Environmental damage costs linked to Hydrofobes raw materials

Master’s thesis in Technology Management and Economics

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SUMMARY

Industries play a major role to the environmental issues we are facing for the past decade and the most frequently used of industrial products is general household cleaning product. Nouryon Company cooperated with IVL Swedish Environmental Research Institute is working on a project to discover the innovative production to enhance sustainability and environmental friendly product. Hence, one strategy to mitigate the environmental impact is changing the raw material source from synthetic to biogenic resources.

This study is focused on investigating different raw materials. In total, four C10 compounds with hydrophobic properties will be assessed. The raw materials to be investigated are first, synthetic 2-propylheptanol. Second, Isodecyl alcohol, Third, is linear synthetic C10 alcohol. And the last one is Natural C10 alcohol from palm kernel, this fatty alcohol is derived from the plant sources which remain a largescale feed stock. A Life Cycle Assessment (LCA) will be performed to see which one of the four raw materials are environmentally preferable by analyzing the environmental impacts and environmental damage cost.

According to the results, biogenic hydrofob provided higher environmental impact and environmental damage cost than the synthetic one because of the agricultural stages (preparation of land use and using fertilizer). For the synthetic hydrofob, the major drivers of the environmental impact and environmental damage costs are from carbon dioxide emission and crude oil used as a resource.

The aspects that can be considered to reduce the environmental issues for hydrofob raw material production are using RSPO-certified palm oil instead of non-certified palm oil, recirculating aluminium powder in the production of linear synthesis C10 alcohol since it is the second largest environmental impact contributor. And studying on different approach to renewable sourcing for route of ethylene because a lot of synthetic route included utilizing pf ethylene.

Keywords: Hydrofob, Fatty alcohol, Surfactant for cleaning product, Life Cycle Assessment, Environmental Priority Strategies (EPS).

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Oraphitchaya Rattanakoch, August 31st of 2020

Contents

List of Abbreviations

LCA	Life Cycle Assessment
EPS	Environmental Priority Strategies
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
EoL	End of Life
f.u.	Functional Unit
ISO	International Organization for Standardization
GWP	Global Warming Potential (kg CO2 eq.)
AP	Acidification Potential (kg SO2 eq.)
EP	Eutrophication Potential (kg Phosphate eq.)
ODP	Ozone Layer Depletion Potential (kg R11 eq.)
POCP	Photochemical Ozone Creation Potential (kg Ethene eq.)
NaV	Nature Capital and Value Creation
U.S.	United States
EU	European Union

1. Introduction

At this stage, environmental problems have become one of the subjects in everyday life's conversation in all age groups (BBC News UK, 2020). People are starting to concern much more about the environment today since environmental warning signs are happening now and then. For instance, the earth is warming up, rainforests are burning at uncommon levels, and species are at risk of extinction. These can be called the issues surrounding climate change. Climate change is attributed directly or indirectly to unsustainable human activities. Not only the climate change but environmental degradation can also have a significant impact on human health such as respiratory diseases. The main important causes come from air pollution and exposure to hazardous chemicals. Additionally, ecosystem destruction is one of the environmental impacts that influences on everything since an ecosystem is a community of all living organisms that rely on each other. Ocean acidification, water pollution, deforestation, habitat loss, overuse natural resources, and others, all of those are threatening the balance of an ecosystem biodiversity and leading to the extinction of many species. Furthermore, the amount of resources available on earth have been used without reuse or recycling for a decade which leads to the depletion of abiotic resources, another one of the important environmental impacts. Many environmental campaigns are conducted to raise people's awareness of environmental issues. There are however the strategies to mitigate the environmental impacts among the industrial field. The reason that industry becomes a focal point is every single industry field, food, energy, automobile, textile, and others can cause environmental issues. And consuming nonrenewable material and energy plays a major role in increasing environmental impacts. Hence, one strategy for mitigation is aiming to apply sustainable production processes in everyday products. It can also be implied to changing from using synthetic raw material to biogenic raw material in production processes. The most frequently used of everyday industrial products are personal hygiene and general house cleaning products. The global household cleaning product market was valued at about 30 billion U.S. dollars in 2019 (Statista, 2020) and it is expected to grow by 15.7 billion U.S. dollars during 2020 and 2024 (Technavio, 2020). Those are the application of surfactant and polymer made from hydrofob raw material. Hydrofob raw material has a wide range of applications not only personal care and cleaning products but also construction materials, paints, and electronic materials. To narrow down the application areas, cleaning will be used as an application segment by reason of it is the most frequently used and it is close to people in everyday life. It would thereby be of interest to study the environmental impacts through the life cycle of both synthetic and biogenic hydrofobes in collaboration with the surfactant and polymer producer Nouryon Company. Moreover, as it was mentioned above, there is an issue in environmental impact from utilizing cleaning product to climate change, greenhouse gas, even to human health, and more so that the bigger picture should be taken in consideration. Therefore, Environmental Priority Strategies (EPS) was decided to use as a weighting method in Life Cycle Assessment (LCA) because it could capture a wide variety of different impact.

1.1 Background

Surfactants and polymers for cleaning are one of the main products from Nouryon Company. Cleaning products are close to people and used every day in household cleaning such as kitchens, bathrooms, and cars to industrial cleansing in factories, schools, and hospitals. Nouryon Company corporate with IVL Swedish Environmental Research Institute is working on a project to discover the innovative production to enhance sustainability and environmentally friendly products. This research project is named Nature Capital and Value Creation (NaV).

1.1.1 Nature Capital and Value Creation (NaV) project

Nature Capital and Value Creation (NaV) is a research project that has been started since November 2018 with the cooperation of IVL Swedish Environmental Research Institute, Chalmers University of Technology, Volvo cars, Volvo group, Nouryon, and Swedish EPA. The project's purpose is to study the effectiveness of the use of different types of resources by using a metric for resource efficiency (sustainable accounting for measuring resource efficiency across life cycle stages). The project is divided into five case studies in total. This study, Environmental damage costs linked to Hydrofobes raw materials, is one of them. The natural capital impact result will be expressed by using Environmental Priority Strategies (EPS) method.

1.1.2 Purpose

The purpose of this project is to inquire into both environmental damage costs and environmental impacts of four raw materials in the production of surfactants and polymers for cleaning application by applying monterarization. The monetary weighting methods within Life Cycle Assessment (LCA) that will be utilized in this project are Environmental Priority Strategies (EPS).

The objectives of this project are:

- Better understanding of what environmental impact and environmental damage costs of hydrofob raw material that can cause in the future.
- To compare the environmental impact of four different hydrofobes raw materials.
- How costs of environmental impact can affect the cost of raw material and possible the end consumer products costs.
- To compare the environmental impacts through the cradle to gate perspective between biogenic hydrofobes (natural C10 alcohol) and synthetic hydrofobes (2-propylheptanol, Isodecyl alcohol, and linear synthetic C10 alcohol).

1.2 Life Cycle Assessment (LCA) methodology

Life Cycle Assessment (LCA), according to Baumann and Tillman (2004), is an assessment tool for studying a whole product system in an environmental viewpoint includes environmental impacts and environmental costs. A whole product system or a product's life cycle begins since the extraction of raw materials, through the manufacturing process, use phase, to waste management steps, and cycles back to the nature or ends up in other products (Bengtsson, 1998) which can be defined as cradle-to-grave.

LCA applications that are listed in international standard of LCA according to Baumann and Tillman (2004) are decision making, learning and exploration the environmental properties of the product system, and communication. The aim of LCA with these three applications are to improve and change throughout the life cycle of products in order to reduce the variety of environmental issues. The environmental issues could be related to natural environment, man-made environment, and human health and resources (Jacob Lindberg, 2014).

The life cycle assessment method is divided into 4 main parts include goal and scope definition, inventory analysis which indicates model construction and calculation, impact assessment where inventory results are converted to environmental values, and interpretation. The whole Life cycle Assessment methodology are described in appendix A1.

1.3 Monetary valuation

Monetarization or monetary weighting method is one of the four optional steps (normalisation, grouping, weighting, and data quality analysis) in life cycle impact assessment (LCIA). After classification and characterization, the weighting step will be processed due to the need for further aggregation of the characterization results. Monetarization is a method to convert environmental impacts to single environmental cost. There are several monetary weighting methods that can be used, for example EPS, LIME, Ecovalue, ExturnE, Step-wise, and Ecovalue (Jacob Lindberg, 2014). The monetary weighting methods that is utilized in this study is Environmental Priority Strategies (EPS). A more description of EPS can be found in the section below.

Environmental Priority Strategies (EPS)

In the year 1989, Bengt Steen proposed a weighting method to investigate the environmental impacts thoroughly the entire life cycle of products. The method known as Environmental Priority Strategies (EPS). The development of EPS started with the collaboration of the Swedish Environmental Research Institute and the Federation of Swedish Industries (The Industrial Green Game, 1997). Environmental priority strategies (EPS) is the method based on endpoint and monetarization. The monetary value of the environmental impact will be estimated by focusing on endpoints, safeguard subjects and then weighting will be performed by considering the monetary values of the endpoints. The endpoint impact categories carry damages to human health, ecosystem production, abiotic stock resources, and biodiversity (Steen, 1999a; Steen, 1999b). Different endpoints are given different monetary weights depend on their severity. The relationship between safeguards subjects, endpoint impact categories, and their specific weighting factors are shown in the table A3.1 in the appendix A.

2. Description of the study

2.1 Hydrophobic and hydrophilic materials

The phenomenon in material is a general result from material property. The diversity of properties brings up several applications of materials. Hydrophilic and hydrophobic are one of the surface properties that could provide a significant impact on the performance of materials. Hydrophilic and hydrophobic materials are defined by the geometry of water on a flat surface which will create different phenomena (David L. Chandler, 2013). On hydrophilic surfaces, water spreads evenly when it hits the surface by the angle between the edge of the droplet and the surface underneath (contact angle) must lower than 90°. Hydrophilic surfaces can be used in many applications, such as filtration, biomedical, heat pipes, and others (Ahmad., Bogaraert., Miller. and Presswell, 2018). Hydrophobic surface has the ability to repel water then the water breads into tiny droplets which means it barely touches the surface and the contact angle is higher than 90 ̊. There are many sectors in application for hydrophobic material according to Ahmad et al. (2018) such as, the removal of petroleum from aqueous solutions, applied to plastic and ceramics for oil removing, hydrophobic surfaces have a strong self-cleaning and improve the anti-freezing behavior. This study will only investigate on surfactant application from hydrophobic material for the cleaning segment due to the fact that the most frequently used of everyday products are personal hygiene and general house cleaning products (Marline et al., 2015).

2.2 Studied chemical information

Fatty alcohol with the dominant chain length of C10 and hydrophobic property is investigated. The name hydrofob raw material will be used to refer to the fatty alcohol. Four hydrofob raw materials to be focused in this study can be divided into 2 types, synthetic hydrofob and biogenic hydrofob.

The synthetic hydrofobs are 2-Propylheptanol, Linear synthesis C10 alcohol, and Isodecyl alcohol. First 2-Propylheptanol, it is also known as 2-PH and 2-Propyl alcohol. It is a branched fatty alcohol that is primarily used in the production of plasticizers, in the lubricants manufacture, in adhesive application, and in surfactants applied in detergent or industrial cleaning products which is the investigated segment in this study. Moreover, as it is known to all that fatty alcohol could be obtained in both branched form and straight chain. So, for the second alternative hydrofob raw material, the linear straight-chain fatty alcohol having 10 carbons is investigated. Nouryon Company has different suppliers for the linear synthesis C10 alcohol. They purchase depending on which offers a better deal in the current market situation. According to the linear synthesis C10 alcohol product data sheet, it is basically a mixture of 10% maximum of octanol, 90% minimum of decanol, and 4% maximum of dodecanol. The last investigated petrochemical source in this study is Isodecyl alcohol or Isodecanol. It may be used in pure form as a solvent in paper manufacturing. However, the dominant application of Isodecyl alcohol is an intermediate liquid used for continue producing various chemicals such as in PVC and detergent production.

Hydrofob raw material could be obtained from renewable sources not only from petrochemical sources. Palm oils, palm kernel oils, coconut oils, and animal fats are the main renewable inputs for the production of fatty alcohol which can also be called oleochemical feedstocks. In this study the derived fatty alcohol from palm kernel oil are investigated as a biogenic hydrofob.

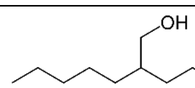
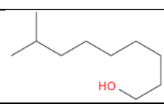
Nouryon Company purchases both synthetic and biogenic hydrofobes (fatty alcoholes) from several global suppliers. The major suppliers of biogenic and synthetic alcohols can be seen in the table 1 below.

Table 1: Major global suppliers of synthetic and biogenic alcohols

Fatty alcohol	Supplier
Synthetic alcohol	BASF Chemical Company
	Evonik Industries
	Exxon Mobil Chemical Company
	Perstorp Oxo AB
	Sasol Chemicals Company
Biogenic alcohol	BASF Chemical Company
	Evonik Industries
	Ecogreen Oleochemicals Company
	Procter & Gamble Company
	Sasol Chemicals Company
	Sinarmas Cepsa Pte. Ltd.
	Wilmar International Ltd.

Table 2 below shows the information on the properties of hydrofobes raw materials including CAS number (a universal assigned number to a chemical substance by the Chemical Abstracts Service), skeletal formula for each hydrofob raw material, example of trade name which is used in the industrial area, and molecular weight and physical property. Hazards classification is also included in the table. All four hydrofobes raw materials are in the equal level in the categories of skin corrosion and irritation and chronic aquatic toxicity. For the serious eye damage and irritation, 2-Propylheptanol and Natural C10 alcohol are in the hazard categories of 2B and 2A, respectively. Category 2A is classified as severe skin irritant and category 2B is classified as mild irritant (ChemSafetyPro, 2019).

Table 2: Properties of studied hydrofobes chemicals

Hydrofobes chemicals	**CAS number**	**Skeletal formula**	**Example of trade name**	**Molecular weight (g/mol)**	**Physical property**	**Hazards classification (Category)**		
						Skin corrosion and irritation	**Serious eye damage and irritation**	**Chronic aquatic toxicity**
2-Propylheptanol	10042-59-8		-	158.28	Colorless liquid	2	2B	3
Linear synthesis C10 alcohol	112-30-1; 85566-12-7		NAFOL 10D	155-162	Clear and colorless liquid	2	2	2
Isodecyl alcohol	68526-85-2		Exxal 10	158.28	Colorless liquid	2	-	3
Natural C10 alcohol	112-30-1; 85566-12-7		Ecorol 10/98	158.28	Colorless liquid	2	2A	3

2.3 Delimitation

There are several applications available for using hydrofob as a raw material in everyday situations such as the use of hydrophobic coating on textiles, TEFLON coating which prevents food to stick to the pan, and the use of hydrophobic coating to improve the quality of plastic and energy efficiency of heat exchanger and heat pipe. The focused application in this study is cleaning products, since cleaning products are close to people and used every day. Moreover, this study only considered four hydrofobes which are 2-propylheptanol, natural C10 alcohol from palm kernel, Isodecyl alcohol, and linear synthetic C10 alcohol.

The environmental damage costs can be analyzed by several assessment methods. In this report, the life cycle assessment (LCA) is selected as an assessment method where the environmental priority strategies (EPS) and Stepwise method are used as a monetary weighting method.

The limitations during the performing of the study may appear mostly in the life cycle assessment. As mentioned, this study aims to compare the use of different hydrofobes as a raw material. To be able to achieve comparable conditions, the assumptions for LCA would be required such as lifetime, use profile (cleaning will be used as an application segment), and the scope of the inventory (cradle-to-gate perspective). With the limitation in data collection, the data of four hydrofobes (2-propylheptanol, natural C10 alcohol from palm kernel, Isodecyl alcohol, and linear synthetic C10 alcohol) will be acquired through data collected and measured directly by Nouryon Company.

3. Life cycle assessment (LCA)

3.1 Goal and scope of the study

3.1.1 Goal for the study

The overall objective of the study is to perform a life cycle assessment in order to compare the environmental damage cost and environmental impacts for hydrofob raw material with a focus on the four raw materials which are 2-propylheptanol, natural C10 alcohol from palm kernel, Isodecyl alcohol, and linear synthetic C10 alcohol. And to answer which raw material is environmentally preferable for producing surfactant in the cleaning segment.

The results are intended to be communicated to Nouryon Company and IVL Swedish Environmental Research Institute since they are the consequential stakeholders. The result of the study will be used as a basis for deciding on developing the surfactant manufacturing at Nouryon Company.

3.1.2 Scope of the study

The scope of the study is presented below with models and choices that are needed in order to fulfill the goal of the study including Functional unit, Choice of impact assessment, Type of LCA. Flowchart of the life cycle of each hydrofob raw material. Assumptions and Limitations, System boundaries, Allocations and avoid allocations and Data quality requirements are shown as well.

3.1.2.1 Functional unit

The functional unit is a quantified description of the studied system. It is a reference that other flows (inputs and outs) in the system are related to (Baumann and Tillman, 2004). Comparison of the environmental impacts for the studied systems can thereby be analysed based on the functional unit.

The functional unit in this study is defined as 1 kg of fatty alcohol. The process data including raw material and energy requirements and environmental emissions are then integrated over the production processes by weighting the material contributions from each process to the functional unit.

3.1.2.2 Choice of impact assessment

Choice of impact assessment represents the environmental impacts that are considered in the study and how the results are designed to be stated (Baumann and Tillman, 2004). The inventory data from the life cycle of the products will be counted in the impact assessment and then will be converted into environmental impacts. Considering this study in comparison of the four raw materials, the five listed impact categories in the table below will be taken into consideration according to that synthetic hydrofob has fossil fuel as a resource so carbon dioxide emissions are expected. Ethylene is consumed during the process mostly in synthetic hydrofobp production and therefore can be expected to be present as an emission. Another important input in biogenic hydrofob production (palm oil plantation process) is fertilizer which can be a result of phosphorus and nitrate running of. Not only the fertilizer uses but the whole agriculture stage is a major contributor to most of the potential environmental impacts. Other activities such as electricity are expected to give the impact as well. Furthermore, monetary weighting (EPS) is applied to convert the environmental impacts to environmental damage cost.

Table 3: Description of each impact categories included in the study (Guinée, 2004).

Impact category	**Unit**	**Method**
Global warming potential	Carbon dioxide (CO_2) eq.	CML2001
Acidification potential	Sulphur dioxide (SO_2) eq.	CML2001
Eutrophication potential	Phosphate (PO_4^{3-}) eq.	CML2001
Ozone layer depletion potential	Trichlorofluoromethane (CFC-11) eq.	CML2001
Photochemical ozone creation potential	Ethylene (C_2H_4) eq	CML2001

3.1.2.3 Type of LCA

The methodology choices of LCA have basically two types, attributional and consequential, which depend on the goal definition that was set at the earlier step (Rebitzer et al., 2004; Finnveden et al., 2009). Attributional study (accounting) has a goal to describe the environmentally relevant flows in the life cycle. Consequential study (change-orientated) has a goal to describe how environmentally relevant flows will change in response to decision making taken in the study (Rebitzer et al., 2004; Finnveden et al., 2009). In this study, attributional type of LCA is used to analyze and get the comparative information about the environmental damage cost associated with the hydrofob component production from four different raw materials throughout the entire life cycle.

3.1.2.4 System boundaries

This LCA study in terms of environmental impacts and environmental costs of different hydrofobes raw materials for producing surfactants (mainly focusing on the cleaning product segment), will consider a cradle to gate perspective, which is shown in the general flowcharts in section 3.1.2.5 Flowchart of LCA. It is easily to find that the life cycles begin when the raw materials are extracted such as the extraction of oil and natural gas, and 'gate' refers to the outgoing of hydrofobes components to the surfactant industrial such as 2-Propylheptanol from suppliers production industrial to surfactant manufacturing process at Nouryon Company.

The use phase (producing surfactant) for hydrofob component occurs in Sweden. The upstream raw material extraction and production are occurring in Germany for the synthetic hydrofob where most of the supplier industrial companies locate. However, the raw material extraction for one part of natural gas C10 alcohol, palm kernel oil production, mainly takes place in Indonesia. Since there are four alternative raw material choices for producing hydrofob component, the time horizon could differ depending on which hydrofob component is considered.

3.1.2.5 Flowchart of LCA

The production processes of the surfactant from different four raw materials until the final cleaning product have the same procedures. Thereby, it is shown in one figure (figure 1). The four alternatives raw materials are produced by different suppliers and then transported to Nouryon Company, Stenungsund to continue with the surfactant production process. The product from Nouryon Company, hydrofobes surfactants, will be transported to the cleaning industry for generating the final cleaning product and supplying to the end users later on.

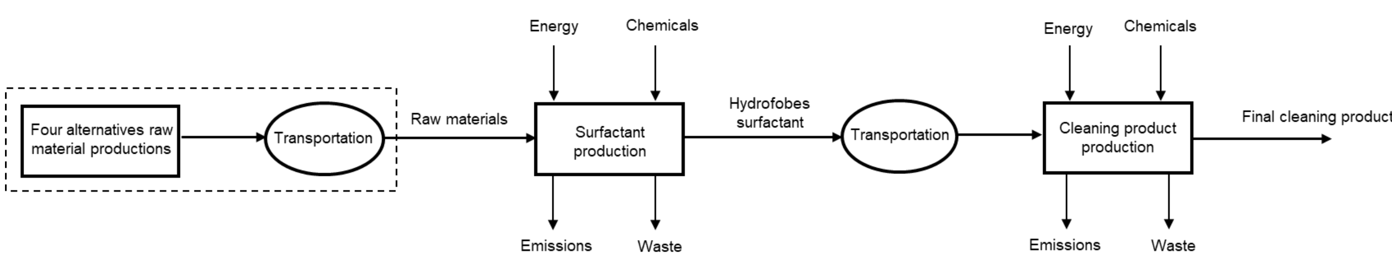


Figure 1: The general flow chart of producing cleaning products.

In this study the system boundaries that will be focusing on is represented within the dotted lines, started since the production of four alternative raw materials until the transportation system to Nouryon Company, Stenungsund.

Figure 2 to 5 below illustrates the general flows and steps that are involved in the production of four raw materials. All four raw materials then will be transported to the surfactant production process separately.

2-Propylheptanol production

2-propylheptanol is generated by performing the commercial production of 2-propylheptanol which is based on valeraldehyde raw material (Scott Jenkins, 2019). Valeraldehyde is one of a number of aliphatic aldehydes industrially prepared by the hydroformylation of butene and synthesis gas (oxo synthesis) and using rhodium catalyst. The production of butene is started with crude oil extraction followed by refining and stream cracking. Rhodium, a rare platinum group metal, is commonly used in the production of oxo-alcohol manufacturing for the reason that it is chemically stable at high temperatures and resistant to corrosion (Terence Bell, 2019). The reaction condition of utilizing rhodium as a catalyst includes the presence of triphenylphosphine (Harris et al., 1980). Triphenylphosphine obtained by reacting phosphorus trichloride with benzene in chloroform and sodium to reduce hydrogen and chloride (Broger, 1981). After the preparation of Valeraldehyde, the following processes are aldol condensation and hydrogenation for producing the final product, 2-propylheptanol. Along the aldolization, caustic soda (sodium hydroxide) is required (Intratec, 2019). The 2-propylheptanol production is shown in Figure 2 below.

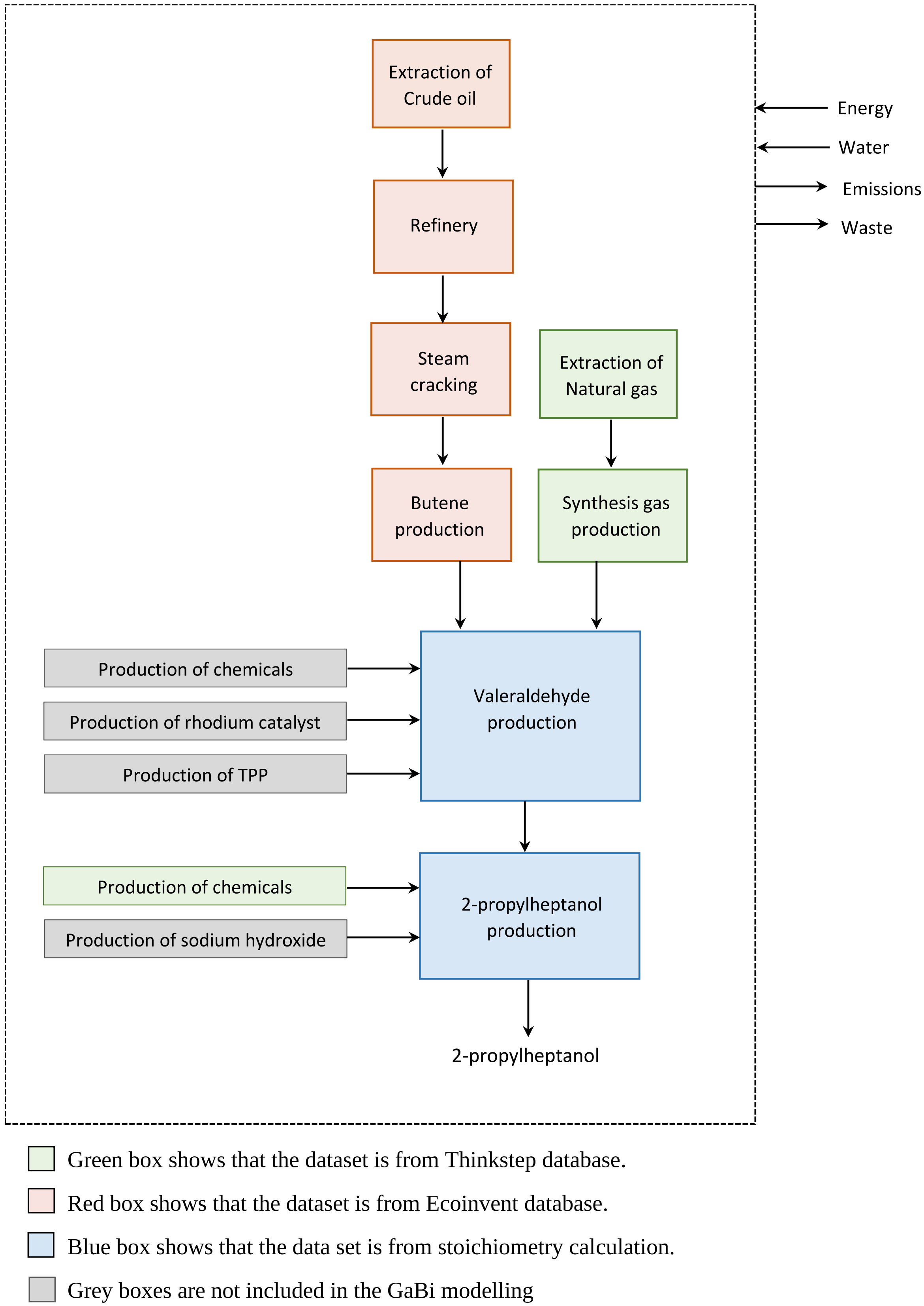


Figure 2: The production flow chart of 2-propylheptanol

The production of 2-Propylheptanol is a multiple step reaction summarized as follows:

1. The hydroformylation of butene and synthesis gas to Valeraldehyde

$$C_4H_8 + CO + H_2 \rightarrow C_5H_{10}O$$

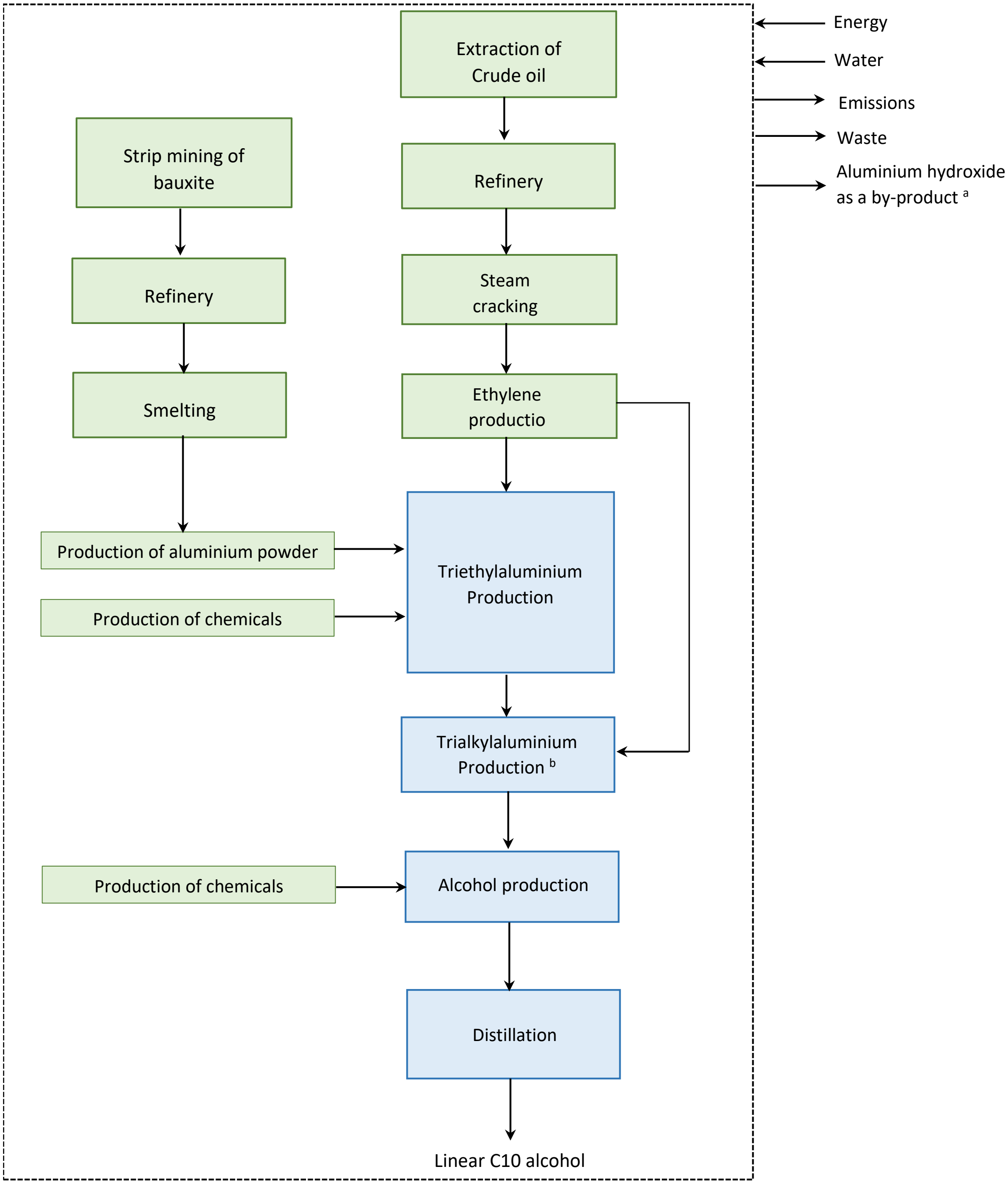
2. Aldol condensation and hydrogenation for producing the final product, 2-Propylheptanol

$$2C_5H_{10} \rightarrow C_{10}H_{18}O + H_2O$$

$$C_{10}H_{18}O + 2H_2 \rightarrow C_{10}H_{22}O$$

Linear synthesis C10 alcohol production

The synthesis route for producing Linear synthesis C10 alcohol is called Ziegler alcohol synthesis which consists of two main steps, oligomerization and oxidation (Noweck and Grafahrend, 2006). The process starts with oligomerization of ethylene by using triethylaluminium as an organoaluminium compound. Ethylene is derived from refining of crude oil. In some cases, natural gas is fed in the small amount depending on the desired composition. Triethylaluminium can be formed by the reaction of aluminium powder, ethylene, and hydrogen gas. The aluminium manufacture consists of two phases. After bauxite being strip mined from the surface of the terrain, the bauxite ore is refined to obtain aluminum oxide which can be called Bayer process (Altenpohl, 1982). Following by smelting the aluminum oxide to release pure aluminum, this step is named Hall-Heroult process. The spent aluminium will be formed a by-product, aluminium hydroxide. After triethylaluminium production, the chain length will be extended by adding ethylene. The process is called trialkylaluminium production with a chain length of C8, C10, and C12. It's difficult to control the exact chain length. Hence, it is in fact achieved a mixture of trioctylaluminium, tridecylaluminium, and tridodecylaluminium. Later that step, trialkylaluminium will be converted to a mixture of alcohol. Then the seperation process is required to distillate the mixture that high in C10.



[a]Aluminium hydroxide is a by-product from

[b]Trialkylaluminium production is an oligomerization process forming a mixture of several trialkylaluminium with chain length as C10 is a dominant component

Green box shows that the dataset is from Thinkstep database.

Red box shows that the dataset is from Ecoinvent database.

Blue box shows that the data set is from stoichiometry calculation.

Grey boxes are not included in the GaBi modelling

Figure 3: The production flow chart of linear synthesis C10 alcohol

The route for linear C10 alcohol is called production of is Ziegler alcohol synthesis summarized as follows:

1. Chemical mechanism for producing triethylaluminium

$$6C_2H_4 + 3H_2 + 2Al \rightarrow 2Al(C_2H_5)_3$$

2. The oligomerization of ethylene to alkylaluminium

$$Al(C_2H_5)_3 + 9C_2H_4 \rightarrow Al(C_8H_{17})_3$$

3. Oxidation of the alkylaluminium product from the first step to desired alcohol

$$Al(C_8H_{17})_3 + 3O + 3H_2O \rightarrow 3C_8H_{18}O + Al(OH)_3$$

$$10Al(C_8H_{17})_3 + 15O + 24H_2O \rightarrow 24C_{10}H_{22}O + 10Al(OH)_3$$

$$Al(C_8H_{17})_3 + 3O + 2H_2O \rightarrow 2C_{12}H_{26}O + Al(OH)_3$$

Isodecyl Alcohol production

According to Isodecyl alcohol production in PVC manufacturing, the production mechanism for producing Isodecyl alcohol consists of 2 main processes. It starts with propene is oligomerized to isononene by heat induced oligomerization (Leeuwen and Claver, 2002). In isodecyl alcohol production process from isononene, it is a formultation process which is similar to the production of valeraldehyde.

The route for Isodecyl alcohol is called production of is a multiple step reaction summarized as follows:

1. Oligomerization of propene to isononene

$$3C_3H_6 \rightarrow C_9H_{18}$$

2. Hydroformylation of isononene and synthesis gas to isodecyl alcohol

$$C_9H_{18} + CO + 2H_2 \rightarrow C_{10}H_{21}OH$$

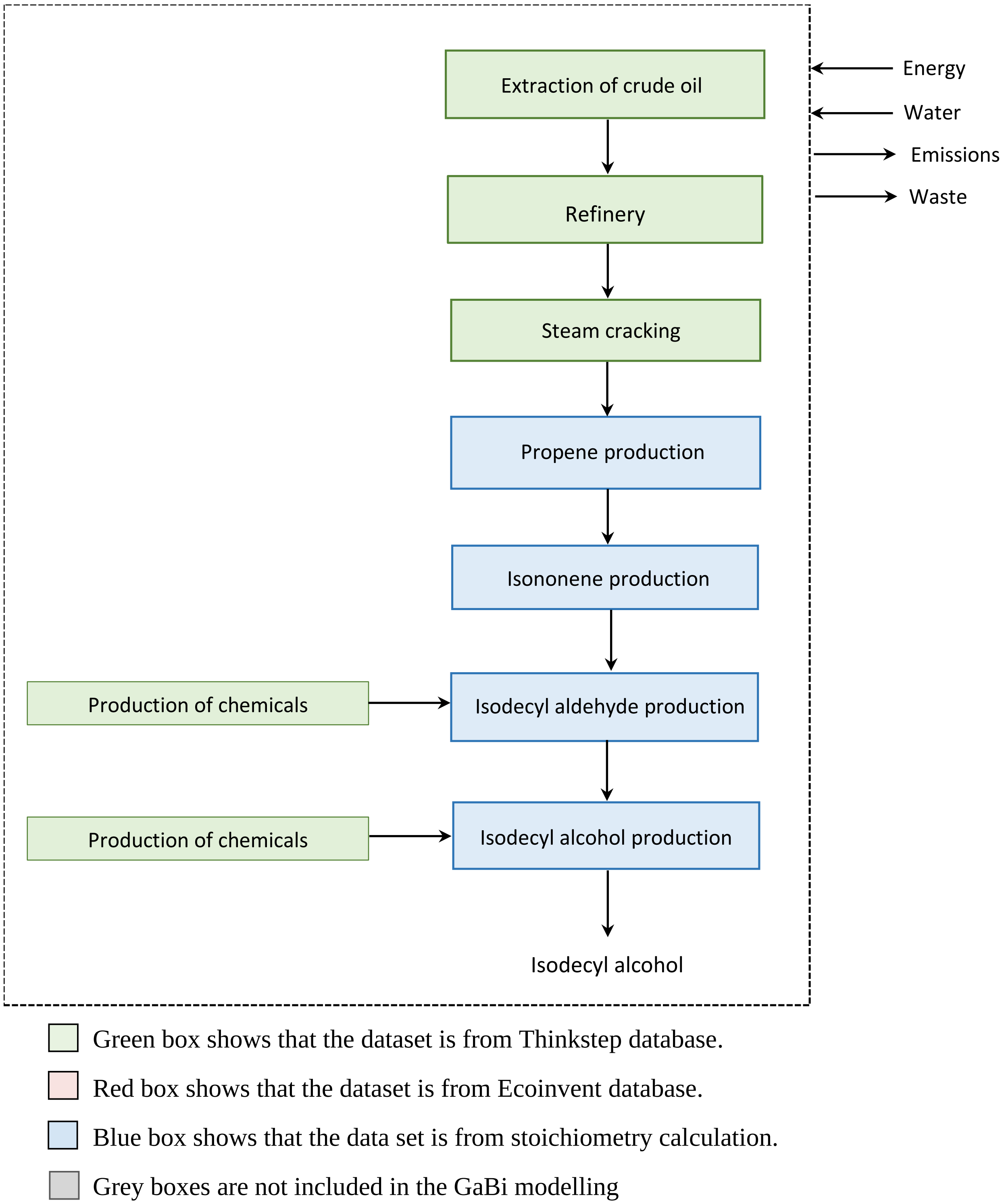


Figure 4: The production flow chart of Isodecyl alcohol

Natural C10 alcohol production

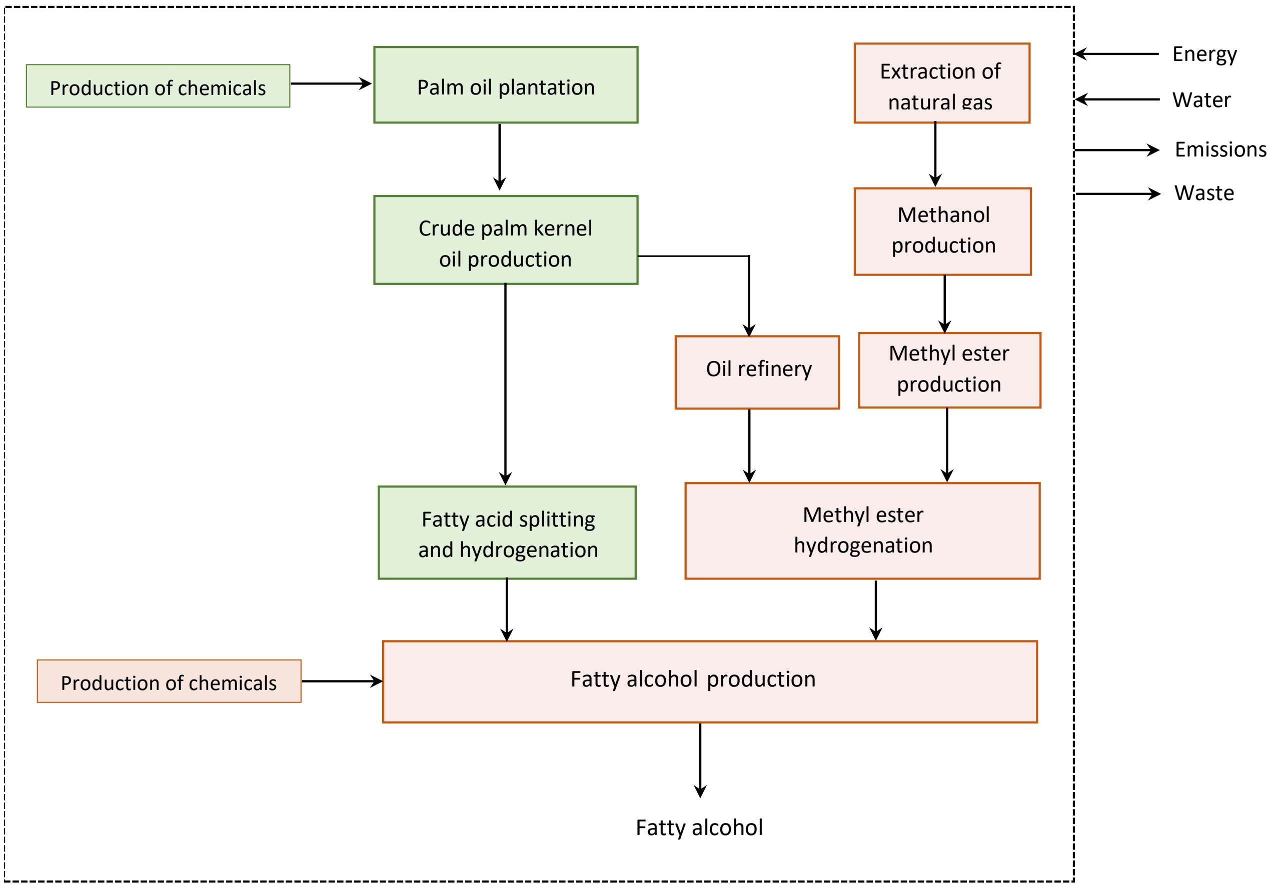
The general flows and steps that are involved in the production of fatty alcohol from palm kernel oil is presented in figure 5, below. The processes are divided into 2 parts; palm kernel oil production and fatty alcohol production. The production of palm kernel oil consists of three mains processes, oil palm plantation, milling process, and palm kernel oil production (Hai, 2002). The production will start with cultivation, converting the forest to plantation area. Oil palm needs enough water for getting higher yields and sometimes pesticides are needed depending on the plantation location along with the fertilizer applying. From the harvesting process, the fresh fruit bunches will be transported to the palm oil mill for further processing and the solid wastes including branches and bark are collected and recycled as a nutrient to cultivation process.

Milling is a procedure where fresh fruit bunches will be processed to crude palm oil and palm kernel cake. The first step of milling is sterilization and threshing of bunches. The prepared bunches will be sent to the oil extraction step. Crude palm oil will be produced then further treated and refined which will not be considered in this study. Another product from the oil extraction step is palm kernel cake which will be processed at palm kernel oil mill. In the palm kernel oil production process, it starts from depricarping, nut cracking, and winnowing. After drying the kernel, the oil inside can be extracted through pressing and solution extraction. In this palm kernel oil process, some solids wastes including fibers and shells could be used for incineration to generate heat for the entire process.

The fatty alcohol production consists of two main processes, fatty alcohols from fatty acid splitting and fatty alcohol from methyl ester production. In this study, 73% of fatty alcohols are produced from methyl ester production which is divided into 56% direct from crude palm kernel oil and 17% out of refined oil. The rest of the 27% of fatty alcohols are produced from fatty acid splitting.

For fatty acid splitting and hydrogenation, it starts with a splitting step. In this process triglycerides are hydrolyzed to fatty acid and glycerin by contacting of crude palm kernel oil with steam at high pressure and temperature conditions (Cryogenics & Lurgi technologies, 2017). Finally, fatty acids from oil splitting will be hydrogenated through Lurgi directed hydrogenation step into fatty alcohols.

For Methyl ester production and hydrogenation, it starts with transesterification, fatty acid methyl esters are produced by conducting the reaction between crude palm oil or refined oil and methanol. Then the fatty alcohols are produced by the hydrogenation of fatty acid methyl esters.



Green box shows that the dataset is from Thinkstep database.

Red box shows that the dataset is from Ecoinvent database.

Blue box shows that the data set is from stoichiometry calculation.

Grey boxes are not included in the GaBi modelling

Figure 5: The production flow chart of fatty alcohol from palm kernel oil

3.1.2.6 Assumptions

Assumption for 2-Propylheptanol production

- 2-Propylheptanol can be produced by different manufacturing routes and different sources of raw material. In this study, commercial production of 2-propylheptanol based on valeraldehyde as a raw material are focused.
- Rhodium catalyst and Triphenylphosphine production processes are not considered in this study. According to U. Marcus Lindström, Organic Reaction in Water, the consumption of rhodium

concentration in aldehyde production is in the ppb range which is approximately zero when compared to aldehyde products.

- Sodium hydroxide (caustic soda) production process is not included in the LCA study. Because sodium hydroxide is aimed to maintain the right level property of the solution (maintain the pH level) and consumed in the small amount which is approximately zero and even circulate it back.
- The aldolization process requires a 50 wt% sodium hydroxide (caustic soda) in water.
- The dataset of some production processes are modelled with a stoichiometric calculation to determine the total mass of the substances. The production processes that are modelled with a stoichiometric calculation are dataset of valeraldehyde and 2-propylheptanol processes.

Assumption for Linear synthesis C10 alcohol production

- NAFOL 10D represents the linear C10 alcohol in this study.
- The alcohol composition (%) of NAFOL 10D is 10% of octanol and 90% of decanol.
- The dataset of some production processes are modelled with a stoichiometric calculation to determine the total mass of the substances. The production processes that are modelled with a stoichiometric calculation are dataset of triethylaluminium, trioctylaluminium, and desired alcohol (octanol, decanol, and dodecanol) productions.

Assumption for Isodecyl alcohol production

- The isodecyl alcohol production process shown in this LCA study is from a part of additive (Di-isodecyl-phthalate) production used in PVC.
- Cobalt based catalyst production processes are not considered in this study. According to the consumption of cobalt based catalyst gives a small impact compared to the overall result from the whole production.

Assumption for Natural C10 alcohol production

- The nursery phase is not considered in this study due to the small impact on the overall result
- In average of 5 % of the POME biogas from palm oil mill is collected and incinerated.
- In the case of EFB mulching, it is the most used treatment option. So, 100% Mulching is assumed for this study
- It was assumed according to literature sources that a mix of 27% of fatty alcohols produced from Fatty Acid Splitting and 73% produced Methyl Ester Production (divided in 56% direct form crude vegetable oil and 17% out of refined oil).
- The palm kernel oil production plant is assumed to be located in Indonesia.

Assumption on transportation

- The distances from supplier companies to Nouryon Compny were obtained by using Google maps to plot the overall road route.
- All 4 alternative raw materials are produced by different suppliers and then transported to Stenungsund. So, the transportation system is assumed to transport mainly from Germany (BASF) and Natherlands (Isodecanol).
- Transportation of 2-Propylheptanol from Perstop Oxo AB to Nouryon Company is through pipeline system since they are neighbor factories.

3.1.2.7 Allocations and avoided allocations

Allocation in this study will be dealt by first, according to that attributional type of LCA is used, the analysis will be performed considering no credits or additional burdens outside of the system. Moreover, since stoichiometric calculation is used to model the dataset of production processes, only the main product which is fatty alcohol will be considered and occurred in the chemical reaction. Therefore, this study was performed by allocating 100% to the desired product.

3.1.2.8 Data quality requirements

Data collected and assessed in this study are from several sources. Due to the LCA is modelled in GaBi Software, some production processes are already existing in the database. Databases that are utilized in this study are from Thinkstep database and Ecoinvent database. However, some dataset of the production processes is modelled with a stoichiometric calculation to determine the total mass of the substances. In the monetary valuation part (weighting step), the data is mainly from Thinkstep database. Regarding the difficulty of requiring and gathering the data from the specific suppliers, data has been collected and calculated in the way that should express the system as suitably and reasonably as possible.

3.2 Life cycle inventory

3.2.1 2-Propylheptanol production process

Synthesis gas production

The dataset uses for this process in this study come from Thinkstep database. The dataset represents the production situation in Germany. In this process, the quantitative specification of carbon monoxide and hydrogen ratio is assumed to be 50% hydrogen and 50% carbon monoxide. The assumption on the energy production was made according to the individual country-specific situation. Thermal energy is produced from light fuel oil and together with process steam. Modelling the electricity consumption is assumed to use electricity grid mix as an electricity source.

Butene production

In this process, the raw material extraction until manufacture of refined petroleum products were occurred in European production sites. The data that use in this study come from Ecoinvent database (Ecoprofiles of the European plastics industry, 2015).

Valeraldehyde production

The dataset for valeraldehde production process is modelled with a stoichiometric calculation to determine the total mass of the substances. The material flow, emission, and energy for valeraldehyde production are presented in the table 4 below. Thermal energy and electricity dataset come from Thinkstep database. By the electricity grid mix (based on EU-28) is used as an electricity source and the energy consumption is come from thermal energy produced from natural gas.

2-Propylheptanol production

The dataset for 2-Propylheptanol production process (both reactions) are modelled with a stoichiometric calculation to determine the total mass of the substances. The material flow, emission, and energy for 2-Propylheptanol production are presented in the table 4 below. The manufacturing of 2-Propylheptanol required energy and electricity which come from the same sources as in Valeraldehyde production.

Table 4: The inventory data for 2-Popylheptanol production by using stoichiometric calculation

Processes	**Components**	**Inlet (kg)**	**Outlet (kg)**
Valeraldehyde production	Butene	0.651	
	Carbon monoxide	0.325	
	Hydrogen	0.024	
	n-Valeraldehyde		1
	Thermal energy	5.44 MJ	
	Electricity	1.09 MJ	
First reaction of 2-PH production	n-Valeraldehyde	1.1168	
	Ctronellal/rhodinal		1
	Water		0.1168
	Thermal energy	4.88 MJ	
	Electricity	0.975 MJ	
Second reaction of 2-PH production	Ctronellal/rhodinal	0.975	
	Hydrogen	0.025	
	2-Propylheptanol		1
	Thermal energy	5 MJ	
	Electricity	1 MJ	

3.2.2 Linear synthesis C10 alcohol production process

Ethylene production

Ethylene production or steam cracking process dataset is from Thinkstep database. This dataset represents the manufacturing in Europe. The assumption on the electricity production was made according to the source of electricity produced in specific countries.

Aluminium powder production

The dataset of aluminium powder production is modelled with aluminium foil production dataset as an input source and electricity. In aluminium foil process, European aluminium ingot import mix with European specific foil production. The electricity used in aluminium foil process is modelled according to multiple sources, i.e. the current national grid and fuel supply. For the electricity input,the electricity grid mix (based on EU-28) is used as an electricity source.

Triethylaluminium production

The dataset for triethylaluminium production process is modelled with a stoichiometric calculation to determine the total mass of the substances. The material flow, emission, and energy for triethylaluminium production are presented in the table 5 below. Thermal energy and electricity dataset come from Thinkstep database. By the electricity grid mix (based on EU-28) is used as an electricity source and the energy consumption is come from thermal energy produced from natural gas.

Trialkylaluminium production

In this process, the dataset is modelled by using a stoichiometric calculation to determine the total mass of the substances for the production process. Table 5 below shows the material flow, emission, and energy for trialkylaluminium production. Thermal energy and electricity used in trialkylaluminium production are modelled with Thinkstep database. The electricity grid mix (based on EU-28) is used as an electricity source and the energy consumption is come from thermal energy produced from natural gas.

Desired alcohol production

The desired alcohol in this LCA study are 10% octanol and 90% decanol. Both alcohol production datasets are modelled by using stoichiometric calculation to determine the total mass of the substances. The material flow, emission, and energy for both alcohol, octanol and decanol, are shown in the table 5 below. The manufacturing of alcohol required energy and electricity which come from the same sources as in Triethylaluminium and Trialkylaluminium production. However, different types of alcohol require different amount of energy.

Table 5: The inventory data for linear synthesis C10 alcohol production by using stoichiometric calculation

Processes	Components	Inlet (kg)	Outlet (kg)
Triethylaluminium production	Ethylene	0.737	
	Hydrogen	0.0265	
	Aluminium powder	0.2365	
	Triethylaluminum		1
	Thermal energy	1.5 MJ	
	Electricity	0.299 MJ	
Trioctylaluminium production	Triethylaluminum	0.311	
	Ethylene	0.689	

	Alkylaluminium		1
	Thermal energy	4.81 MJ	
	Electricity	0.962 MJ	
Octanol production	Alkylaluminium	0.938	
	Oxygen	0.123	
	Water	0.138	
	Octanol		1
	Alumnium hydroxide		0.199
	Thermal energy	0.5 MJ	
	Electricity	0.1 MJ	
Decanol production	Alkylaluminium	0.965	
	Oxygen	0.126	
	Water	0.114	
	Decanol		1
	Alumnium hydroxide		0.205
	Thermal energy	4.5 MJ	
	Electricity	0.9 MJ	

3.2.3 Isodecyl alcohol production process

Propene production

In propene production process, the dataset come from Thinkstep database and represents the manufacturing situation in Europe. The assumption on thermal energy and process steam production were made according to the source of thermal energy produced from light fuel oil and process steam produced from natural gas.

Isononene production (Oligomerization)

The amount of thermal and electricity energy is needed in this process. The thermal energy is assumed to be produced from natural gas. And the electricity is assumed to be produced by using electricity grid mix (based on EU-28) as an electricity source.

Isodecyl alcohol production (Hydroformylation)

Isodecyl alcohol production or hydroformylation process dataset is modelled by using stoichiometric calculation to determine the total mass of the substances. Thermal energy and electricity dataset come from Thinkstep database. By the electricity grid mix (based on EU-28) is used as an electricity source and the energy consumption is come from thermal energy produced from natural gas as same as oligomerization process. The material flow, emission, and energy are shown in the table 6 below.

Table 6: The inventory data for Isodecyl alcohol production by using stoichiometric calculation

Process	**Components**	**Inlet (kg)**	**Outlet (kg)**
Isononene production (Oligomerization)	Propene	1	
	Isononene		1
	Thermal energy	3.99 MJ	
	Electricity	0.797 MJ	
Isodecyl alcohol production (Hydroformylation)	Isononene	0.797	
	Carbon monoxide	0.177	
	Hydrogen	0.025	
	Isodecyl alcohol		1
	Thermal energy	5 MJ	
	Electricity	1 MJ	

3.2.3 Natural C10 alcohol production process

Palm kernel oil production

The dataset used for this process in this study come from Thinkstep database. The dataset represents the global production mix by based on the two dominant regions of production which are Malaysia and Indonesia. As they produce more than 80% of the global production volume (47% Malaysian and 53% Indonesian products). The energy needed for the manufacturing are provided by the Malaysia electrical grid mix.

Fatty alcohol production

Fatty alcohol production dataset is from Ecoinvent databases which is based on European production. In this dataset, the medium voltage electricity is used as an electricity source. The energy consumption is come from thermal energy produced mainly from natural gas.

4. Monetary valuation results

The results from the monetary valuation are divided onto three parts. In the first part the environmental costs are analyzed and compare for the four alternatives hydrofob raw materials, 2-Propylheptanol, Linear synthesis C10 alcohol, Isodecyl lcohol, and Natural C10 alcohol. The second part focuses on each hydrofob raw material, where their life cycle contributions are presented and together with the environmental information of the environmental costs for each hydrofob raw material. In the third part, the environmental damage cost for 1 kg of each four hydrofob rawmaterial (fatty alcohol) are compare with the real cost (product market price).

4.1 Total environmental damage costs

Figure 5 below present the total environmental costs for the monetary weighting method: Envieonmental Priority Strategies (EPS) in the four alternatives hydrofob raw materials.

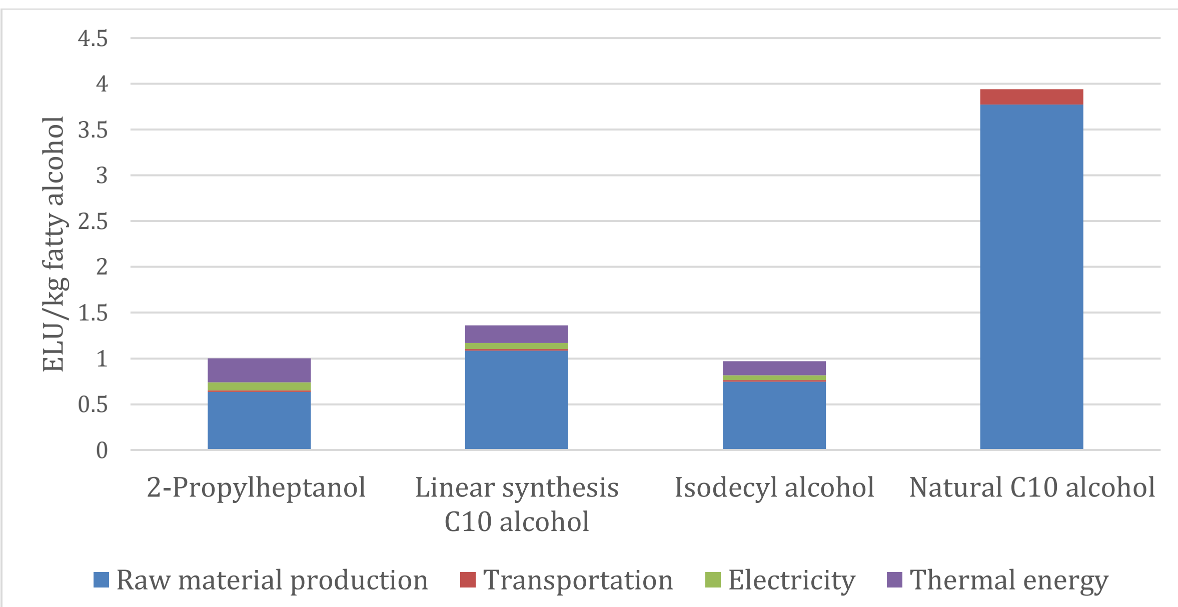


Figure 5: Comparison of the environmental costs between the four hydrofob raw materials

In the above Figure 5, the cost differences between the alternatives can be seen. Natural C10 alcohol obtains the highest environmental costs followed by linear C10 alcohol, isodecyl alcohol, and 2-Propylheptanol. Natural C10 alcohol gives around 72% higher value than all other hydrofob components. A possible reason for this can be that the dataset for natural C10 alcohol is existed in the database system which based on the actual industrial information. But for another three hydrofob components, most of the process dataset are from stoichiometric calculation which are not exactly equal to actual industrial data. Other explanations are possible, which are further investigates in the second part of the result presentation in the figures below, breakdowns of the above results are shown.

4.2 Dominance analysis on four alternatives raw materials

As the focus in the second part is about environmental damage cost on each hydrofob raw material, figure 6 to 13 below present their life cycle contributions and the environmental information of the environmental costs for each hydrofob component.

4.2.1 2-Propylheptanol production

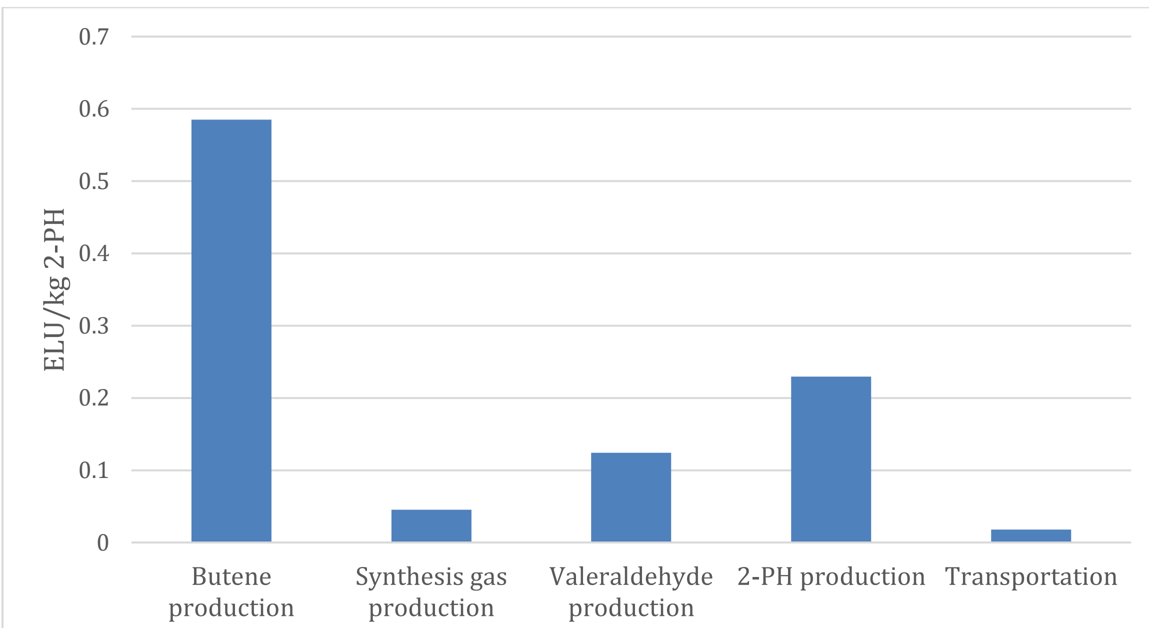


Figure 6: Processes contributing to the environmental damage cost for 2-Propylheptanol production

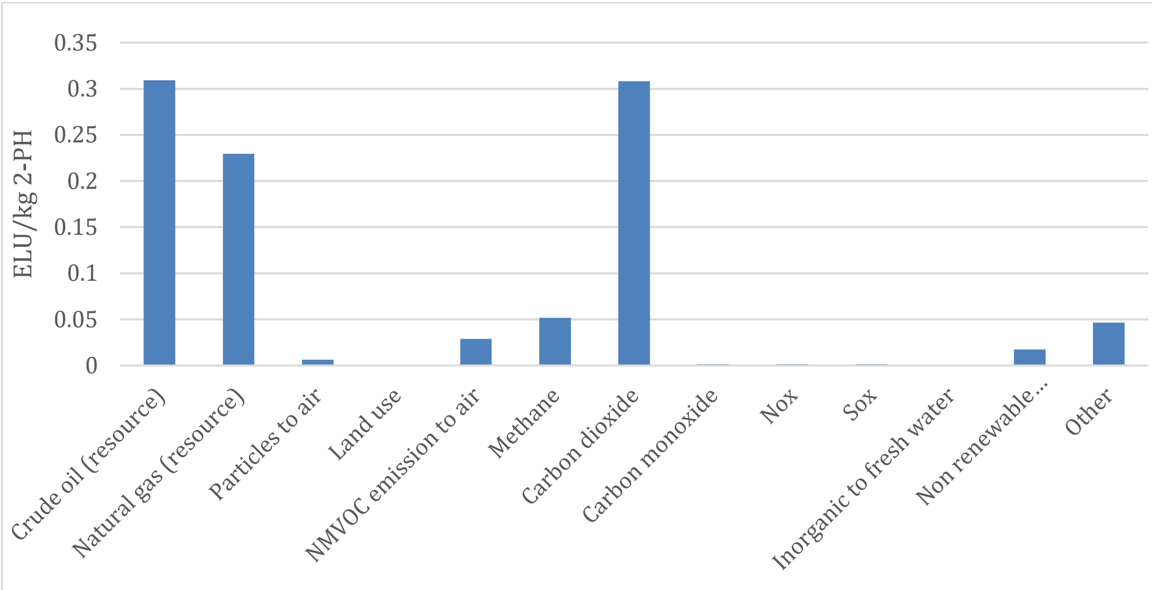


Figure 7: Flows contributing to the environmental damage cost for 2-Propylheptanol production

Figure 6 presents each product's and process's contribution to the environmental costs and how the environmental cost differ between processes in the life cycle of 2-Propylheptanol. First of all it could be seen that butene production contributes with the major parts of the environmental damage costs. For the 2-Propylheptanol process, thermal energy production plays the main role and gives a highest environmental cost followed by electricity production.

Figure 7 shows the results where the contributions are given for various material and energy resource and also for inorganic emission to air and fresh water. The dominant environmental damage costs are utilizing crude oil and carbon dioxide emissions to air followed by utilizing natural gas. Crude oil is mainly used as a raw material in butene production same as the carbon dioxide emissions and natural gas used. That is also related to the result from the Figure 6 that butene production contributes with the major parts of the environmental damage cost in the life cycle of 2-Propylheptanol.

4.2.2 Linear synthesis C10 alcohol production

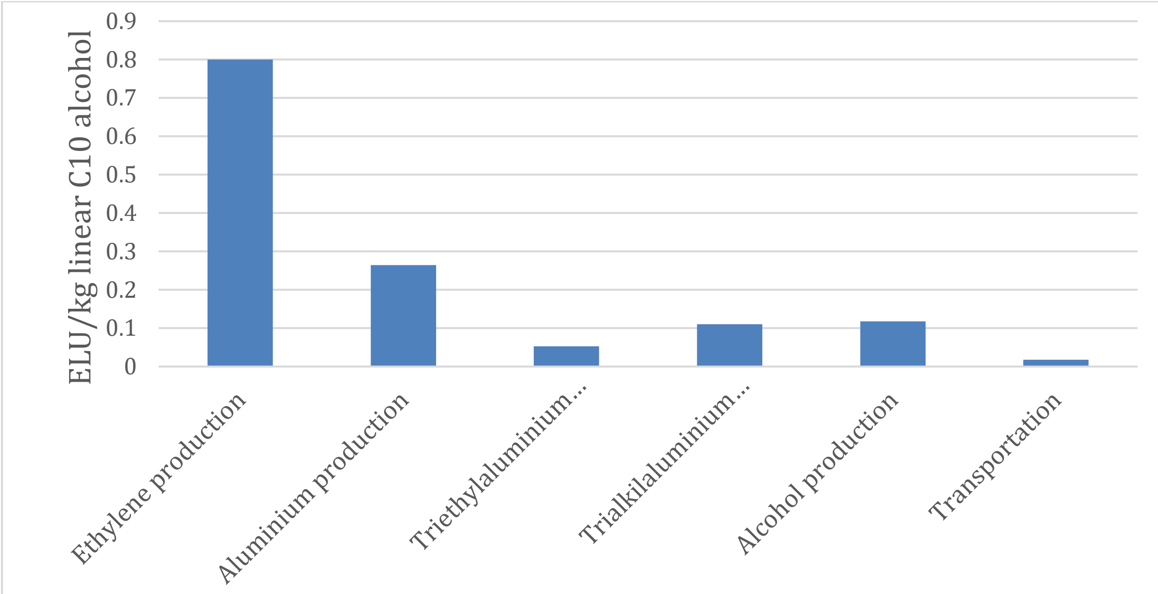


Figure 8: Processes contributing to the environmental damage cost for Linear synthesis C10 alcohol production

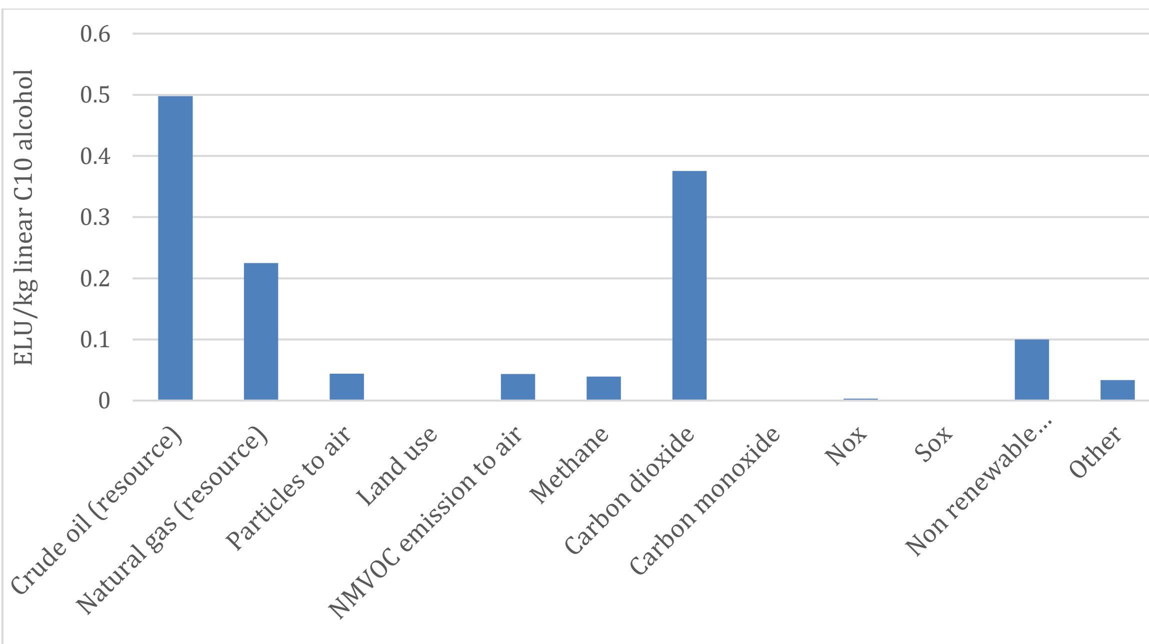


Figure 9: Flows contributing to the environmental damage cost for linear C10 alcohol production

Figure 8 presents each product's and process's contribution to the environmental costs and how the environmental cost differ between processes in the life cycle of linear synthesis C10 alcohol. Ethylene production gives a higher environmental cost than others followed by aluminium production.

The contribution results for linear C10 alcohol production life cycle are given in Figure 9 above. The major cost driers are utilizing crude oil followed by carbon dioxide emissions, utilizing natural gas, and nonrenewable resource use. Those three mains drivers are mainly used and occurred in the same process which is Ethylene production. For carbon dioxide emissions to air, not only occur in ethylene production but also in aluminium foil production.

4.2.3 Isodecyl alcohol production

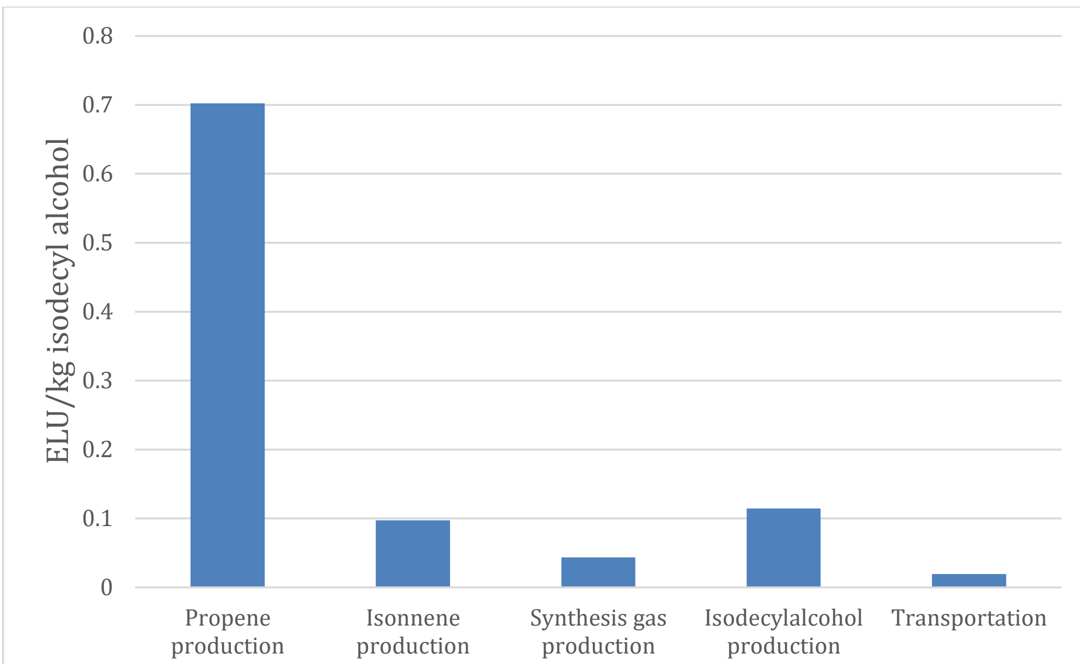


Figure 10: Processes contributing to the environmental damage cost for Isodecyl alcohol production

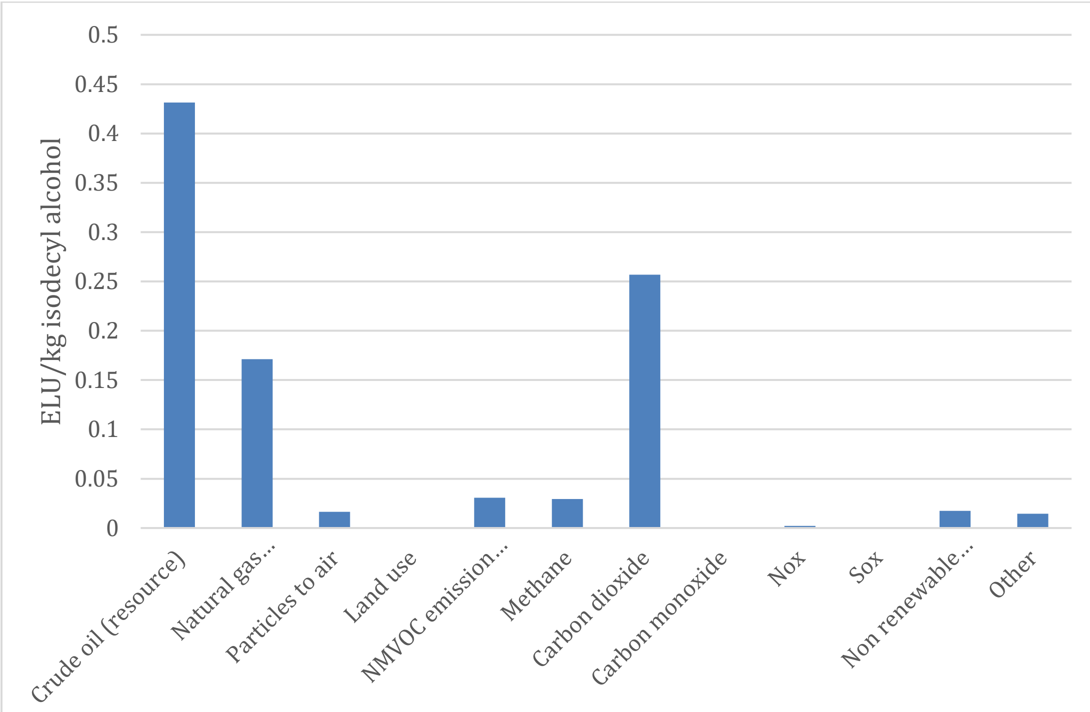


Figure 11: Flows contributing to the environmental damage cost for isodecyl alcohol production

The above figure shows product's and process's contribution to the environmental costs and how the environmental cost differ between processes in the life cycle of isodecyl alcohol. It could be identified that propene production contributes with the major parts of the environmental costs in this life cycle. The environmental costs from hydroformylation or Isodecyl alcohol production mainly arise from extraction and production of synthesis gas used in the process.

As can be seen in the above figure, alike the result from the production of 2-Propylheptanol. The majority of the environmental costs are from utilizing crude oil followed by carbon dioxide emissions to air and natural gas used as a resource. Natural gas is mainly used as raw material in propene production. Crude oil and Carbon dioxide emissions are mainly used and occurred, respectively in propene and synthesis gas production.

4.2.4 Natural C10 alcohol production

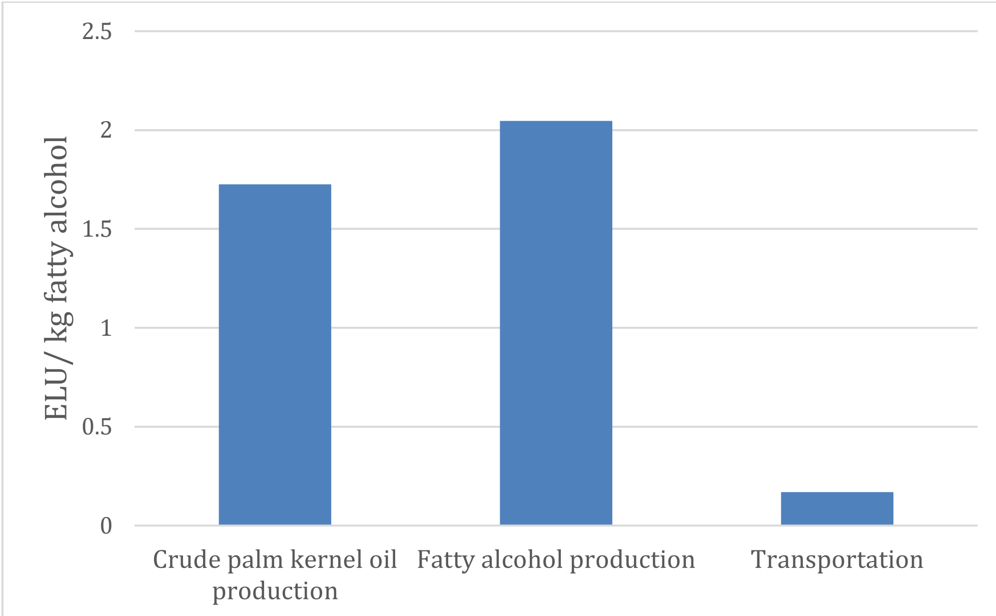


Figure 12: Processes contributing to the environmental costs for Natural C10 alcohol production

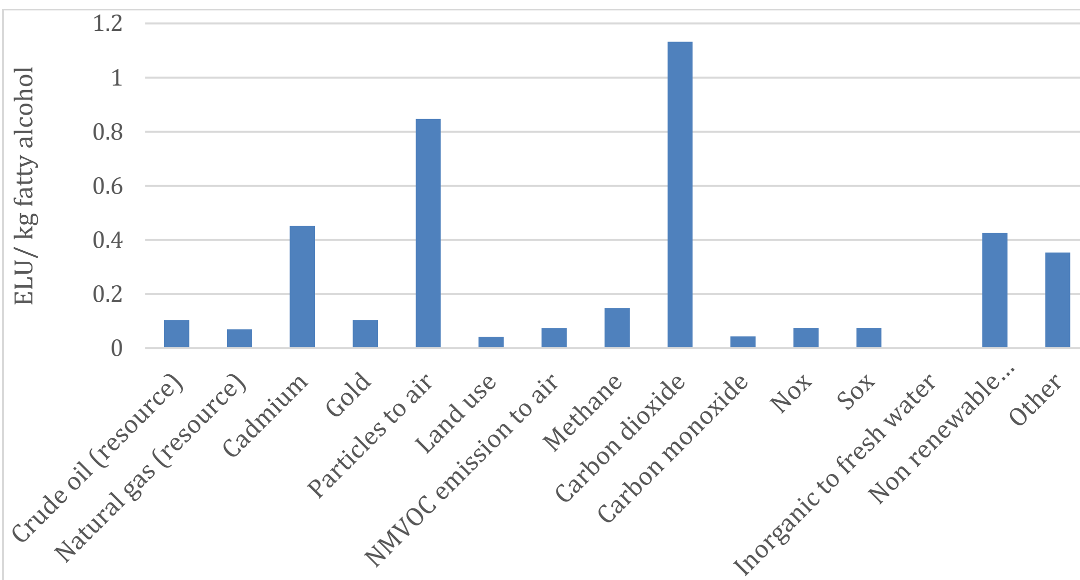


Figure 13: Flows contributing to the environmental costs for Natural C10 alcohol production

From Figure 12, it can be implied that fatty alcohol production, after receiving crude palm kernel oil from manufacturing, is a major driver for giving the environmental costs where it has about 30% higher value than crude palm kernel oil manufacturing. Further breakdown of the environmental costs are found in Figure 13.

Figure 13 shows the results of each environmental costs from various material and energy resources and also from inorganic emissions to air. The dominant environmental damage costs are carbon dioxide followed by particles to air and utilizing cadmium. Carbon dioxide emissions to air are mainly from land use change in crude palm kernel oil manufacturing (cultivation). Particles release to air are also mainly from crude palm kernel oil manufacturing. The common particular matter that released to air is PM2.5. Cadmium as a nonrenewable element is used in fatty alcohol production as a special catalyst in selective hydrogenation in the form of cadmium oxides. The presence of gold in life cycle is caused in the process of selective oxidation of glycerol by using gold catalyst. Gold based catalyst appears to be more resistance to poisons (oxygen poisoning) which results in higher catalytic activity and selectivity (Cristina et al., 2012).

4.3 Comparison of environmental damage costs with product prices

In the last part of the results, the comparison between the environmental costs and the product market prices for four hydrofob components are displayed in Figure 14 below. The environmental damage cost is expressed as Environmental Load Units (ELU). One ELU represents one Euro in willingness to pay to avoid environmental damage at the endpoint level.

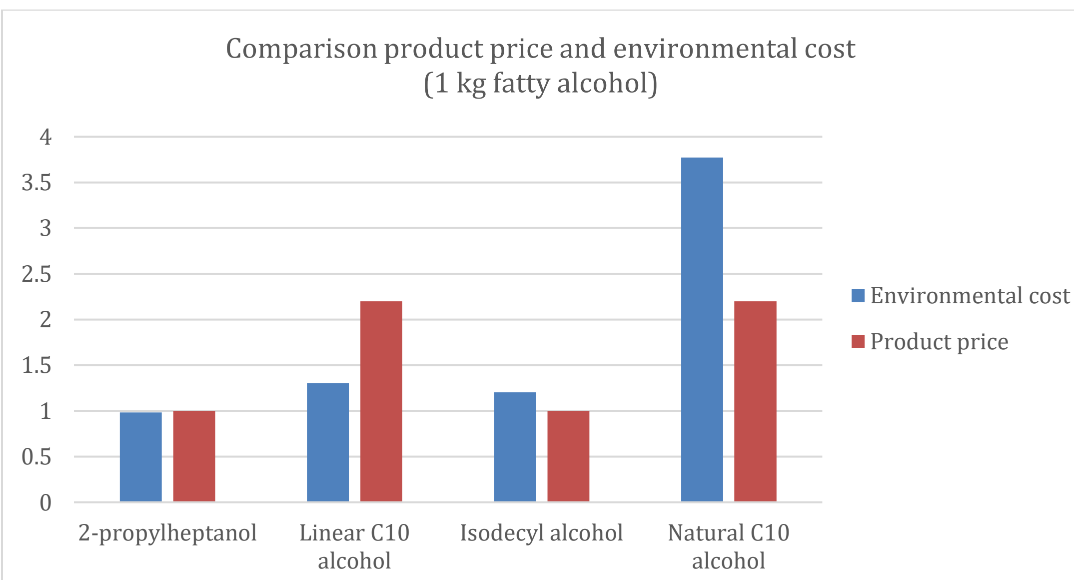


Figure 14: Comparison between the hydrofobes' environmental costs and products' market price

As indicated in Figure 14, the environmental costs constitute a similar value with the total product market price except the natural C10 alcohol. For 2 –propylheptanol and isodecyl decanol, the environmental costs are especially close to product market prices. But for linear C10 alcohol, the environmental cost is lower than product market price about 44%. IN the other hand for natural C10 alcohol, the environmental cost is higher than the product market price about 40%. This could illustrate that the environmental costs could be added in the future to the product price, such as through the policy measures.

5. Impact assessment results

The results from impact assessment include the synthetic-based cases compared to the bio-based case in terms of the five impact categories (Global Warming Potential, Acidification Potential, Euthrophication Potential, Ozone Layer Depletion Potential, and Photochemical Ozone Creation Potential). The results and discussion are presented below where the impact from each main activity in the life cycle is investigated.

5.1 Global warming potential

Figure 15 and table D1 in appendix D present the results of Global Warming Potential (GWP). The figure shows that the Natural C10 alcohol establishes the highest GWP and the lowest goes to isodecyl alcohol. Moreover, the largest contributor to GWP is raw material production for all four hydrofob components. The transportation gives a small contribution in the overall system except for the natural C10 alcohol due to the distance between the crude palm kernel oil manufacturing plant (Indonesia) and the fatty alcohol manufacturing plant (Germany), mainly from the diesel consumption by trucks and ships.

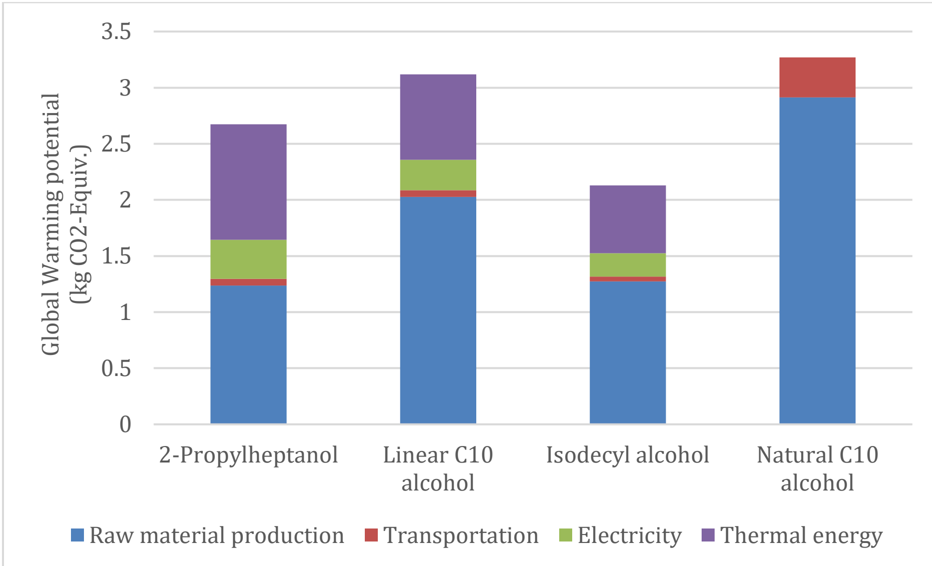


Figure 15: Stacked barcharts indicating the results of Global Warming potential (GWP) for the activities involved in the life cycle of each hydrofob component.

5.2 Acidification potential

Figure 16 presents the characterization results for Acidification Potential (AP) for the main activities in the life cycle are depicted. The results are also presented in table D2 which can be found in appendix D. It can be seen in the figure that AP for the synthetic-based hydrofob components constitute less than half of AP for the bio-based one. Furthermore, the greatest contributor to AP for all four hydrofob components is raw material production. Moreover, it can be seen that the contribution from transportation, and electricity and thermal energy used are similar in size for the synthetic-based hydrofob components.

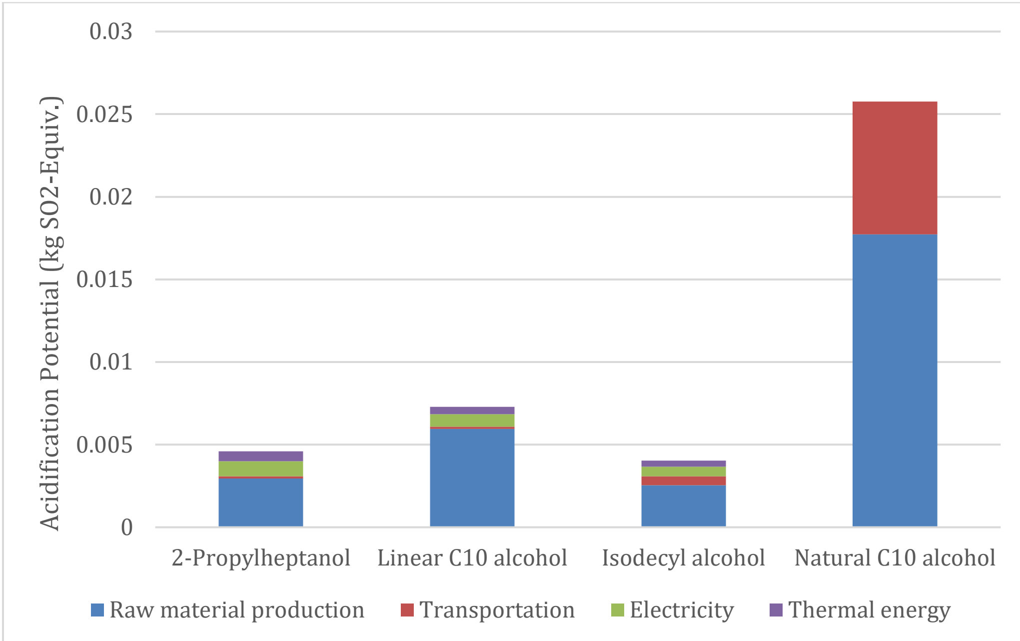


Figure 16: Stacked barcharts indicating the results of Acidification Potential (AP) for the activities involved in the life cycle of each hydrofob component.

5.3 Eutrophication potential

The characterization results for Eutrophication potential (EP) where the contribution from the main activities in the life cycle are depicted, are presented in figure 17 and in table D3 in appendix D. The figure illustrates clearly that natural C10 alcohol greatly contribute to EP impact more than the synthetic-based hydrofobes components. Due to agricultural practices, when fertilizers are used, nitrate and phosphorous are leaching.

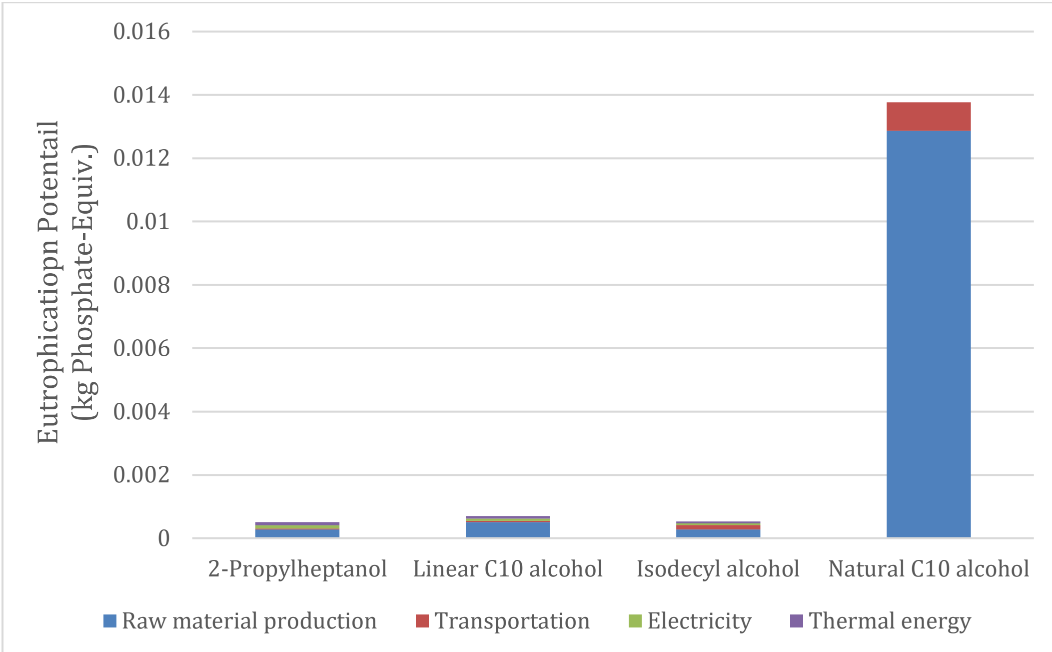


Figure 17: Stacked barcharts indicating the results of Eutrophication Potential (EP) for the activities involved in the life cycle of each hydrofob component.

5.4 Ozone layer depletion potential

The characterization results for Ozone Layer Depletion Potential (ODP) where the contribution from the main activities in the life cycle are depicted, are presented in figure 18 and in table D4 in appendix D. First, the absolute number of the results are extremely small overall which means the results are not dependable in a way. Second, the figure illustrates clearly that natural C10 alcohol greatly contribute to ODP more than the synthetic-based hydrofobes components. The reason could be the atmospheric chemistry effect of nitrogen compound emission from production and application of fertilizers.

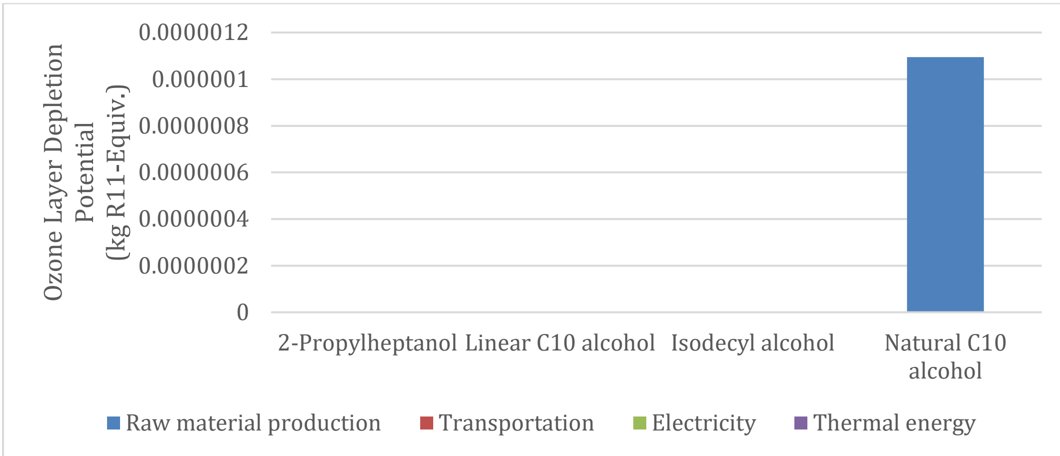


Figure 18: Stacked barcharts indicating the results of Ozone Layer Depletion Potential (OLDP) for the activities involved in the life cycle of each hydrofob component.

5.5 Photochemical ozone creation potential

Figure 19 and table D5 in appendix D presents the results of Photochemical Ozone Creation Potential (POCP). The figure shows that natural C10 alcohol gains higher POCP impact than the less synthetic-based hydrofob components. However, similar to OLDP impact, the absolute number of the results are extremely small overall which means the results are insignificant to the whole picture.

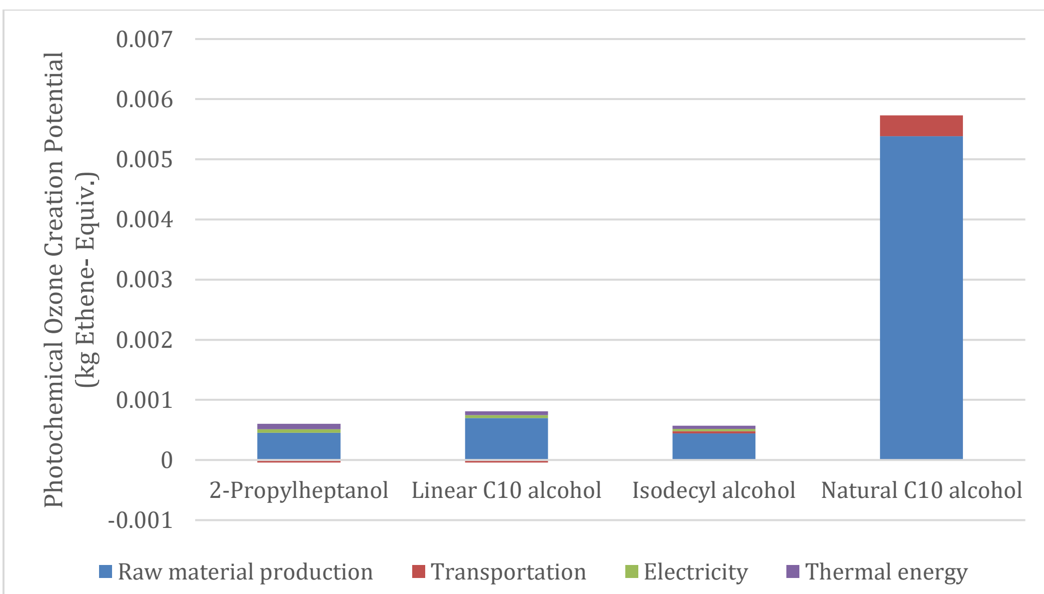
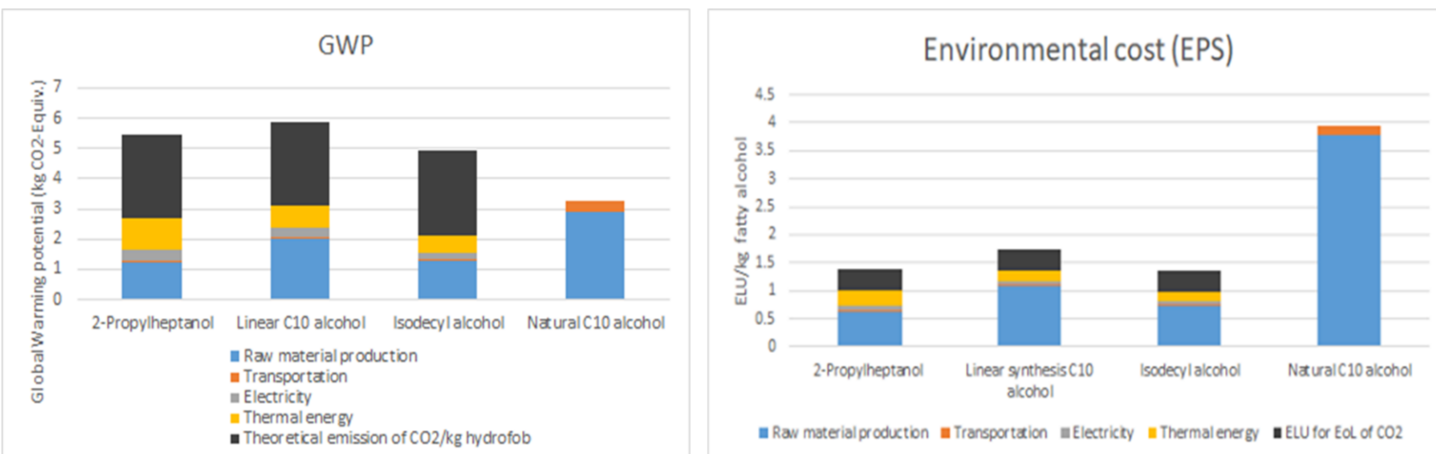


Figure 19: Stacked barcharts indicating the results of Photochemical Ozone Creation Potential (POCP) for the activities involved in the life cycle of each hydrofob component.

From chapter 4 and 5, Monetary valuation results and Impact assessment results, the results indicate that natural product which is natural C10 alcohol is awfully worse than the synthetic hydrofob. Those results were performed according to the cradle to gate perspective. Therefore, the end of life stage of carbon dioxide emission was performed to examine the different between two perspectives. The theoretical carbon dioxide emission was calculated and added to the end of life stage in the synthetic hydrofob in both global warming potential impact and environmental damage cost value. In figure 20, the black bars indicate the theoretical carbon dioxide emission. The results in figure 20 (a), it could be implied that natural C10 alcohol would be the favorable product when the end of life perspective is considered due to the major change to global warming potential when theoretical carbon dioxide emission is added. On the other hand, considering the theoretical carbon dioxide emission in the end of life stage will not have much of the effect to the environmental damage cost value, which can be seen in the figure 20 (b).



(a) (b)

Figure 20: A figure illustrating the theoretical carbon dioxide emission in the end of life stage by (a) shows the result on Global Warming potential (GWP) and (b) shows the result on the environmental damage cost (EPS).

6. Sensitivity analysis

A sensitivity analysis was performed to further understanding how the results are affected based on changes in other variables. In this study, four different sensitivity analyses have been conducted and the results are shown below. The first sensitivity analysis includes the effects of changing electricity sources and amount of input electricity. The second one involves the different bio-based material. The third one is the comparison between different manufacturing of crude palm kernel oil (RSPO certified and non-certified production). The last sensitivity analysis is the effect of recirculating aluminium used in linear synthesis C10 alcohol.

6.1 Sensitivity analysis on electricity

The contribution analysis for monetary valuation has been extended, from comparing the electricity sources and the assumption amount of electricity inputs only in 2-Propylheptanol production scenario. The results found from the sensitivity analysis are presented below the figure 21.

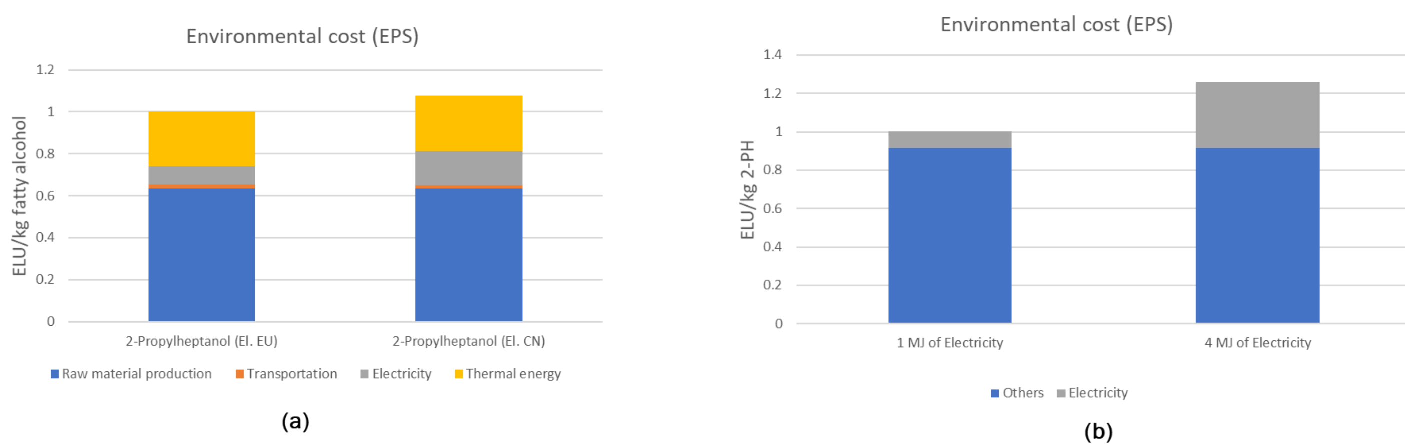


Figure 21: A figure illustrating the electricity impacts by (a) shows the comparison of different electricity sources and (b) shows the comparison of assumption amount of input electricity.

Figure 21 (a) illustrates the comparison of the different electricity sources from mix grid European countries and mix grid from China. The grey level indicates the environmental cost occurred from electricity used. The electricity from China (0.086 ELU/kg fatty alcohol) gives higher environmental cost two times higher of the electricity mix grid from European countries (0.16 ELU/kg fatty alcohol). Figure 21 (b) illustrates the comparison of the assumption amount of input electricity between 1 and 4 MJ. The blue bar names ‘others’ indicates the summation of environmental cost from raw material production, transportation, and thermal energy. The result of the environmental cost is four times higher than the 1 MJ assumption which is related to the amount input.

6.2 Sensitivity analysis on bio-based material

Bio-based resources and products have been increasingly recognized and researched over two decades. Researches present the result of the beneficial from bio-based resources in plenty of fields including the surfactant field for cleaning product. According to the research's result from Erich E Dumelin, The Environmental Impact of Palm Oil and Other Vegetable Oils (2009), biogenic hydrofobes can be produced from a variety of bio-based feedstock. The figure 22 below shows the relation of five environmental impact categories between three vegetable oil sources.

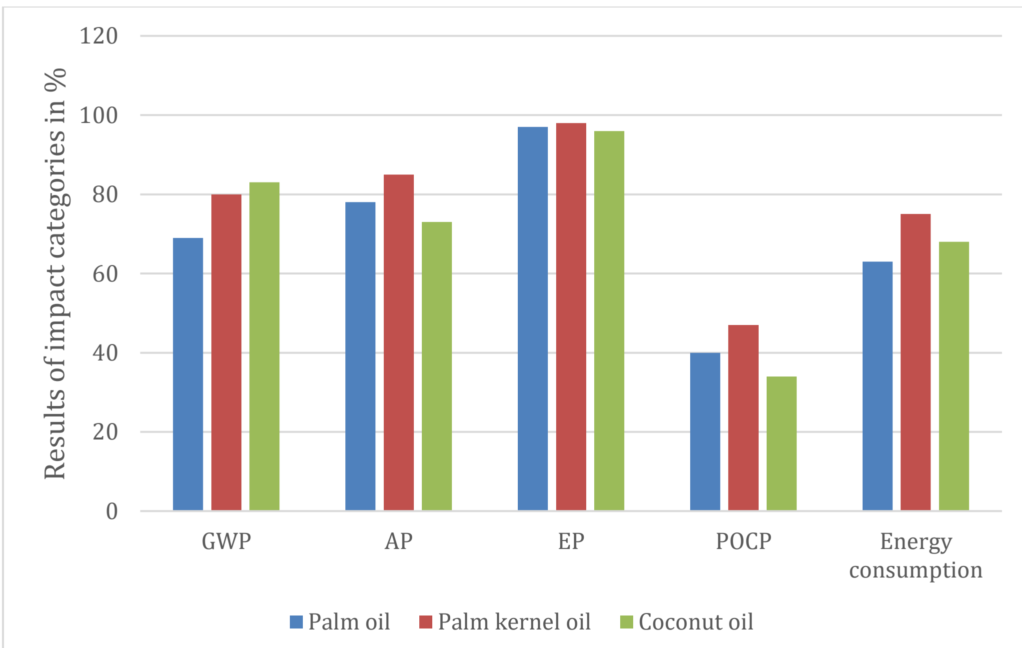


Figure 22: The individual impact categories in % of three bio-based alternatives material (Erich E Dumelin, 2009)

These three sources are the most important vegetable oil used in surfactant production which are palm kernel oil, palm oil, and coconut oil. The result shows that it does not give a significant different from changing one vegetable oil to another. Moreover, in this case coconut oil is relatively similar to the palm source.

6.3 Sensitivity analysis on different manufacturing of crude palm kernel oil

Since 2014, oil palm producers, processors, consumer goods manufacturers, and environmental and social non-govermental organisations (NGOs) decided to develop and implement global standards for sustainable palm oil and palm kernel oil called Roundtable on Sustainable Palm Oil (RSPO). RSPO certification indicates that the standard of palm oil production is followed the Principles and Criteria for Sustainable which means the product is producing without causing harm to the environment and society (Leegwater and Duijin, 2012). When the users consume RSPO certified Palm Oil products for producing their product, they will be able to label on sustainability of the palm oil in their product. Furthermore, there will be the additional costs for RSPO certified when comparing with non-certified Palm Oil. RSPO certified Palm Oil does need costs to keep material identifiable through several processes in the life cycle chain. It can be said that the more complex the product, the further increased of the price.

The contribution analysis for each type of palm oil manufacturing, RSPO certified Palm Oil and non-certified Palm oil, has been conducted by 2.-o LCA consultants in Crowdfunded project. The results found from the sensitivity analysis are presented below the figure.

Figure 23 illustrates results from three main impact categories, global warming, nature occupation (biodiversity), and respiratory inorganics. It's clearly shown that non-certified palm oil production gains higher global warming and nature occupation impact.

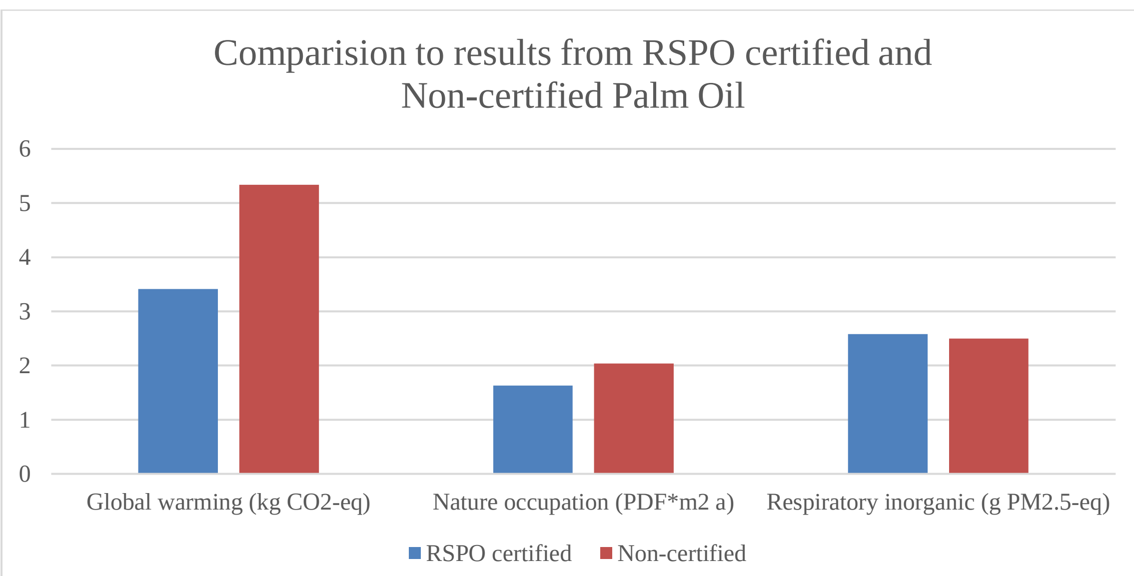


Figure 23: A figure illustrating the impact categories from RSPO certified and non-certified Palm Oil (Schmidt and Rosa, 2019)

According to Adoption of Principles and Criteria for the Production of Sustainable Palm Oil (2013), one of the RSPO principles is environmental responsibility and conservation of natural resources and biodiversity by following the criteria:

- Monitoring and mitigation the negative impacts from plantation and mill management.
- Reducing, recycling, re-using, and disposing waste in an environmentally manner
- Using fuel and energy in the efficiency way
- Reducing pollution and emission

These principles and criteria indicate that RSPO certified palm oil provides more sustainable product than the non-certified one.

For the respiratory inorganics impacts or respiratory health effects that refer to emissions of particulates (mostly are PM2.5), ammonia, NO_x and SO_2, RSPO certified palm oil has an insignificantly higher impact than non-certified palm oil. RSPO certified production shows an impact of 2.58 while non-certified shows 2.5 g PM2.5-eq. As the fact that RSPO certified palm oil production has major amount of fertilizer inputs due to intensive agricultural practices, leading to an increase in nitrogen loss per unit of product.

6.4 Sensitivity analysis on recirculating aluminium used in linear synthesis C10 alcohol

According to the section 4.2.2 Monetary valuation result from linear synthesis C10 alcohol production, aluminium production gives the second highest environmental damage cost. It can be also seen in the figure 24. Hence, the concept of the last sensitivity analysis is to discover the better alternative to producing linear synthesis C10 alcohol by comparing the original production scenario with the production with recirculating aluminium used scenario.

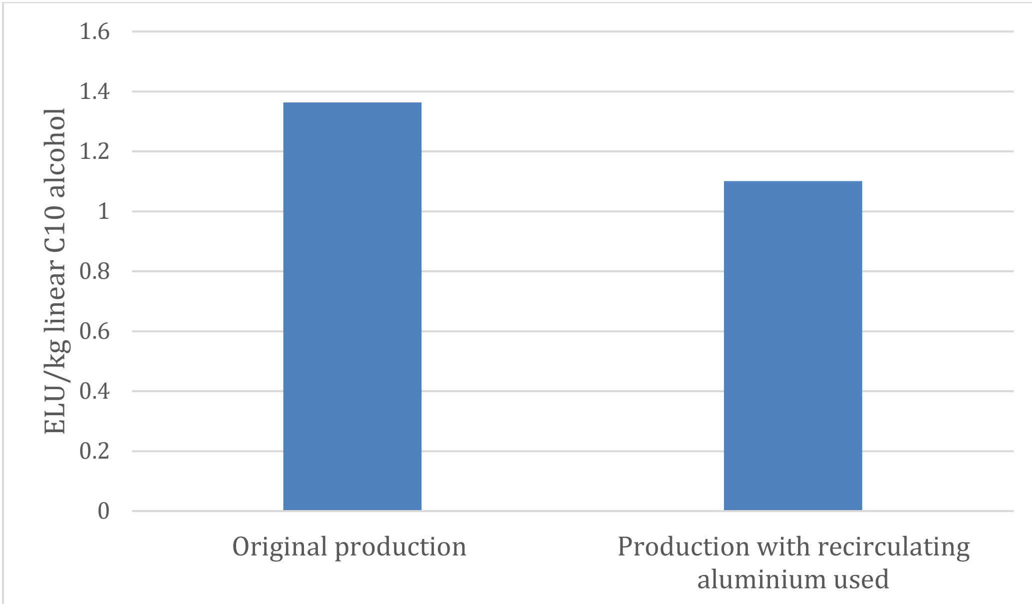


Figure 24: The comparison of environmental damage cost of Linear synthesis C10 alcohol production with and without recirculating aluminium process.

The second scenario, production with recirculating aluminium used, was performed and determined the environmental damage cost. The comparison result is shown in the figure 24 above. The graph is identifying that the lower environmental damage cost will be provided when the aluminium is recirculated and the production of aluminium powder is removed.

7. Conclusions

Hydrofob component is a raw material which could be a feedstock for surfactant (surfactant for cleaning product segment is focused in this study). The hydrofobes raw materials were categorized into synthetic and biogenic hydrofob. The different types of hydrofobes have different environmental impacts. The purposes defined for this study will be assessed in this chapter according to the study's results.

The results from comparing the environmental impacts and environmental damage cost in the life cycle by using cradle to gate perspective between biogenic and synthetic hydrofobes by using Environmental Priority Strategies (EPS) indicated that biogenic hydrofob production delivered larger environmental damage cost than synthetic hydrofob production as a result of that there are several parameters contributed significantly. For example, the presence of cadmium used in life cycle due to the requirement of cadmium as a special catalyst in selective hydrogenation step in the production of fatty alcohol from palm kernel oil. And also, the emission of particulate that comes from fertilizer inputs during cultivation process of palm oil. Furthermore, the results of the sensitivity analysis showed a better result in term of GWP when RSPO certified palm oil is considered instead of non-certified palm oil. Hence, the differ between RSPO certified and non-certified palm oil could be further researched.

Among three synthetic hydrofobes, linear synthesis C10 alcohol caused the highest environmental impacts and environmental damage cost. The majority of the environmental damage cost are from carbon dioxide emission and crude oil used as a resource. This conclusion applies to all of the synthetic hydrofobes included in this study. Moreover, further developments in different approach to renewable sourcing for route of ethylene might improve the environmental impacts because a lot of synthetic route included utilizing pf ethylene.

8. Reference

1. Kurt Kosswig (2005). "Surfactants" in Ullmann's Encyclopedia of Industrial Chemistry, Wiley-VCH, Weinheim. DOI:10.1002/14356007.a25_747
2. Kocal, Joseph A., Vora, Bipin V. and Imai Tamotsu (2001). Production of linear alkylbenzenes. Applied Catalysis A: General. 221 (1–2): 295–301. DOI: 10.1016/S0926-860X(01)00808-0.
3. Adewale Daniel Omojowo 2016, Climate Change: A result of Human unsustainable Activities Threatens word Peace and Development, The Organization for World Peace, viewed 30 January 2020, <https://theowp.org/climate-change-a-result-of-human-unsustainable-activities-threatens-word-peace-and-development/>.
4. David L. Chandler (2013). Explained: Hydrophobic and hydrophilic, MIT News Office, viewed 13 February 2020, http://news.mit.edu/2013/hydrophobic-and-hydrophilic-explained-0716
5. Darem Ahmad., Inge van den Bogaraert., Jeremey Miller. and Roy Presswell. (2018). Hydrophilic and hydrophobic materials and their applications, pp. 2686-2725. DOI: 10.1080/15567036.2018.1511642
6. Marline, L., Squance., Glenn Reeves., John Attia., Howard Bridgman. and Maya Guest. (2015). Self-reported Lupus flare: Association with everyday home and personal product exposure, vol 2, pp. 880-888. DOI: 10.1016/j.toxrep.2015.05.010
7. The Editors of Encyclopaedia Britannica (2020). Surfactant compound, BRITANNICA, viewed 13 February 2020, <https://www.britannica.com/science/surfactant>.
8. Thierry Benvegnu., Daniel Plusquellec. and Loïc Lemiègre. (2008). Chapter 7 - Surfactants from Renewable Sources: Synthesis and Applications, pp. 153-178. DOI: 10.1016/B978-0-08-045316-3.00007-7
9. Adam Stephan Bland (2019). Global Surfactants Industry, IHA Markit, viewed 13 February 2020, <https://ihsmarkit.com/research-analysis/global-surfactants-industry.html>
10. Schowanck, D., Borsboom-Patel, T., Bouvy, A., Colling, J., Antonio de Ferre, J., Eggers, D., Groenke, K., Gruenenwald, T., Martinsson, J., Mckeown, P., Miller, B., Moons, S., Niedermann, K., Pérez, M., Schneider, C. and Viot J. (2017). New and updated life cycle inventories for surfactants used in European detergents: summary of the ERASM surfactant life cycle and eco footprinting project, pp. 867-886. DOI: 10.1007/s11367-017-1384-x

11. US Senate Committee on Agriculture Nutrition and Forestry, 2006. Energy Title (Title IX) of the Farm Security and Rural Investment Act of 2002, viewed 14 February 2020, <http://www.agriculture.senate.gov/imo/media/doc/107-171%20-%20Farm%20Security%20And%20Rural%20Investment%20Act%20Of%202002.pdf>
12. Douglas, G., Hayes. and George A. Smith. (2019). Biobased Surfactants: Overview and Industrial State of the Art, pp.3-38. DOI: 10.1016/B978-0-12-812705-6.00001-0
13. Jignesh Shah., Erdem Arslan., John Cirucci., Julie O'Brien. and Dave Moss. (2016). Comparison of Oleo- vs Petro-Sourcing of Fatty Alcohols via Cradle-to-Gate Life Cycle Assessment. DOI: 10.1007/s11743-016-1867-y
14. Judi Shapiro (2018). An Easy Guide to Understanding Surfactants, International Products Corporation, viewed 20 February 2020, <https://www.ipcol.com/blog/an-easy-guide-to-understanding-surfactants/>
15. Ethan (2018). What's are Anionic and Nonionic Surfactants?, Safe Household Cleaning, viewed 20 February 2020, <https://www.safehouseholdcleaning.com/anionic-nonionic-surfactants/>
16. Jacob Lindberg (2014). Monetarization – A Life Cycle Assessment weighting methodology, Monetize environmental impacts of paint with and without modified colloidal silica for AkzoNobel (Master's thesis). Available from Chalmers Open Digital Repository database. (Report No. 2014:10)
17. Baumann, H. and Tillman, A-M. (2004). The Hitch Hiker´s Guide to LCA. Lund, Sweden: Studentlitteratur AB.
18. Finnveden, G., Hauschild, M. Z., Ekvall, T., Guinée, J., Heijungs, R., Hellweg, S., Koehler, A., Pennington, D. and Suh, S. (2009). Recent developments in Life Cycle Assessment. Journal of Environment. vol. 91:1, pp.1-21. DOI: 10.1016/j.jenvman.2009.06.018.
19. Rebitzer, G., Ekvall, T., Frischknecht, R., Hunkeler, D., Norris, G., Rydberg, T., Schmidt, W.-P., Suh, S., Weidema, B.P. and Pennington, D.W. (2004). Life cycle assessment Part 1: Framwork, goal and scope definition, inventory analysis, and applications. Environmental International. vol. 30:5, pp. 701-720. DOI: 10.1016/j.envint.2003.11.005.
20. Scott Jenkins (2019). Technology profile: production of 2-propylheptanol, viewed 5 March 2020, <https://www.chemengonline.com/production-2-propylheptanol/>
21. Norman Harris., Alan J. Dennis. and Thomas F. Shevels (1980). Hydroformylation process for the production of n-Valeraldehyde. (Application No. US06/132,292)

22. Terence Bell (2019). Rhodium, a Rare Platinum Group Metal, and Its Applications, viewed 27 April 2020, <https://www.thoughtco.com/metal-profile-rhodium-2340151>
23. Emil A. Broger, Magden, Switzerland (1981). Process for manufacturing triphenylphosphine. Official Gazette of the United States patent and trademark office. vol. 1003. (Application No. 40,950)
24. Intratec (2019). 2-Propylheptanol Production Process Report 2-PH E11A Basic Cost Analysis, Intratec
25. Hai, T. (2002). The palm oil industry in Malaysia. From seed to frying pan, viewed 3 May 2020,<https://www.researchgate.net/publication/237447627_The_palm_oil_industry_in_Malaysia_From_seed_to_frying_pan?fbclid=IwAR3LK7UulITqjp3_wnpsVMyGfxqG_I5hMtrVoRdvvMr3ZM9lJAQ78GE8fFc>
26. Cryogenics & Lurgi technologies (2017). Oleochemicals Optimized For The Highest Quality Output, Air Liquid Engineering construction, viewed 3 May 2020, <https://www.engineering-airliquide.com/sites/activity_eandc/files/2017/11/22/air-liquide-e-c-oleochemicals-september-2017.pdf>
27. Sasol Olefins & Surfactants, SASOL reaching new frontiers, viewed 5 May 2020, <http://www.sasoltechdata.com/tds/nacol_nafol.pdf>
28. Klaus Noweck, Wolfgang Grafahrend (2006). "Fatty Alcohols". Ullmann's Encyclopedia of Industrial Chemistry. Weinheim: Wiley-VCH. doi:10.1002/14356007.a10_277.pub2.
29. Deschenes L., Lafrance P., Villeneuve JP., Samson R., (1996) Adding sodium dodecyl sulfate and Pseudomonas aeruginosa UG2 biosurfactants inhibits polycyclic aromatic hydrocarbon biodegradation in a weathered creosote-contaminated soil. Appl Microbiol Biotechnol 46:638–646
30. Sharrel Rebello., Aju K. Asok., Sathish Mundayoo.r, and M.S. Jish., (2003). Surfactants: chemistry, toxicity and remediation Chapter 5, pp. 277-324
31. Hall WS, Patoczka JB, Mirenda RJ, Porter BA, Miller E (1989) Acute toxicity of industrial surfactants to Mysidopsis bahia . Arch Environ Contam Toxicol 18:765–772
32. Goel G, Kaur S (2012) A study on chemical contamination of water due to household laundry detergents. J Hum Ecol 38:65–69
33. C.L. Yuan., Z.Z. Xu., M.X. Fan., Y.H. Xie. and T.Zhu (2014). Study on characteristics and harm of surfactants, Journal of Chemical and Pharmaceutical Research, 2014, 6(7):2233-2237
34. AL Michael (1991). Water Research, 25(11), 1425-1429

35. Jovanic BR, Bojovic S, Panic B, Radenkovic B, Despotovic M (2010). The effect of detergent as polluting agent on the photosynthetic activity and chlorophyll content in bean leaves. Health 2:395–399
36. Xiaoli Y, Xuegang L, Changbin S, Shihong C, Qiang W (2000) The effects of surfactants on the activity of invertase and superoxide dismutase of soybean leaf in vitro and in vivo. Colloids Surf A 175:249–255
37. Doyle C (2010). Powerful choices podcast: dispelling cancer myths, viewed 14 May 2020, <www.cancer.org>
38. U. Marcus Lindström (2007). Organic Reactions in Water; Principles, Strategies and Applications, Wiley Online Library. DOI: 10.1002/9780470988817
39. Bengtsson, M. (1998) Värderingsmetoder i LCA: Metoder för viktning av olika slags miljöpåverkan - en översikt. Gothenburg, Sweden: Chalmers University of Technology. (Department of Environmental system analysis). In CPM report 1998:1
40. Isabelle Blanc and Damien Friot (2010). Evaluation of Environmental Accounting Methodologies for the assessment of global environmental impacts of traded goods and services, viewed 24 May 2020, <http://www.imea-eu.com/documents/IMEA_Final_Report_septembre_2010.pdf>
41. The Industrial Green Game: Implications for Environmental Design and Management (1997). Pp. 124-131, viewed: 24 May 2020, <https://www.nap.edu/read/4982/chapter/11>
42. Steen, B. (1999a) A Systematic approach to environmental priority strategies in product development (EPS). Version 2000-general system characteristics. Gothenburg, Sweden: Chalmers University of Technology (CPM report 1999:4).
43. Steen, B. (1999b) A Systematic approach to environmental priority strategies in product development (EPS). Version 2000-Models and data of the default method. Gothenburg, Sweden: Chalmers University of Technology. (CPM report 1999:5).
44. Piet W.N.M. vn Leeuwen and Carmen Claver (2002). Rhodium Catalyzed Hydroformylation, Catalyst by Metal Complexes, Chapter 8. Vol. 22, pp. 223-227
45. Martin, B., Johannes, K., Eloise, B., Cecillia, M., Thilo, K., Niels, F., Niki, B., Annegrethe,H., Teresa, B., Veronica, B., Jenna, W. and Mar, M. (2004). Life Cycle Assessment of PVC and of principal competing materials, Final Report, viewed: 26 May 2020, <https://ec.europa.eu/environment/waste/studies/pdf/pvc-final_report_lca.pdf>

46. Jan Conway (2020). Size of the global household cleaners market from 2017 to 2020, Statista, viewed 29 May 2020, <https://www.statista.com/statistics/935010/household-cleaners-market-value-worldwide/>
47. Global Household Cleaning Products 2020-2024, Growing Primary and Secondary Housing Markets to Boost the Market Growth (2020). Technavio, viewed 29 May 2020, <https://www.businesswire.com/news/home/20200203005294/en/Global-Household-Cleaning-Products-2020-2024-Growing-Primary>
48. Altenpohl Dietrich (1982). Aluminum Viewed from Within: An Introduction into the Metallurgy of Aluminum Fabrication (English translation). Dusseldorf: Aluminium-Verlag, 1982.
49. Cristina Della Pina, Ermelinda Falletta, and Michele Rossi (2012), Chemical SSociety Review, Update on selective oxidation using gold, viewed 27 July 2020, <https://pubs-rsc-org.proxy.lib.chalmers.se/en/content/articlelanding/2012/cs/c1cs15089h#!divAbstract>
50. Marieke Leegwater and Gerrit van Duijin (2012), Traceability of RSPO-certified Sustainable Palm Oil, viewed 27 July 2020, Retrieved from https://app.knovel.com
51. Jannich Schmidt and Michele De Rosa (2019), New crowd-funded project: LCA of RSPO certified and non-certified Palm Oil, 2.-o LCA consultants, Denmark
52. Principles and Criteria for the Production of Sustainable Palm Oil (2013), Roundtable on Sustainable Palm oil, viewed 5 August 2020, <www.hallbarpalmolja.se/wp-content/uploads/2016/12/RSPO_Principles_Criteria_for_the_Production_of_Sustainable_Palm_Oil_2013.pdf>
53. GHS Classification Criteria for Eye Irritation and Serious Eye Damage (2019), ChemSafety Pro, viewed 10 June 2020, <https://www.chemsafetypro.com/Topics/GHS/GHS_Classification_Criteria_for_Serious_Eye_Damage_and_Eye_Irritation.html>
54. Guinée, J. B. (2004), Handbook on life cycle assessment, Kluwer Academic Publishers, viewed 10 June 2020, <http://proxy.lib.chalmers.se/login?url=http://search.ebscohost.com/login.aspx?direct=true&db=ir01368a&AN=cpl.89360&site=eds-live&scope=site>
55. Climate change: What is it and why is everyone talking about it? (2020), BBC News UK, viewed 25 April 2020, <https://www.bbc.co.uk/newsround/45880633>

APPENDIX

Appendix A: Underlying background information

A1: Life Cycle Assessment methodology

The whole procedure is illustrated in the figure A1.1 below by the unbroken line indicates the order of procedural steps and the dotted lines show iteration.

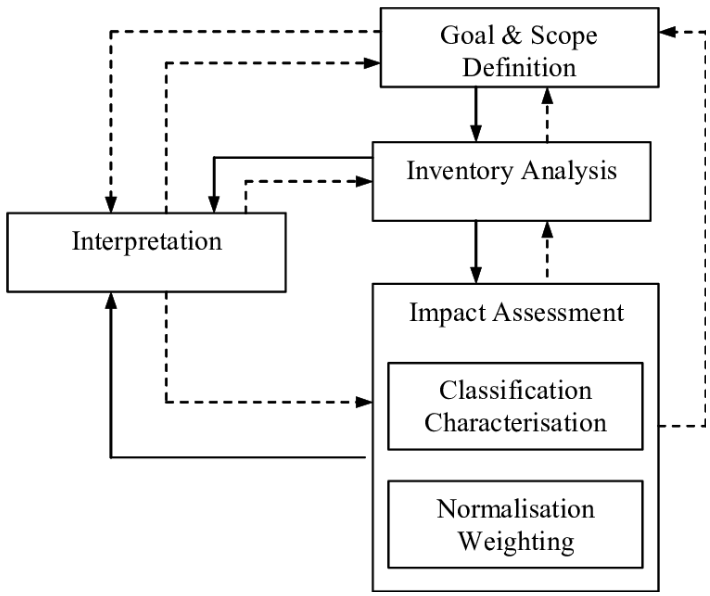


Figure A1.1: Working procedure for a Life Cycle Assessment (Baumann and Tillman, 2004).

Goal and scope

The LCA procedure starts with the definition of goal and scope of an LCA study. In this early stage, choices, specifications, requirements on the modelling are appointed (Baumann and Tillman, 2004). The result from stating goal and scope should provide adequate answers to questions in the context of the study such as why and how the study is conducted and who the intended audience are. Answering these question would help making relevant methodology choices in the modelling step because a specific purpose is considered instead of a general goal.

In the scope definition step, the modelling specification is decided which includes functional unit, type of environmental impact, method for impact assessment, system boundary, allocation description, and level of the details, and data quality requirement. The detail and aspect in each choice considered in this study are descripted in depth in Chapter 2 Goal and scope below.

Life Cycle Inventory (LCI)

The second procedure after goal and scope definition is Life Cycle Inventory (LCI). It is practically building the system model by constructing the flow model which is related to the system boundaries decided in the goal and scope definition. Collecting data is one of the actions in the LCI process and one of the most time consuming processes accordance with the concern for what type of data to collect and data sources. Due to the challenging and lacking of data, many databases have been developed in order to manage this issue. However, the data source (primary and secondary), location, production technology, and age of the data have to be concerned. When the flow model is constructed and the data are collected, the subsequent phase is calculation procedure. The calculation of the amount of resource use and pollutant emission of the system in relation to functional unit that are mentioned in goal and scope definition will be done in this part. The calculation steps, according to Baumann and Tillman (2004), contain normalizing the data, calculating the flows linked between processes in the flow model, calculating the flow passed the system boundary, summing up the resource use and emission, and documenting the calculations.

Life Cycle Impact Assessment (LCIA)

The impacts of the environment loads quantified in the inventory analysis are described in this part by using the conventional impact categories and turn the inventory result into more environmentally relevant information and easier comparable results by classification according to the type of environmental impact and characterization which is calculating the relative contributions of the emissions and resources consumption. The environmental problems are generally modelled by the web-like cause-effect chains. It is illustrated in figure A1.2 below.

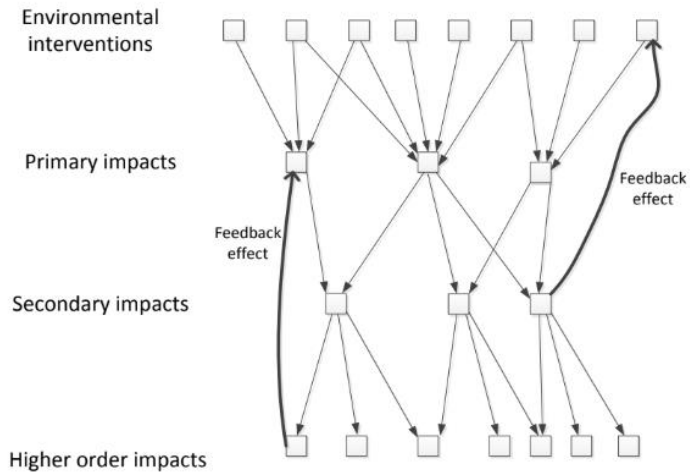


Figure A1.2: Cause-effect chain of environmental impacts (Baumann and Tillman, 2004)

The general structure of LCIA methods are presented in the figure A1.2. According to ISO 14042 (2000), the procedure of LCIA contains mandatory elements and optional elements along with sub-phases. The first step in mandatory elements is impact category definition considered relevant to the study. Impact categories are divided into two types which are midpoint level (potential impact in the cause-effect chain) and endpoint level (damages at the areas of protection). The second step is classification. The results from LCI are grouped and assigned to impact categories they lead to. The last step in mandatory elements is characterization. The environmental impact values are calculated from LCI data by using equivalency factor which represented the number of different impact categories such as CO_2-equivalents for global warming the impact category.

In the optional mandatory elements, three steps are mentioned in Blanc and Friot (2010) and one additional step is discussed in Baumann and Tillman (2004) which is data quality analysis. These steps could be performed independent from each other. Normalization is one of them, the impact results will be related to reference value to get a better understanding from environmental impacts from the whole system. The second one is grouping, where the characterization are grouped and assigned according to their importance such as emissions to fresh water or emissions to air. Another step is weighting, the environmental impacts are weight against all the other by using relative weights called weighting factors (Baumann and Tillman, 2004). The weighting method can be performed by using several kinds of principles for example monetarisation, authorized targets, authorized panels, proxies, or technology abatement. The weighting procedure will be descripted more in section 1.2.5 monetary valuation. The last one is an additional step named data quality analysis. The aim of this step is to greater understand the uncertainties and sensitivities of the system.

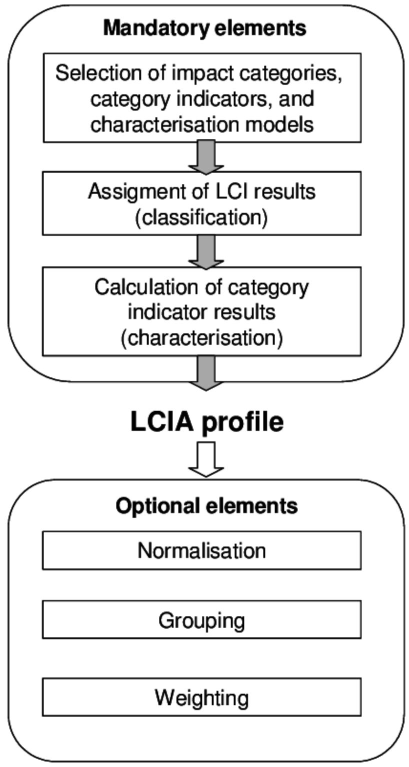


Figure A1.3: Life Cycle Impact Assessment (LCIA) according to Blanc and Friot (2010)

Interpretation of the results

The interpretation is a process to assess and conclude the results from the study by following the defined goal and scope definition from beginning of the process. According to Baumann and Tillman (2004), the structure of the interpretation phase will be helpful for analyzing and presenting the results from LCA study. The structure phase contains identification of significant issues to approach goal and scope, evaluation to establish confident in the results (selectivity and consistency check) to better understand the results accuracy, and conclusion which included limitations and recommendations.

A2: Environmental priority strategies (EPS)

The table A2.1 below shows the relationship between safeguards subjects, endpoint impact categories, and their specific weighting factors.

Table A2.1: Relationship between safeguards subjects, endpoint impact categories, and their specific weighting factors (Steen, 1999a; Steen, 1999b).

Safeguard subjects	Impact category	Category indicator	Indicator unit	Weighting factor (ELU/indicator unit)
Human health	Life expectancy	YOLL (years of life lost)	Person*years	85000
	Severe morbidity	Severe morbidity	Person*years	100000
	Morbidity	Morbidity	Person*years	10000
	Severe nuisance	Severe nuisance	Person*years	10000
	Nuisance	Nuisance	Person*years	100
Ecosystem production	Crop growth capacity	Crop	Kg	0.15
	Wood growth capacity	Wood	Kg	0.04
	Fish and meant production capacity	Fish and meat	Kg	1
	Soil acidification	Base cat-ion capacity of soil	Mole $H^{+,-}$ equivalents	0.01
	Production capacity for irrigation water	Irrigation water	Kg	0.003
	Production capacity for drinking water	Drinking water	Kg	0.03
Abiotic stock resources	Depletion of reserves	Reserves	Kg of elememt	0-594000000
	Depletion of coal reserves	Fossil oil	Kg	0.506
	Depletion of natural gas reserves	Fossil coal	kg	0.0498
Biodiversity	Species extinction	Natural gas	g	1.1
Cultural & recreational values	-	-	-	-

The environmental cost calculation in EPS method is descripted below in equation 1 based on Steen (1999b). The results from EPS environmental cost calculation is expressed in ELU, stand for Environmental Load Unit. ELU is basically known as currency Euro (Steen, 1999a).

$$\text{Substance emission (kg)} \times \frac{\text{Impact category (Indicator unit)}}{\text{Substance emission (kg)}} \times \frac{\text{Value (ELU)}}{\text{Impact category (Indicator unit)}} = \text{Value (ELU)} \qquad (1)$$

A3: Surfactant

Surfactants are the substances that reduce the interfacial tension between two liquids or between liquid and solid, by that increasing spreading and wetting properties of those phases (Britannica, 2020). Those properties provide a wide range of surface chemistry functions which are detergency, wetting, emulsifying, solubilizing, and softening (Benvegnu., Plusquellec. and Lemiègre, 2008). Due to the behaviour of surfactants, it can be utilized in the variety of applications in household, industry, and agriculture areas. Surfactants are mainly used to separate dirt and oil from various surfaces. The surfactant usage has been fast growing since last decade. The current worldwide production of surfactants reaches 16 million tons in 2018 which can be converted to $39 billion and it is expected to grow at an average annual rate of 2.6% (Adam Stephan Bland, 2019). The most application sector is household detergents for approximately 46% followed by industry and institutional, then personal care, and the smallest application sector is fabric softeners (Adam Stephan Bland, 2019).

Surfactants can be derived from both oleochemical feedstock and petrochemical feedstocks (Schowanck et al., 2017). US Senate Committee on Agriculture Nutrition and Forestry (2006) defined bio-based surfactant as a surfactant that is derived in whole or significant part of biological products or renewable domestic agricultural materials (including plant, animal, and marine materials) or forestry materials. The most frequently used sources for producing nonfood applications of bio-based surfactant are palm kernel, palm oil, and coconut oils (Douglas, G., Hayes. and George A. Smith, 2019). For food applications, corn, olive, or soybean oils are commonly used instead. Algae is another potentially valuable source by converting sunlight and CO_2 into carbohydrates and oil through photosynthesis (Douglas et al., 2019). For petrochemical feedstocks, they can be derived from crude oil, natural gas, or coal either by Ziegler process or by oxo process (Shah et al., 2016).

Surfactants can be categorized into four groups, cationic, anionic, amphoteric, and nonionic depending on the charge of the hydrophilic head (surfactants have a hydrophobic tail and hydrophilic head). A study by

Judi Shapiro (2018) summarized the type of surfactants. Anionic surfactants have a negative electric charge and are the most frequently used surfactants. For example, methyl ester sulfonates and sodium laureth sulfate. Cationic surfactants have a positive charge which is useful in fabric softeners for anti-static effect. Amphoteric surfactants have both positive and negative charges and are often used in personal care products. The commonly used amphoteric surfactants are alkylamidopropyl betaines (Douglas et al., 2019). Nonionic surfactants contain no charge and they are the second most widely used surfactants after anionic surfactants (Ethan, 2018).The most common nonionic surfactants are fatty alcohol ethoxylates, amine oxides, and sulfoxides.

A4: Toxicity of surfactants

Surfactants have gained huge importance in various industrial applications. However, it was seen that surfactants can cause some negative effects due to the surfactant toxicity on its usage and disposal. Surfactants are omnipresent effluents which can lead to the accumulation of potential toxicity or harmful substances and cause serious environmental problems (Deschenes et al., 1996). Not only the Industries but also human activities such as bathing and laundry discharge used and untreated surfactants or any other effluents to the rivers which increase the concentration of surfactants in the water bodies (Sharrel et al., 2003). The level of toxicity depends and varies with the chemistry of the pollutant surfactant, its ethylene oxide (EO) molar ratio. The EO ratio for the toxic surfactants is less than 15. To be the less toxic surfactants, the EO ratio must be in between 30 to 50 (Hall et al., 1989).

As it was mentioned in section 2.2, surfactants can be derived from both oleochemical feedstock and petrochemical feedstocks. Both types of surfactants result in environmental problems in different ways. The commonality they all share are the results in atmospheric emission (NOx, CO2, SO2, and hydrocarbons), eutrophication, and acidification to water bodies (Sharrel et al., 2003).

Surfactants derived from petrochemical feedstocks positively cause serious dangerous harm on ecosystems a lot more than the effect of oleochemical derived surfactants. The use of surfactants gives the chemical contamination in water and leads to significant increase in the pH level, chlorides, sulfate, carbonate, bicarbonate, and total dissolved solids (TDS) and decrease in the portability of wash water (Goel and Kaur, 2012). Surfactants have widely effects on various fields such as aquatic systems, plants and animals, and the human body.

Effects of surfactants to aquatic system

The major effect of surfactants is water pollution problems. When surfactants contaminate in water bodies, the bubbles and foam are formed. Therefore, the water surface will be turned into an insulating layer which reduces the exchangeability between water body and gas atmosphere land leads to reduction of dissolved oxygen (C.L. Yuan et al., 2014). Moreover, when the surfactant concentration exceeds the critical micelle concentration (the concentration when surfactant's surface tension remains constant or changes in the slower rate), the pollutants in water will be higher and change the water properties (AL Michael, 1991). Contamination of surfactants can kill microorganisms in the aquatic system as well which hinders the other toxic substances degradation because aquatic organisms play the role of taking up pollutants. The long term exposure to a contaminant of the aquatic system can lead to chronic toxicity. It is a toxicity that affects aquatic organisms including changes in growth, reproduction and behavior.

Effects on plants and animals

Agricultural system uses irrigation for planting. The source of water for irrigating is from the water body. From the effects of surfactants on aquatic systems, the water body can easily be contaminated with surfactants. Consequently, irrigation of agricultural systems can allow aggregation of surfactant residues in soil and plants. Physical and chemical properties of soil could be damaged even with the low concentration of surfactants polluted in the water (Sharrel et al., 2003). Surfactants basically affect the roots of the plants, reduce the photosynthetic rate (Jovanic et al., 2010), and hinder the specific activities in plants, for example, the hydrolysis of sucrose into fructose and glucose of soybean leaf (Xiaoli et al., 2000). Animals can normally be exposed to surfactants especially aquatic animals. Therefore, the toxicity of surfactants will transfer to animals either by feeding or penetration through skin (AL Michael, 1991). For example, exposing the surfactants of fishes. According to the body surface and gills, fish is very easy to take in surfactants. Furthermore, the contaminated fish will go through the food chain and enter the human body.

Effects on the human body

People are exposed to surfactants almost every day throughout the household cleaning product and personal care products. Long term exposure can cause skin irritation followed by some degree of damage. Surfactants can also transfer into human's body and affect the activity, enzyme, and physiological function (AL Michael, 1991). But there is still no research to confirm that surfactants are one of the cancer risk factors (Doyle, 2010).

Appendix B: Monetary valuation results

This appendix shows two different types of data table including their life cycle contributions and the environmental information of the environmental damage cost for each hydrofob raw material. Results depicted in batrcharts can be found in the monetary valuation results chapter.

Table B1: The environmental damage cost for 2-Propylheptanol production

The contributors to the environmental damage cost	**ELU**
Butene production	0.584881858
Synthesis gas production	0.045572321
Valeraldehyde production	0.123970291
2-PH production	0.229754365
Transportation	0.017991375
The environmental information of environmental damage cost	
Crude oil (resource)	0.309084079
Natural gas (resource)	0.22960678
Particles to air	0.006188732
Land use	0.000382143
NMVOC emission to air	0.028850912
Methane	5.17E-02
Carbon dioxide	3.08E-01
Carbon monoxide	1.52E-03
NOx	1.31E-03
SOx	1.31E-03
Inorganic to fresh water	8.88E-07
Non renewable resources/element	1.74E-02
Other	4.65E-02

Table B2: The environmental damage cost for Linear synthesis C10 alcohol production

The contributors to the environmental damage cost	**ELU**
Ethylene production	0.8000052
Aluminium production	0.2648073
Triethylaluminium production	0.0525808
Trialkilaluminium production	0.1103086
Alcohol production	1.18E-01
Transportation	0.0179914
The environmental information of environmental damage cost	
Crude oil (resource)	0.497677009
Natural gas (resource)	0.225029175
Particles to air	0.04417157
Land use	0.000597437
NMVOC emission to air	0.043290547
Methane	0.039102325
Carbon dioxide	3.75E-01
Carbon monoxide	1.09E-03
NOx	3.09E-03
SOx	4.71E-04
Non renewable resources/element	0.100111282
Other	3.35E-02

Table B3: The environmental damage cost for Isodecyl alcohol production

The contributors to the environmental damage cost	**ELU**
Propene production	0.702313
Isonnene production	0.097216
Synthesis gas production	0.043596
Isodecylalcohol production	0.11463
Transportation	0.019326
The environmental information of environmental damage cost	
Crude oil (resource)	0.43141587
Natural gas (resource)	0.17125192
Particles to air	0.01647759
Land use	0.00019218
NMVOC emission to air	0.03060534
Methane	0.02947573
Carbon dioxide	2.57E-01
Carbon monoxide	7.01E-04
NOx	2.21E-03
SOx	2.10E-04
Non renewable resources/element	1.75E-02
Other	1.44E-02

Table B4: The environmental damage cost for Natural C10 alcohol production

The contributors to the environmental damage cost	**ELU**
Crude palm kernel oil production	1.725493
Fatty alcohol production	2.046667
Transportation	0.168892
The environmental information of environmental damage cost	
Crude oil (resource)	0.10363681
Natural gas (resource)	0.0686076
Cadmium	0.45156946
Gold	0.10321182
Particles to air	0.84698957
Land use	0.04140414
NMVOC emission to air	0.07352008
Methane	0.14781458
Carbon dioxide	1.13E+00
Carbon monoxide	4.26E-02
NOx	7.53E-02
SOx	7.53E-02
Inorganic to fresh water	0.00017087
Non renewable resources/element	0.42511013
Other	3.54E-01

Appendix C: Impact assessment results

This appendix shows all of the characterization results from each studied impact category with respect to all four alternatives hydrofobes raw materials. Results depicted in batrcharts can be found in the impact assessment results chapter.

Table C1: Results for Global Warming Potential expressed in table form.

	GWP (kg CO2 eq.)				
	Raw material production	Transportation	Electricity	Thermal energy	Total
2-Propylheptanol	1.236159	0.05954	0.34723	1.030906	2.673835
Linear C10 alcohol	2.0253241	0.059996	0.271011	0.761058	3.1173891
Isodecyl alcohol	1.273253	0.043332	0.208819	0.60472	2.130124
Natural C10 alcohol	2.91199	0.358119	-		3.270109

Table C2: Results for Acidification Potential expressed in table form.

	AP (kg SO2 eq.)				
	Raw material production	Transportation	Electricity	Thermal energy	Total
2-Propylheptanol	0.0029448	0.000139	0.000914	0.000597	0.0045948
Linear C10 alcohol	0.005944309	0.000139	0.000765	0.0004408	0.007289309
Isodecyl alcohol	0.002545	0.000542	0.000589	0.00035	0.004026
Natural C10 alcohol	0.01772	0.008044	-	-	0.025764

Table C3: Results for Eutrophication Potential expressed in table form.

	EP (kg phosphate eq.)				
	Raw material production	Transportation	Electricity	Thermal energy	Total
2-Propylheptanol	0.000273377	0.0000347	0.0000964	0.0001055	0.000509977
Linear C10 alcohol	0.000512845	3.47E-05	0.00007163	0.00007784	6.97E-04

Isodecyl alcohol	0.00027864	1.34E-04	0.0000552	0.0000619	5.30E-04
Natural C10 alcohol	0.012871	0.0008947	-	-	0.0137657

Table C4: Ozone Layer Depletion Potential expressed in table form.

	ODP (kg R11 eq.)				
	Raw material production	Transportation	Electricity	Thermal energy	Total
2-Propylheptanol	3.3901E-10	9.77E-18	7.05E-15	7.04E-17	3.39E-10
Linear C10 alcohol	5.70526E-15	9.77E-18	7.55E-15	5.197E-17	1.33E-14
Isodecyl alcohol	1.422E-15	5.68E-18	5.82E-15	4.13E-17	7.28898E-15
Natural C10 alcohol	0.000001095	4.767E-17	-	-	1.095E-06

Table C5: Photochemical Ozone Creation Potential expressed in table form.

	POCP (kg ethene eq.)				
	Raw material production	Transportation	Electricity	Thermal energy	Total
2-Propylheptanol	0.00045035	-4.03E-05	0.0000593	0.0000914	0.00056075
Linear C10 alcohol	0.000695489	-4.03E-05	0.00004848	0.00006751	7.71E-04
Isodecyl alcohol	0.0004441	3.68E-05	0.0000374	0.0000536	0.0005719
Natural C10 alcohol	0.005385	0.0003467			0.0057317

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