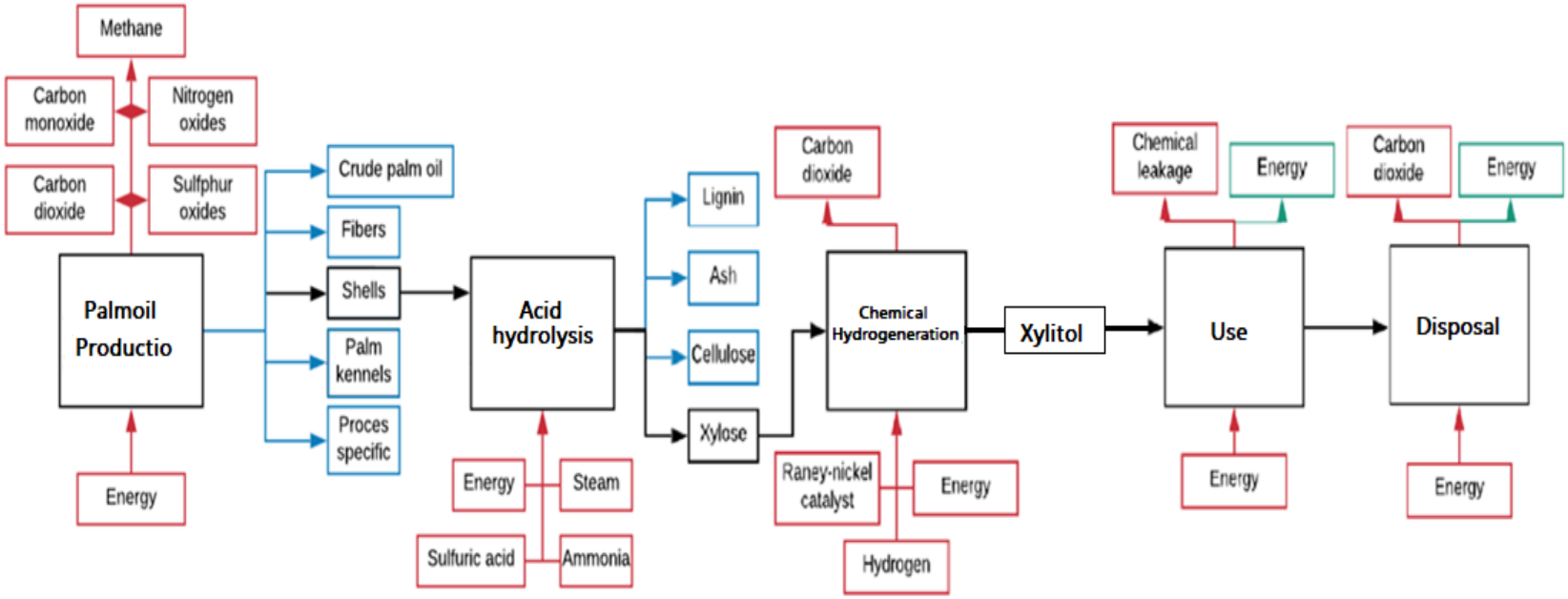

Figure 9: Simplified production chain from cradle to grave for Xylitol with system flows

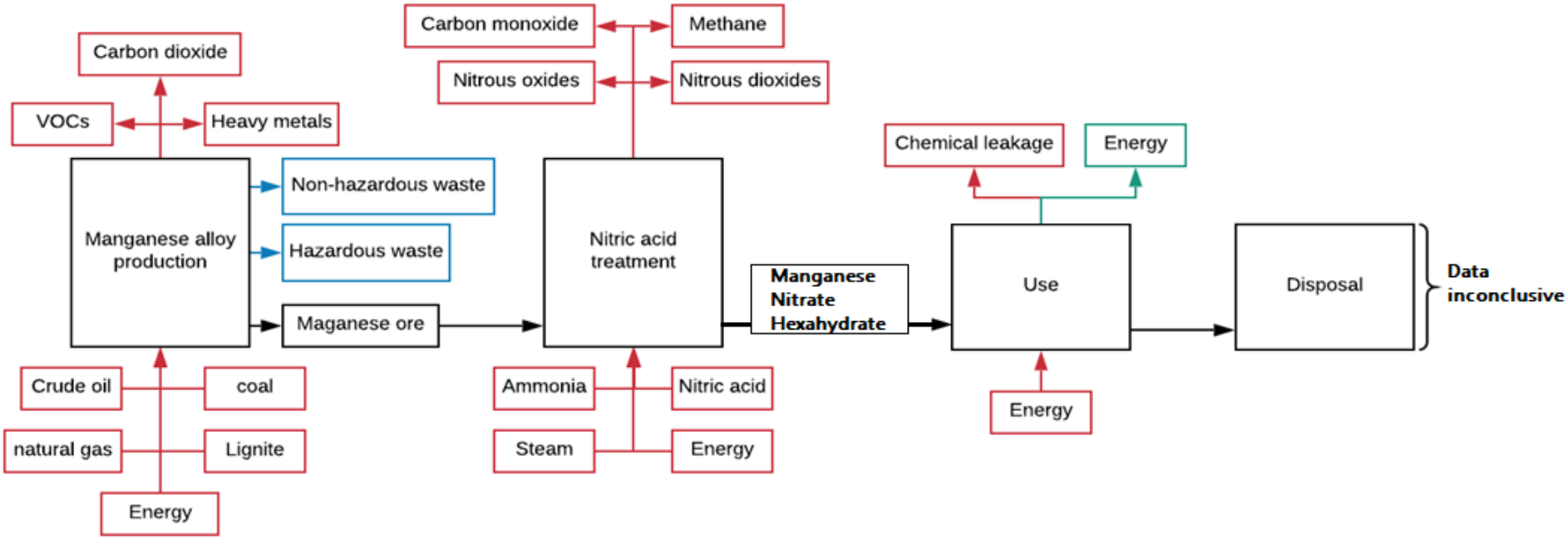

Figure 10: Simplified production chain from cradle to grave for Manganese Nitrate Hexahydrate with system flows

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3.4 Impact categories

3.4.1 Global Warming Potential (GWP)

GWP is a measurement of how much heat a greenhouse gas traps in the atmosphere relative to carbon dioxide over a period of 100 years. It is measured in carbon dioxide equivalents, $CO_{2,eq}$ where the unit is tonnes. GWP is calculated over a specific time, commonly selected as 20, 100 or 500 years, which will show different results as different greenhouse gases dissolves at different rates. The specific time used in this report is 100 years, thus denoted by GWP_{100}. The calculation for GWP_{100} is done using data given by the IPCC Fifth Assessment report, 2014 (AR5) [67], multiplying the amount of greenhouse gas by its conversion factor. Emitted gases that are lacking data in the report and will be viewed as non-greenhouse gases as and was consequently not considered when performing the calculations as they are assumed to have a negligible impact on the final result.

3.4.2 Cumulative Energy Demand (CED)

CED is a measurement of how much indirect and direct energy usage is required in order to produce the relevant amount of the product. In order to calculate this, the sum of all energy inputs in the manufacturing process from the LCI data is calculated.

3.4.3 Energy Payback Time (EPBT)

For this study, we are assuming that the selected PCMs are used in the same TES system and conditions, assuming that the only difference are the inherent enthalpies of fusion for the different PCMs. This is a rough approximation but will however present a relevant picture of the EPBT will behave for the selected materials (i.e. which one is the most likely to have the lowest actual EPBT). For this calculation, it was assumed that a PCM were to undergo 52 cycles (taking in and releasing energy) during one year, i.e. one cycle per week. The values are calculated according to Equation 1, where E_{in} is the total CED for the PCM and $E_{out.a}$ is the annual energy output for the PCM, which is calculated using the theoretical enthalpies of fusion. $E_{out.a}$ depends of the energy storage capacity of the PCM times the amount of annual cycles. The energy storage capacity, Q, of a PCM is defined according to Equation 2 [14]. To calculate Q for each given PCM, the initial temperature is assumed to be $T_{PC} - 1\ [K]$ and the final temperature is assumed to be $T_{PC} + 0.1\ [K]$.

Equation 1

$$EPBT = \frac{E_{in}}{E_{out.a}}$$

Equation 2

$$Q_{PCM} = \int_{T_1}^{T_{PC}} m * C_{P\ solid}(T) * dT + m * \Delta H_m + \int_{T_{PC}}^{T_2} m * C_{P\ liquid}(\mathrm{T}) * \mathrm{dT}$$

4. Result and Discussion

4.1 LCI

4.1.1 LCI for Octadecane

The values from Table 5 are taken from a previous LCI for the extraction of crude oil [48] and have been converted from total extraction of oil over one year to the amount of oil needed to produce 1 kg of paraffin wax. The amount needed is calculated from data stated in a previous LCI for diesel production [49] and the molecular weight of diesel and Octadecane. The values for the production are all multiplied with a factor of 1.51 taken from the ratio of the molar masses between the average diesel composition ($C_{12}H_{24}$) and Octadecane ($C_{18}H_{38}$) according to Equation 3. These factors are estimations and will contribute to some error in the interpretation and conclusion. Due to no data could be found in how much bauxite is needed to filter 1 kg of paraffin wax and how often the bauxite is replaced and how it is disposed, no conclusive results can be drawn from Table 5. By reasoning about the effects of bauxite and the energy needed to extract it the impact value can be considered high and are therefore considered as a negative effect going in to the LCIA and the interpretation. The Energy storage capacity are calculated with **Error! Reference source not found.** by using the heat capacity and enthalpy stated in Table 2.

Equation 3

$$\frac{\text{molar mass } C_{18}H_{38}}{\text{molar mass } C_{12}H_{24}}$$

The emissions from disposal are calculated from the balanced chemical reaction of combusting 1 kg (3.93 moles) of Octadecane in oxygen as shown in Equation 4.

Equation 4

$$3.93C_{18}H_{38}(s) + 108.075\ O_2\ (g) \rightarrow 70.74\ CO_2(g) + 74.76\ H_2O\ (g)$$

The energies emitted are calculated from Equation 4 where the difference of the formation enthalpies of the reactants (left side side) and the products (right side) and the energy needed for the combustion are taken from Octadecanes' enthalpy of vaporization [50] as shown in Equation 5 where ΔH_x are the enthalpies and n_x are the amount of moles in the balanced reaction.

Equation 5

$$(n_{octadecane} \cdot \Delta H_{Octadecane} + n_{Oxygen} \cdot \Delta H_{Oxygen}) - (n_{Carbondioxide} \cdot \Delta H_{Carbondioxide} + n_{Water} \cdot \Delta H_{Water})$$

Table 4: Enthalpies of formation relevant for combustion of octadecane

$\Delta H_{Octadecande}$	$92\ \frac{kJ}{mol}$	[50]
ΔH_{Oxygen}	$0\ \frac{kJ}{mol}$	[68]
$\Delta H_{Carbondioxide}$	$16.7\ \frac{kJ}{mol}$	[69]
ΔH_{Water}	$40.66\ \frac{kJ}{mol}$	[70], [71]

Table 5:LCI data for environmental impacts for 1 kg paraffin wax produced

Octadecane	Quantity [kg]	Source
Raw materials		[49]
Coal	$2.22 \cdot 10^{-2}$	
Oil	$6.43 \cdot 10^{-3}$	
Natural Gas	$5.94 \cdot 10^{-2}$	
Uranium	$5.30 \cdot 10^{-7}$	
Perlite (SiO_2)	$3.71 \cdot 10^{-4}$	
Limestone	$4.20 \cdot 10^{-3}$	
Water	$1.46 \cdot 10^{-3}$	
Bauxite (Filtering process)	*Data inconclusive*	[51]
Coproducts		[49]
Lubricant oils (ca 1.3 w.%[13] of the oil)	$8.38 \cdot 10^{-2}$	
Asphalt (ca 3.83 w.% of the oil)	0.24	
Other fuel (ca 94.69 w.% of the oil)	6.11	
Extraction of crude oil		
Energy usage	183.9 [MJ]	[48]
Air Emissions		[48]
Methane, Bromo trifluoro-, Halon 1301	$2.48 \cdot 10^{-7}$	
Methane, trifluoro-, HFC-23	$9.93 \cdot 10^{-7}$	
Water Emissions		[48]
Biological Oxygen Demand (BOD5)	$8.02 \cdot 10^{-3}$	
Chemical Oxygen Demand (COD)	$8.02 \cdot 10^{-3}$	
Dissolved Organic Carbon (DOC)	$5.31 \cdot 10^{-3}$	
Total Organic Carbon (TOC)	$5.31 \cdot 10^{-3}$	
Oils (unspecified)	$2.09 \cdot 10^{-3}$	
Soil emission		[48]
Oils (unspecified)	$3.20 \cdot 10^{-3}$	
Waste		[48]
Solid	~0	
Water	~0	
Production/ Refinery		
Energy usage		[49]
Primary Energy	4.27 [MJ]	
Fossil Energy	4.24 [MJ]	
Fuel Energy	65.7 [MJ]	
Air emissions		[49]
Carbon dioxide (CO_2)	$5.44 \cdot 10^{-1}$	

[13] Percent of total weigh of extracted oil.

Methane (CH_4)	$4.68 \cdot 10^{-4}$	
Nitrogen oxides (NO)	$1.14 \cdot 10^{-3}$	
Carbon monoxide (CO)	$3.78 \cdot 10^{-4}$	
Other hydrocarbons	$1.60 \cdot 10^{-3}$	
Formaldehyde	$1.70 \cdot 10^{-8}$	
Particulates (PM10)	$1.28 \cdot 10^{-5}$	
Particulates (unspecified)	$6.93 \cdot 10^{-4}$	
Sulphur Oxides (SO_x)	$3.86 \cdot 10^{-3}$	
Nitrous oxides (N_2O)	$1.10 \cdot 10^{-5}$	
Hydrogen Chloride (HCl)	$1.19 \cdot 10^{-5}$	
Hydrogen Fluoride (HF)	$1.49 \cdot 10^{-6}$	
Water emissions		[49]
Biochemical Oxygen Demand (BOD5)	$1.10 \cdot 10^{-3}$	
Chemical Oxygen Demand (COD)	$9.26 \cdot 10^{-3}$	
Metals (unspecified)	$1.36 \cdot 10^{-5}$	
Ammonia (NH_3)	$1.60 \cdot 10^{-4}$	
Nitrates (NO_3^-)	$1.88 \cdot 10^{-8}$	
Waste		[49]
Water	$1.46 \cdot 10^{-3}$	
Solids (hazardous)	$3.56 \cdot 10^{-3}$	
Solids (non-hazardous)	$1.39 \cdot 10^{-2}$	
Use		
Energy storage capacity	0.32 [MJ]	[50]
Disposal/combustion		
Energy used	0.09 [MJ]	
Energy emitted	8.86 [MJ]	
Emission from combustion		
Carbon dioxide	3.11	

As seen in Table 5:LCI data for environmental impacts for 1 kg paraffin wax produced the emittance of greenhouse gases are low in all stages while the biochemical oxygen demand (BOD5) and chemical oxygen demand (COD) are significantly higher which are an indicator of the quality of the surrounding water, where a higher BOD5 and COD values indicates a higher degree of water pollution. The amount of energy needed in both extraction and production/refinery for 1 kg of paraffin wax are very high but considering that the waxes are a by-product of the fuel (mainly diesel) production the value are reasonable although one may discuss if the value should represent the paraffin as an independent substance or as a coproduct to diesel. In this paper, wax have been treated as a coproduct which argues that the total emittance of the whole oil extraction and refinery processes are included in manufacturing of the paraffin. For the usage stage only the energy storage capacity have been analysed as the leakage of chemicals are considered to be a health and safety hazard aspect and will therefore be discussed in Table 6: Health and safety impact data for Octadecane. No data could be found on how to dispose of paraffin waxes except for ordinary wax candles which are disposed as household waste and thereafter combusted for energy. This together with paraffins' thermal properties at combustion (exothermic reaction) results in the assumption of disposal by combustion being recognized as plausible. The value representing the carbon dioxide emittance during combustion are high due to the high contents of carbon in one chain of Octadecane and may be elevated from real values due to the simplicity of the chemical reaction analysed for combustion of Octadecane shown in Equation 4 with only

carbon dioxide and steam as products when other gases and substances are likely to exist such as methane and coal.

For health and safety impacts various papers and surveys on the work environment in the oil industry are summarized and reflected in the first section of Table 6 (Extraction and refinery). For the second section of Table 6 (Use) safety risks of chemical leakage during use are reflected by the Material Data Safety Sheet of Octadecane. No data could be found concerning the disposal of Octadecane.

Table 6: Health and safety impact data for Octadecane

Octadecane	Hazard	Source
Extraction and refinery		
Accidents		
Hearing loss	76% of all workers	[72]
Immune disease	Exposed to harmful chemicals and particles, may cause death	[73]
Infectious disease	Exposed to harmful chemicals and particles, may cause death	[73]
Dermal disease	Exposed to harmful chemicals and particles, may cause death	[73]
Respiratory disease	80% of workers exposed to a higher rate of crystalline silica, may cause lung disease and cancer	[74]
Fatalities	1189 fatalities (2003-2013)	[75]
Use		
Chemical leakage		[76]
Flammability	Flash point 160-330.8 °C; emits CO and CO_2 when ignited	
Inhalation	May cause respiratory irritation, may be fatal if inhaled	
Skin contact	Causes skin irritation	
Eye contact	Causes eye irritation	
Ingestion	May be fatal if ingested	
Carcinogenicity	Not listed in any countries	
Disposal		
Managing waste	*Data inconclusive*	

The accidents for extraction and refinery are very high due to the heavy manual labour and high level of noise from the apparatus controlling the drilling. One can argue if paraffins should be considered an independent substance responsible for the accidents caused exclusively by the production of the wax or as a coproduct, as in this paper, where all the accidents for the entire operation are included. During use chemical leakage (not including water) are analysed by the MSDS for Octadecane which have a higher flammability risk due to its low flash point. The health risks of Octadecane are moderate if not ingested.

4.1.2 LCI for Xylitol

The data for the palm oil production in

Table 8 have been taken from a previous LCI for said process and have been recalculated by an average of the LCI results from the different palm mills and multiplying with a factor of 0.0056 to conform the values from 1 tonne of crude palm oil which gives an average of 1.16 tonnes of empty fruit bunches (EFB) to 6.58 kg of EFB which is needed to produce one kilogram of Xylitol. The calculations are shown in Equation 6. The average of the LCI results and the factor are estimates and can give reason to odd values. For the methane emission the value has been recalculated from cubic meters to kilograms by multiplying with the density of methane (0.668 kg/m^3) [62].
No data could be found of any other emissions than carbon dioxide to produce xylitol from xylose. Therefore, an assumption of other emissions are made due to the difficulty to achieve a reaction where all components are absorbed by the final product or products, however no numerical value is given to this category. The energy storage capacity
was calculated using Equation 2 and the enthalpy and heat capacity values stated in Table 1: Material data for the inorganic PCMs. The emissions from disposal are calculated from the balanced chemical reaction of combusting 1 kg (6.57 moles) of Xylitol in oxygen in Equation 7.

Equation 6

$$\frac{6.58\ kg\ EFB\ needed\ for\ 1kg\ of\ Xylitol}{1160\ kg\ EFB\ gathered\ from\ 1000\ kg\ of\ crude\ palm\ oil} \approx 0.0056$$

Equation 7

$$6.57\ C_5H_7(OH)_5\ (s) + 36.135\ O_2(g) \rightarrow 32.85\ CO_2(g) + 39.42\ H_2O\ (g)$$

The energy emittance is calculated from the difference in formation enthalpies of the reactants and products according to Equation 8. The energy needed for the combustion are taken from Xylitol's enthalpy of vaporization [56].

Equation 8

$$(n_{Xylitol} \cdot \Delta H_{Xylitol} + n_{Oxygen} \cdot \Delta H_{Oxygen}) - (n_{Carbondioxide} \cdot \Delta H_{Carbondioxide} + n_{Water} \cdot \Delta H_{Water})$$

Table 7: Enthalpies relevant for combustion of Xylitol

$\Delta H_{Xylitol}$	$111.1\ \frac{kJ}{mol}$	[56]
ΔH_{Oxygen}	$0\ \frac{kJ}{mol}$	[68]
$\Delta H_{Carbondioxide}$	$16.7\ \frac{kJ}{mol}$	[69]
ΔH_{Water}	$40.66\ \frac{kJ}{mol}$	[70], [71]

It is important to note that Xylitol production is a small part (and coproduct) of palm oil production and thus a relatively low part of the impact category data can be directly associated to it.

Table 8: LCI data for environmental impact for 1 kg of Xylitol produced

Xylitol	Quantity [kg]	Source
Raw materials		[53]
Empty Fruit Bunches (EFB)	6.58	
Sulfuric acid	0.13	
Ammonia	0.07	
Rayne-nickel catalyst	0.06	
Hydrogen	0.02	
Water	33.5	[53] , [54]
Coproducts		[53]
Lignin	1.29	
Cellulose	1.74	
Ash	0.24	
Extraction (palm oil production)		
Energy used:		[54]
Turbine (internal)	2.60 [MJ]	
Electricity	0.03 [MJ]	
Air emissions		[54]
Carbon dioxide	0.47	
Carbon monoxide	$4.57 \cdot 10^{-4}$	
Sulphur oxides	$8.80 \cdot 10^{-6}$	
Nitrogen oxides	$7.59 \cdot 10^{-4}$	
Methane	0.24	
Production		
Energy used		[53]
Electricity	0.12 [MJ]	
Heat	18.8 [MJ]	
Air emissions		[55]
Carbon dioxide	0.33	
Other	*Data inconclusive*	
Use		
Energy storage capacity	$9.28 \cdot 10^{-2}$ [MJ]	[56]
Disposal/combustion		
Energy used	0.108 [MJ]	
Energy emitted	1.421 [MJ]	
Air emissions		
Carbon dioxide	1.445	

As seen in

Table 8 the emittance of greenhouse gases in the extraction of palm oil are high, especially methane and carbon dioxide, which will give reason to higher values for GWP_{100} and may be elevated due to the adaption of Xylitol as a coproduct of palm oil, lignin, cellulose and ash and not as an independent substance responsible for the emittance exclusively for the collection of EFB to produce Xylitol. During production the energy needed from heat are very high due to the same reason. As discussed in 4.1.1 LCI for Octadecane only the energy storage capacity are included in the usage stage due to chemical leakage are considered a health and safety aspect and therefor discussed in Table 9: Health and safety impacts for Xylitol. For disposal no conclusive data could be found and an assumption of combustion due to the exothermic reaction at combustion of Xylitol are made. The values representing this stage may be elevated due to the simplicity of the reaction shown in Equation 7 where only carbon dioxide and steam are representing the products when there is a possibility there may occur other substances such as methane and coal.

In Table 9: Health and safety impacts for Xylitol the health and safety issues during extraction of palm oil production of xylitol, usage of Xylitol in TES and disposal of Xylitol are represented. The data have been adapted from MSDS for Xylitol [41] and an article about safety concerns in the palm oil industry [77].

Table 9: Health and safety impacts for Xylitol

Xylitol	Hazard	Source
Extraction		
Accidents		[77]
Chemical leakage	Leakage of n-Hexane which caused fire. 1 fatality (2011)	
Explosions	Bio-gas tank explosion. 1 fatality (2010), Sterilizing machine explosion, fatalities 4 (2013)	
Production		[41]
Skin contact	May cause irritation, may be harmful if absorbed though skin	
Inhalation	May cause respiratory irritation	
Ingestion	Low risk for industrial workers, may cause irritation in the digestive tract	
Carcinogenicity	*Data inconclusive*	
Eye contact	May cause irritation	
Flammability	*Data inconclusive*	
Use		[41]
Skin contact	May cause irritation, may be harmful if absorbed though skin	
Inhalation	May cause respiratory irritation	
Ingestion	May cause irritation in the digestive tract	
Carcinogenicity	*Data inconclusive*	
Eye contact	May cause irritation	
Flammability	*Data inconclusive*	
Disposal		
Managing waste	*Data inconclusive*	

Compared to the extraction and refinery of crude fossil based oil the accidents of extraction are very low and are occurring in isolated events caused by extreme circumstances, even if the data represented in the table are a few years old a number of three accident have been reported in a period of three years and considering the amount production sites the value is acknowledged as very low. The chemical leakage (except for water) during usage are mild due to the bio capability of Xylitol.

4.1.3 LCI for Manganese Nitrate Hexahydrate

The LCI data for Manganese Nitrate Hexahydrate is unavailable at the moment of writing, therefore an approximate of the LCI for the Cradle-to-Grave process is made by using information taken from *Lifecycle Assessment of Global Manganese Alloy production*, created by the International Manganese institute [57] The report assesses the LCI of average manganese alloy production. It can be shown that for the average manganese alloy, approximately 0.487 kg of unprocessed manganese ore, MnO_2 is left as a waste product.

Manganese Nitrate is created through nitric acid treatment of MnO, following the stoichiometric relation [58]:

Equation 9

$$MnO + 2HNO_3 \rightarrow Mn(NO_3)_2 + H_2O$$

MnO_2 can be reduced to MnO through several steps under temperatures up to 1700 ℃, following the stoichiometric relation [59], [60]:

Equation 10

$$2MnO_2 \rightarrow 3MnO + \frac{1}{2}O_2$$

Using these relations, we can calculate that in order to produce 1 kg of Manganese Nitrate, approximately 0.396 kg of MnO and 0.704 kg of $2HNO_3$ is required according to Equation 9. According to Equation 10, approximately 0.485 kg of MnO_2 is required to obtain 0.396 kg of MnO in the reduction process. We can thus approximate the LCI of manganese nitrate hexahydrate by combining the values taken from *Lifecycle Assessment of Global Manganese Alloy production* with separate LCIs for gate-to-gate nitric acid production [61], which requires further LCI information due to ammonia input [62], and thereafter its crude oil [63], coal [64] and natural gas inputs [65]. Using this data and recalculating the given values, we can obtain values for The LCI of Manganese Nitrate hexahydrate. This LCI is however an estimation as data components are missing (for example energy demands for the nitric acid treatment) and the fact that the data obtained from *Lifecycle Assessment of Global Manganese Alloy production* is misrepresented for our purposes as it based on several processes that would, for Manganese Nitrate production, be redundant and unnecessary. This should result in higher values of emissions and energy consumption than otherwise should be expected.

Table 10: LCI data for environmental impacts for 1kg of Manganese alloy produced

Manganese Alloy	Quantity [kg]	Scale	Source
Total raw material input	37.5		[57]
Crude oil	0.133		
Hard coal	1.85		
Lignite	$8.55 \cdot 10^{-2}$		
Natural gas	0.119		
Uranium	$1.75 \cdot 10^{-4}$		
Renewable resources	$8.24 \cdot 10^{-5}$		
Non-renewable elements	$1.85 \cdot 10^{-2}$		
Non-renewable resources	18.1		
Renewable resources	17.2		
Total material output	40.95		[57]
Waste for recovery	1.05		
Manganese ore	0.487		
Hazardous waste	1.25		
Non-hazardous waste	38.7		
Total Energy Usage	[MJ/kg]		
Non-renewable sources	71.1		[57]
Crude oil	5.63		
Hard coal	49.5		
Lignite	1.02		
Natural gas	5.14		
Uranium	9.81		
Renewable sources	2.35		[57]
Other	$4.70 \cdot 10^{-3}$		
Emissions to air	[kg]		
Total emissions to air	20.3		[57]
Heavy metals to air	$1.9 \cdot 10^{-5}$		
Inorganic emissions to air	5.88		
Ammonia	$1.85 \cdot 10^{-5}$		
Ammonium	$8.60 \cdot 10^{-12}$		
Carbon dioxide	5.80		
Carbon monoxide	$2.07 \cdot 10^{-2}$		
Hydrogen chloride	$7.07 \cdot 10^{-4}$		
Nitrogen dioxide	$2.68 \cdot 10^{-3}$		
Nitrogen monoxide	$2.63 \cdot 10^{-10}$		
Nitrogen oxides	$1.60 \cdot 10^{-2}$		
Nitrous oxide	$9.31 \cdot 10^{-5}$		
Sulphur dioxide	$3.09 \cdot 10^{-2}$		
Sulphur hexafluoride	$1.28 \cdot 10^{-9}$		
Organic emissions to air (VOC)	$1.15 \cdot 10^{-2}$		
Other emission and particles	1.45		
Other emission and water losses	[kg]		
Total emissions to fresh water			[57]
Analytical measures	$5.78 \cdot 10^{-3}$		
Ecoinvent long-term	$2.91 \cdot 10^{-4}$		
Heavy metals	$1.88 \cdot 10^{-3}$		
Inorganic emissions	$1.61 \cdot 10^{-2}$		
Organic emissions	$8.25 \cdot 10^{-5}$		
Particles	$3.42 \cdot 10^{-3}$		
Total emissions to seawater			[57]
Analytical measures	$1.17 \cdot 10^{-4}$		
Heavy metals	$3.30 \cdot 10^{-6}$		
Inorganic emissions	$3.17 \cdot 10^{-3}$		

Organic emissions	$1.48 \cdot 10^{-5}$		
Other emissions	$1.60 \cdot 10^{-9}$		
Particles	$1.75 \cdot 10^{-3}$		
Emission to agricultural and industrial soil			[57]
Heavy metals	$4.74 \cdot 10^{-6}$		
Inorganic emissions	$1.15 \cdot 10^{-4}$		
Organic emissions	$7.29 \cdot 10^{-5}$		
Other emissions	$3.88 \cdot 10^{-6}$		
Use	[MJ/kg]		
Energy storage capacity	$4.49 \cdot 10^{-2}$		
Disposal	[MJ]		
Data inconclusive			

Table 11: LCI data for environmental impacts for 0.704 kg of Nitric acid produced (gate to gate)

Nitric Acid	Quantity	Source
Total Material input	[Kg]	[61]
Ammonia	0.190	
Steam	No data available	
Total energy usage	[MJ/kg]	[61]
District heat	No data available	
Electricity	No data available	
Emissions	[kg]	[61]
Nitrous oxide	$6.35 \cdot 10^{-3}$	
Nitrogen dioxide	$7.11 \cdot 10^{-4}$	

Table 12: LCI data for environmental impacts for 0.19 kg of Ammonia produced (gate to gate)

Ammonia	Quantity	Source
Total material input	[kg]	[62]
Coal	0.749	
Crude oil	1.01	
Total energy usage	[MJ/kg]	[62]
Electricity	$5.70 \cdot 10^{-2}$	
Natural gas	6.00	
Emissions	[kg]	[62]
N-tot (nitrogen to water)	No data available	

Table 13: LCI data for environmental impacts for 0.7486 kg of coal extracted

Coal	Quantity	Source
Total material input	[kg]	[64]
Raw Coal	1.41	
Process air	3.38	
Process water	2.13	
Total energy input	[MJ/kg]	[64]
Electricity	$7.49 \cdot 10^{-2}$	
Emissions	[kg]	[64]
Methane	$7.49 \cdot 10^{-3}$	
Chlorides	$2.47 \cdot 10^{-4}$	
Carbon monoxide	$5.24 \cdot 10^{-5}$	
Ammonium	$2.99 \cdot 10^{-5}$	
Nitrogen oxide	$9.77 \cdot 10^{-5}$	

Particulates	$3.74 \cdot 10^{-5}$	
Sulfur dioxide	$7.49 \cdot 10^{-6}$	
Sulphates	$5.98 \cdot 10^{-3}$	
VOC	$1.50 \cdot 10^{-5}$	
Other (non-gases)	6.1407	

Table 14: LCI data for environmental impacts for 1.0127 kg of crude oil extracted

Crude Coal	Quantity	Source
Total Energy input	[MJ/kg]	[63]
Thermal energy	0.7696	
Emissions	[kg]	[63]
Carbon dioxide	$5.663 \cdot 10^{-2}$	
Oil	$1.587 \cdot 10^{-5}$	

Table 15: LCI data for environmental impacts for 6.004 kg of Natural gas extracted (assuming density of 0.84 kg/Nm3)

Natural gas	Quantity	Source
Total energy input	[MJ/kg]	*[65], [66]*
Hydro power	$3.40 \cdot 10^{-2}$	
Coal	0.230	
Crude oil	1.67	
Natural gas	11.6	
Emissions and residue	[kg]	*[65]*, [66]
Benzene	$3.40 \cdot 10^{-4}$	
Ammonium	$2.40 \cdot 10^{-3}$	
Carbon dioxide	0.870	
Chlorodifluoromethane	$1.00 \cdot 10^{-8}$	
Hydrochloric acid	$1.30 \cdot 10^{-6}$	
Hafnium	$2.00 \cdot 10^{-7}$	
Nitrous oxide	$1.80 \cdot 10^{-5}$	
NMVOC	$5.20 \cdot 10^{-4}$	
Nitrogen oxides	$4.00 \cdot 10^{-3}$	
Particles	$6.60 \cdot 10^{-5}$	
Sulfur oxides	$6.70 \cdot 10^{-4}$	
Hazardous waste	$8.70 \cdot 10^{-3}$	
Other waste	$7.90 \cdot 10^{-2}$	

The LCI for Octadecane is shown in table 11 to table 15. The data shows high values for both greenhouse gas emissions as well as energy input for the whole process, which were to be

expected considering that table 11 is based on the average manganese alloy production which can be considered to be a lot more energy intensive process relative to manganese nitrate production and thus shows higher values than should be expected for the total LCI. Throughout the process, the LCI shows a high amount of industrial leakage (according to table 11), chemical and metal, to agricultural soil, fresh- and seawater as well as air emissions. It is worth to note that the LCI data for ammonia production (table 12), coal extraction (table 13), crude oil extraction (table 14) and natural gas extraction (table 15) are not as comprehensive as the LCI data for the Manganese alloy production (table 11). Due to no data being available for disposal, landfill is assumed (inconclusive).

Table 16: Health and safety impacts for Manganese Nitrate Hexahydrate

Manganese Nitrate Hexahydrate	Hazard	Source
Use		
Chemical leakage (Manganese nitrate hexahydrate)		[29]
Skin contact	May cause irritation. May be harmful if absorbed.	
Inhalation	Causes respiratory tract irritation. May be harmful if inhaled.	
Ingestion	May cause irritation of the digestive tract. May be harmful if swallowed. May cause nausea, vomiting and diarrhoea.	
Carcinogenicity	*No available data*	
Eye contact	May cause irritation.	
Flammability	May intensify fire	
Disposal		
	Inconclusive	

Data of industrial accidents directly related to manganese nitrate production, as well as manganese extraction was not available. The hazard risks in event of chemical leakage/human interaction is based a material data safety sheet for Manganese nitrate hexahydrate and obtains a moderate level of risk according to the previously established system in section 3.2.2.

4.2 LCIA

Given the LCI data from section 4.4 for the separate PCMs, we can now evaluate the information and establish a comparison for the selected materials. This is done by calculating the GWP_{100}, CED and EPBT values as well as comparing the health and safety impacts for each PCM.

The global warming potential of each material is plotted in Figure 11, given the LCI data, it can be seen that the production and disposal of Manganese Nitrate Hexahydrate produces the most amount of $CO_{2,eq}$ and has therefore the largest impact on climate change of the selected materials.

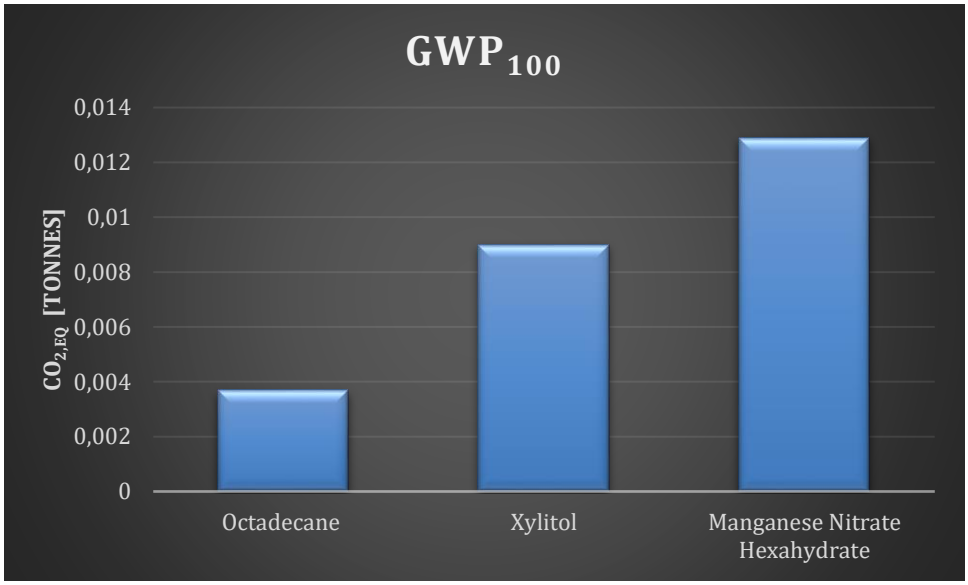

Figure 11: Plot of GWP100 values for the selected PCMs

The results for the CED calculations can be seen in Figure 12. Given the LCI data, it was found that the production of Octadecane requires the most energy, while Xylitol require comparatively little energy for its production.

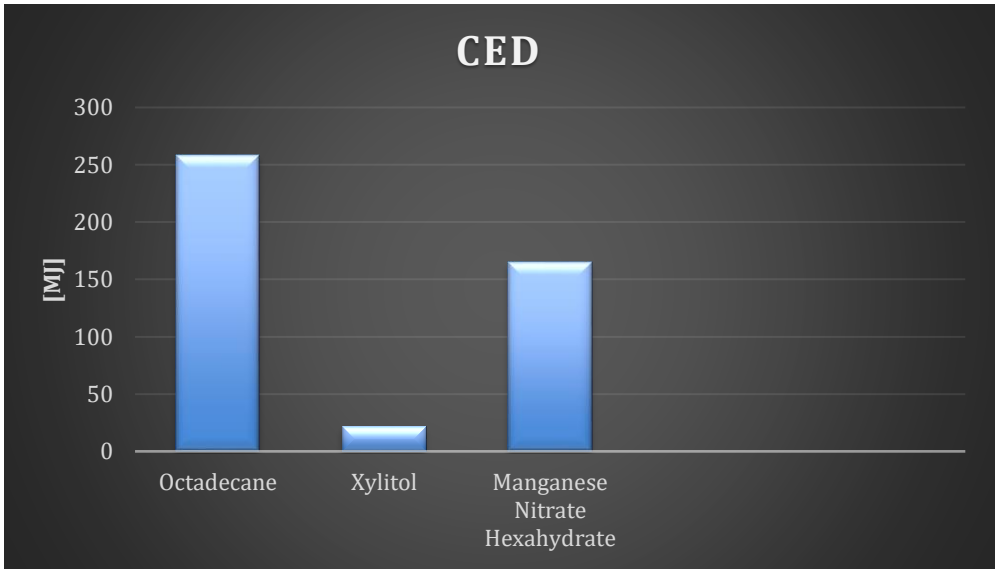

Figure 12: Plot of the CED values for the selected PCMs

The EPBT results of the can be seen in Figure 13. According to the calculation method described in section 3.4.3, Xylitol shows the least amount of time in order to achieve a net-zero energy investment.

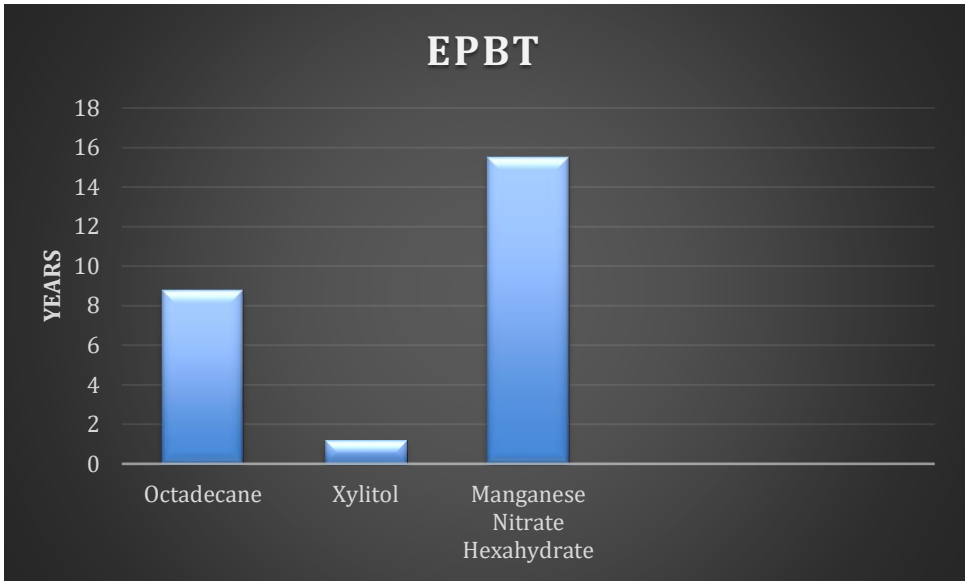

Figure 13: Plot of the estimated EPBT values for the selected PCMs

The safety impact category is, as stated, harder to quantify and therefore difficult to compare relative to the other impact categories of this LCA. The previously established system in section 3.2.2 was made in order to ease comparison between the finished products, not including the safety risks associated with the manufacturing process. The result of the evaluation can be seen in Table 17. As the table shows, the PCM that shows the highest level of risk is Octadecane, due to it being potentially fatal if swallowed or entering airways. Xylitol and Manganese Nitrate Hexahydrate has been given a 2 and 3 respectively and are therefore recognized as relatively safe to interact with.

Table 17: Level of risk associated with the selected PCMs

PCM	Level of Risk
Octadecane	6 (Fatal)
Xylitol	2 (Mild)
Manganese Nitrate Hexahydrate	3 (Moderate)

The safety and health risks associated with the manufacturing process of the separate PCMs are harder to quantify but are important to discuss regardless in order to obtain a satisfactory conclusion. A way to obtain a better view of the relevant manufacturing sector could be to look at the chemical leakage of the industry, emissions to air, water and soil during extraction and manufacturing, as well as the safety standards for the workers.

4.3 Life Cycle Interpretation

From the data presented in previous chapter interpretations of the most promising PCM in each category can be made. The data for the use and disposal comes from assumptions and the production LCI data comes from different approximation methods given different starting conditions, these methods are explained in section 3.3. The selected materials were compared using different impact parameters, where further assumptions were made in order to develop a comparison of the PCMs. The results indicate that Xylitol is the better choice for a PCM used for TES purposes, as Xylitol was given the more favourable result in three out of four impact categories, CED (Figure 12), EPBT (Figure 13) and level of risk (Table 17). The category where Xylitol does not show the best results in was GWP_{100} (Figure 11), where Octadecane have the advantage but the fact that Octadecane is produced using fossil resources and lacking data for the bauxite needed for filtering indicates that the result for this impact category should be discussed further. The material showing least potential according to our findings is Manganese nitrate hexahydrate which other than high GWP and EPBT is known to emit heavy metals in to drinking water during the manufacturing process.

The health and safety impact categories have been investigated and using our defined method of rating the PCMs according to their GHS hazard statements established in section 3.2 we can see that for the finished products (i.e. post-manufacturing phase), Octadecane shows the highest level of risk. It should however be noted that Octadecane was given this level of risk due to it being potentially fatal if swallowed or entering airways [31]. It also of interest to note that Octadecane has been shown to have high flammability, this is certainly a factor that needs to be given great consideration for Octadecane applications within TES systems. This is not a proclamation that Octadecane is unsuited for PCM usage, but the result should be considered if Octadecane were to be used for commercial applications, conveying more importance to the security aspects of such a system.

To evaluate the safety and health aspects of the manufacturing phase of each material was considered but it was deemed too big of a task to establish a system for quantification of this impact area given the scope of this study. Creating a fair comparison between the different manufacturing sectors is a hard task due to, amongst other things, the difference in scale of the sectors. One can for example look at separate instances of accidents, such as shown in the LCI for Octadecane, however comparing these number of instances to the manufacturing process for Xylitol and Manganese nitrate hexahydrate is an unjust method, due to the difference of amount of workers in the sectors and the relative lack of proper documentation. It would be a more just comparison to evaluate the general safety standards for workers of each industry, as opposed to separate incidents. The health impact category can be discussed from a risk analysis point of view, i.e. in which ones of the manufacturing process is there a risk of chemical leakage that affects the health of individuals, and how big the risk of said leakage is. Considering this approach one can refer to amount of global oil spills when discussing the manufacturing Octadecane, which in 2018 amounted to approximately 116,000 tonnes (the largest recorded in 24 years) solely due to oil tankers [78], and the health effects of such, which can be indicated by studies following the Deepwater Horizon offshore drilling

rig disaster [79]. In contrast, the leakage of heavy metals to fresh water, seen in Table 10, for the manufacturing phase of manganese alloys is also a topic of interest in this area. Manganese leakage itself has shown indications to be harmful to human as the manganese content of drinking water has increased [80]. Discussing and developing a quantifiable measurement for the risk of harmful chemical leakage is certainly an interesting option and something that would be recommended for future work.

In order to obtain the given results, several assumptions and approximations were made throughout the report. These were made in order to translate the given LCI data for the respective manufacturing processes and in doing so, several aspects of the products manufacturing process were neglected such as transportation as well as energy usage for several processes (for example the energy requirements for the processes shown by Equation 9 and Equation 10). Further approximations were also made in the EBPT-calculations given that a simplification of the enthalpy storage calculation was made. It is also of note that the final melting temperature of the selected PCMs are not equal as the melting temperature of Xylitol is considerable higher than that of the Octadecane and Manganese nitrate hexahydrate, implying that xylitol may not be suited for the same applications as the other two materials. As a result, it may not be appropriate to assume the same TES system properties for each of the respective PCMs. Considering the approximations and assumptions discussed above, it would not be appropriate to view the results of the impact categories as accurate, as they should instead be interpreted as indicative to an extent.

To obtain data for the LCIs of the different materials' large amounts of assumptions and approximations have been made due to the lack of available resources. The resources to facilitate a proper LCA with restricted assumptions are a LCI database such as EcoInvent [81] or LCA software such as SimaPro [82] which have been used in previous work. For further research in this area a LCI database is recommended if no contact with a manufacturing or producing company are obtained and an LCA software. Alongside this database and software an elaborate methodology for quantifying health and safety aspects of the life cycle are also recommended.

5. Conclusion

A definite PCM most suitable for TES cannot be determined due to the number of assumptions and approximations made in this report as well as due to a lack of suitable LCI data sources. However, the results indicate that Xylitol shows relatively high promise for TES usage and it is therefore recommended that further research on Xylitol as PCM for TES should be conducted.

6. Recommendations and Future work

For future work in the area help from software and databases are recommended and to develop a more adequate method of quantifying health and safety aspects of the production chain between different manufacturing areas as well as the hazards of the finished products in order to adequately compare a larger number of PCMs concerning these impact categories.

7. Acknowledgements

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Appendix

GHS hazard statements

Global Harmonized System (GHS) hazard statements are a phrase connecting to a code stating the nature and severity of the chemical hazard. The codes for these phrases all start with the letter H and followed by three numbers. H2xx stands for physical hazards, H3xx stands for health hazards and H4xx stands for environmental hazards [83]. The GHS hazards used in this report are stated and explained bellow.

H300: Fatal if swallowed
H301: Toxic if swallowed
H302: Harmful if swallowed
H303: May be harmful if swallowed
H304: May be fatal if swallowed and enters airways
H305: May be harmful if swallowed and enters airways
H310: Fatal in contact with skin
H311: Toxic in contact with skin
H312: Harmful in contact with skin
H313: May be harmful in contact with skin
H314: Causes severe skin burns and eye damage
H315: Causes skin irritation
H316: Causes mild skin irritation
H317: May cause an allergic skin reaction
H318: Causes serious eye damage
H319: Causes serious eye irritation
H320: Causes eye irritation
H330: Fatal if inhaled
H331: Toxic if inhaled
H332: Harmful if inhaled
H333: May be harmful if inhaled
H335: May cause respiratory irritation
H340: May cause genetic defects
H341: Suspected of causing genetic defects
H350: May cause cancer
H351: Suspected of causing cancer
H360: May damage fertility or the unborn child
H361: Suspected of damaging fertility or the unborn child
H361d: Suspected of damaging the unborn child
H362: May cause harm to breast-fed children
H370: Causes damage to organs
H371: May cause damage to organs
H372: Causes damage to organs through prolonged or repeated exposure
H373: May cause damage to organs through prolonged or repeated exposure

Calculations

Sample calculations:

Equation 11: calculation of energy released during combustion of Octadecane

$$(3.93 \cdot 92 + 108.075 \cdot 0) - (70.74 \cdot 16.7 + 74.76 \cdot 40.66) = -3859.5396\ kJ \approx -8.859\ MJ$$

Equation 12: Calculations of energy released during combustion of Xylitol

$$(6.57 \cdot 111.1 + 36.135 \cdot 0) - (32.85 \cdot 16.7 + 39.42 \cdot 40.66) = -1421.4852\ kJ \approx -1.421\ MJ$$

Equation 13: sample calculation of GWP_{100} for Octadecane

$$\frac{1}{1000} \cdot (1 \cdot 0.54422665 + 265 \cdot 0.0000109928 + 6290 \cdot 0.000000248 + 12400 \cdot 0.000000993 + 3.93) = 0.003671012862 \frac{tonnes\ CO_{2,eq}}{tonnes\ Octadecane} \approx 3.67 \frac{kg\ CO_{2,eq}}{kg\ Octadecane}$$