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Renewable raw materials in the bioeconomy (340b)

Ecological assessment (LCA) of biomass conversion by hydropyrolysis to middle distillates in molten salts (ABC-Salt process)

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Abstract

Since climate change is becoming more acute and transport fuels are a mayor contributor of GHG emission, a substitute for those fuels is becoming increasingly important. Therefore, in this study, the product of the ABC-Salt process is examined for its environmental impact. The environmental impacts were evaluated by an LCA. As functional unit 1 MJ of fuel was used. The ABC-Salt process is a biomass-to-liquid process that aims to produce alternative fuels with a focus on a reduced climate change impact. For biomass a waste stream of kraft lignin from a Swedish pulp mill is used. The process starts with liquification and the usage of newly developed molten salts, and afterwards a hydropyrolysis developed by project partners. In the end the product is stabilized with hydrodeoxygenation. However, an economically and energetically allocation was done for Culbertsons approach. For the Bernier approach, 65.53 g CO_2-eq. per MJ product (base case) and 50.77 g CO_2-eq. per MJ product (integrated) can be determined. Furthermore, for the Culbertson approach, 41.90 g CO_2-eq. per MJ product (economic) and 67.25 g CO_2-eq. per MJ product (energetic) for the base case and 34.79 g CO_2-eq. per MJ product (economic) and 66.16 g CO_2-eq. per MJ product (energetic) for the integrated scenario could be recorded. Furthermore, trade-offs can be observed, with uranium mining and the use of salts having the greatest influence on acidification, ecotoxicity and resource use. In the future, further GHG emissions could be avoided by increasing the oil yield, as well as more efficient extraction of kraft lignin, as this has the greatest impact on climate change.

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List of abbreviations

AB	Activity Browser
ABC	Advanced Biomass Catalytic Conversion
bw2	brightway2
DLR	Deutsches Zentrum für Luft- und Raumfahrt
EF	environmental footprint
e.g.	example given
EN	European standard
EU	European Union
FEP	freshwater eutrophication potential
FTS	Fischer-Tropsch synthesis
GHG	greenhouse gases
GUI	graphical user interface
GWP	global warming potential
g CO_2-eq.	grams of CO_2 equivalents per MJ product
HDO	hydrodeoxygenation
i.e.	in example
IPCC	The Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
LCA	Life Cycle Assessment

LHV	lower heating value
MEP	marine eutrophication potential
NF	Normalization factors
NREL	National Renewable Energy Laboratory
ODP	ozone depletion potential
RISE	Research Institute Sweden
RUG	University of Groningen
SBSK	Southern bleached softwood kraft
TEPET	Techno-Economic Process Evaluation Tool
TRL	technology readiness level

1. Introduction

Global warming is a serious threat to millions of people and animals. In the last decades a lot of evidences and datasets for global warming were collected. Those evidences lead to many signals of climate change (NASA, 2021). Those signals are described by the IPCC:

"Warming of the climate system is unequivocal, and since the 1950s, many of the observed changes are unprecedented over decades to millennia. The atmosphere and ocean have warmed, the amounts of snow and ice have diminished, sea level has risen, and the concentrations of greenhouse gases have increased." - (IPCC, 2013)

Global Climate Change will be a major problem for the upcoming decades as more catastrophic climate events will happen more regularly (NASA, 2021). For example, the sea level will rise and a lot of people will need to search for refuge (NASA, 2021). As we can see with recent catastrophic events, which are also based on the global warming, the whole globe is hit by this crisis. Only some events get into the media or into our minds such as the inferno in Australia and USA, the flooding in central Europe (Germany, Belgium) and the melting glaciers in Iceland, Greenland as well as in Arctica and Antarctica. Furthermore, the melting of permafrost like in Canada and Siberia (Russia). According to NASA (2021) a well-known driver for climate change is fossil fuel, as carbon was secured millions of years ago and now it is been released in incredible amounts back into the atmosphere as for example Carbon dioxide (CO_2). All this shows us the need for renewable fuels and more environmentally friendly ways to travel.

Therefore, this master thesis focuses on the ecological valuation of a newly developed biomass-to-liquid process (ABC-Salt) that aims to produce alternative fuels with reduced climate change impact. The evaluation will be done by a Life Cycle Assessment (LCA). The whole life cycle will be modeled as realistically as possible with primary data from experiments and simulation based on those, done by project partners, as well as from secondary data like literature and LCA-Databases. The LCA model is based on an Aspen Plus process simulation. The greatest challenge of this LCA lies in the still low technology readiness level (TRL) of the process, which limits data availability for the production scale. Therefore scale-up effects have to be considered. Since the process steps are carried out by different project partners on a lab scale, there is not yet a coherent pilot plant build. The scale-up effects are taken into account by the Aspen Plus simulation. This is done by modeling individual steps into one coherent process based on the laboratory results of the ABC-Salt partners. For the ecological evaluation the open-source LCA software brightway2 will be used. From a variety of impact categories and methods a relevant number is selected for the process evaluation.

The approaches of Bernier's (2013) and Culbertson's (2016) LCAs were used during this thesis and adapted for the ABC-Salt process. These improvements are based on the first LCA results and new data from involved project partner Research Institutes of Sweden (RISE). Further, the biggest drivers of the impact categories are therefore considered. In particular, the greenhouse gas emissions of the biofuel are looked at to determine, whether the greenhouse gas (GHG) emissions can be reduced by 65% compared to a fossil fuel reference to comply with the revised renewable energy directive (RED II). Another focus will be the evaluation of the impact of an increasing oil yield and the different kraft lignin supply scenarios on the LCA results.

Therefore, following research questions accrue:

How much does the biofuel of the ABC-Salt process reduce the greenhouse gas emissions in comparison to fossil fuels?

What possibilities arise in order to reduce further impacts on the environment, in particular GWP and how does this effect other impact categories?

2. Production of renewable fuels

2.1 Biodiesel

Biodiesel is a renewable substitute to fossil fuels such as fossil diesel. It is made out of a lot of potential resources. For example, newly developed biodiesel productions use non-edible feedstock, such as Jatropha, Castor Beans or waste materials as well as algae just to name a few of them (Bera, 2020). In Figure 1 the different generations of biodiesel are shown.

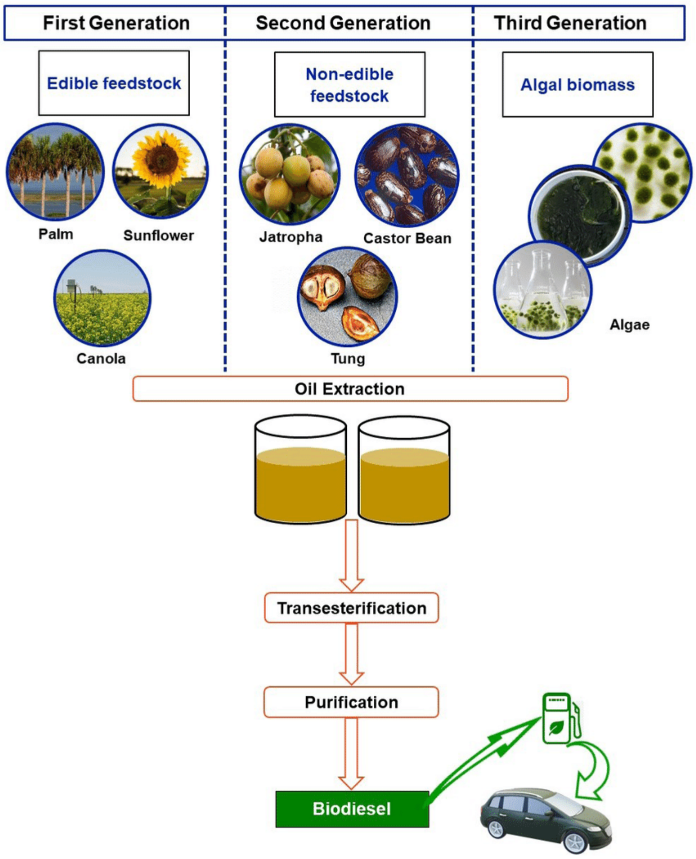


Figure 1: The different generations of feedstock and general way of biodiesel production (Bera, 2020)

2.1.1 State of the art production

Mostly, biodiesel is produced by transesterification reactions (see. Figure 1) which is a single step process and catalyzed by alkali catalysts. In this way of production, the triglycerides are reacted with alcohols, in the presence of a catalyst. Those catalyst function as a reaction promoter, to produce fatty acid methyl esters (Rizwanul Fattah et al., 2020). For example, triglycerides are stepwise converted to diglycerides, monoglyceride and in the end glycerin (or glycerol) (Rizwanul Fattah et al., 2020).

The second generation biodiesel production consists of several reactions which are consecutive, reversible and catalyzed. However, with depending on free fatty acid and water content, sometimes a two-step reaction is required (see. Figure 2 A). In this way of biodiesel production esterification is needed before the transesterification process (Ashraful et al., 2014). The flow diagram for the one- and two-step biodiesel production is expressed in Figure 2.

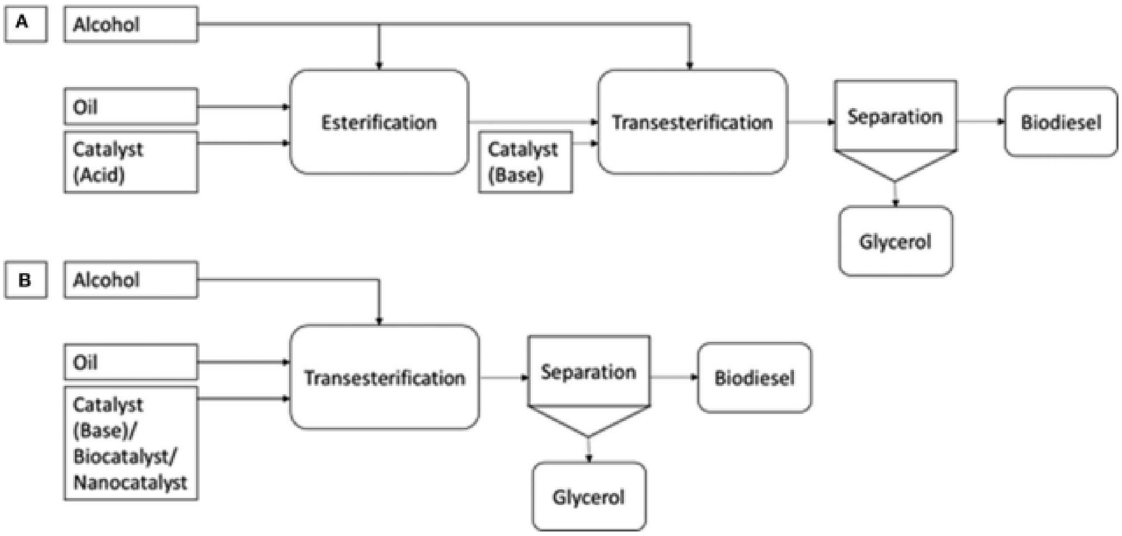


Figure 2: Biodiesel production from feedstock: (A) two-step process; (B) one-step process (Rizwanul Fattah et al., 2020)

2.1.2 Availability

The availability of biodiesel still depends on the region of the world. Rizwanul Fattah (2020) describes that the accessibility of biodiesel depends especially on a combination of climate, geographical location, local soil conditions but also on local agricultural practices. Furthermore, biodiesel is not widely available around the globe yet. But some countries do produce and consume this kind of fuel actively. Nowadays, biodiesel is available in the United States and Brazil commercially. In these countries it is only somewhat more expensive than its fossil counterpart. Furthermore, many American farmers who raise oil-seeds blend also biodiesel into equipment and tractors. This is done as a matter of the farmers policy to boost production of fuel and raise public environmental awareness (myBiodiesel, 2021).

Additionally, in Brazil the first commercial biodiesel refinery has opened in March 2005. According to myBiodiesel (2021) a variety of soybeans, sunflower seeds, or castor beans are used. In reference to Figure 1 the plant is capable to produce biodiesel from edible (first generation) and nonedible (second generation) feedstock (Bera, 2020). The finished product of the plant is a blend of gas oil with 2% biodiesel and it is expected to rise for a blend in up to

5% biodiesel. Both blended fuels are usable in unmodified diesel engines built after 2011 (myBiodiesel, 2021). Furthermore, cheap palm oil is produced in Indonesia, what is a “good” and also cheap solution for biodiesel production. In this study its environmental burdens of the cultivation are discussed later.

2.2 Bioethanol

The way how bioethanol is produced depends on its inputs as for example corn, sugarcane, wheat, straw or miscanthus. It is important to look at the input substrate as it contains different amounts of sugar, starch, cellulose and hemicellulose (Bera, 2020). Those components determine the way of production as well as its classification in first, second and third generation, as shown in Figure 3 (Bera, 2020). The state-of-the-art production is ethanol made of nonedible lignocellulosic feedstock. Therefore wood, energy grasses or crop residues could be used.

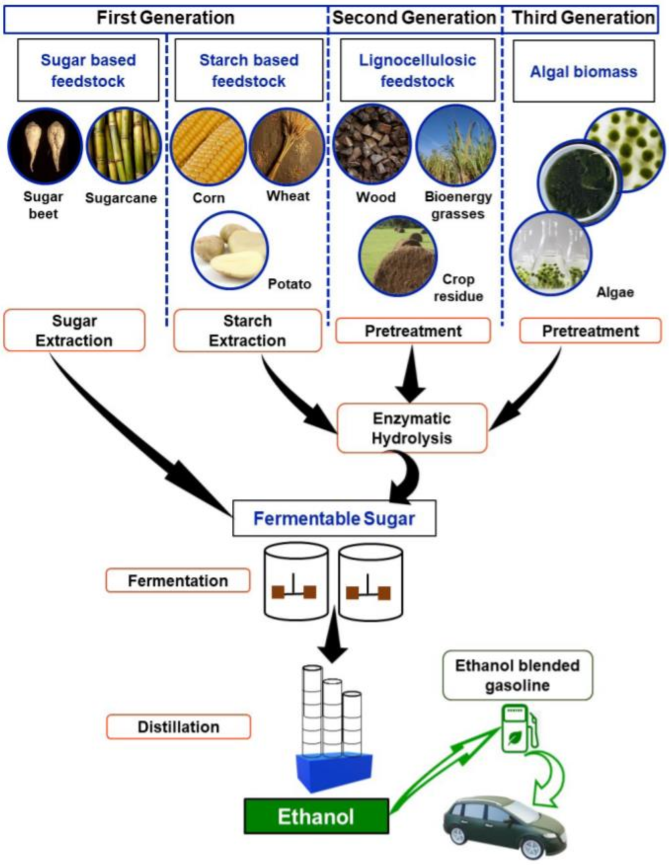


Figure 3: The different generations of feedstock and general way of bioethanol production (Bera, 2020)

2.2.1 State of the art production

Generally, the second generation bioethanol production starts with the pretreatment. Therefore, the typical agricultural waste needs size reduction. For this a simple mechanical (physical) pretreatment is done. Breaking up the structure of lignin, cellulose and hemicellulose is done for second generation feedstock, resulting in degradation of the crystallinity degree to achieve the required conditions before hydrolysis. After this pretreatment it is possible to do enzymatic hydrolysis. This hydrolysis is commonly catalyzed by enzymes or acids. In this step the long chains of carbohydrates (cellulose or starch) are separated with addition of water. This is the most important step for bioethanol production since the achieved quality of hydrolysate will affect further processes and therefore the ethanol quality in the end. The hydrolysis is needed because the microorganisms used during fermentation cannot digest complex sugars and need therefore shorter and simpler carbohydrates to ferment them (Aditiya et al., 2016).

The actual bioethanol production takes place during fermentation, the ethanol is produced directly from the metabolic activity of the implemented fermentation agents such as yeast or bacteria. One type of glucose-fermenting bacteria is for example Zymomonas mobilis. This bacteria prefers glucose-rich hydrolysate as feedstock and leaving ethanol as the product (Aditiya et al., 2016).

The ethanol solution contains a relative high water content. Therefore, the solution must be processed further in order to reduce the water content. In the end you can get a high-quality product of ethanol. “Drying” of this solution is commonly done by distillation (Aditiya et al., 2016).

2.2.2 Availability

The availability of ethanol produced of biomass is similar to the availability of biodiesel as it depends on the region too. Aditiya (2016) claimed, that for validation of the establishment of bioethanol refineries have to cover availability of *“feedstock, domestic demand, feedstock collection scheme, proper feedstock storage and transportation”*, similar to Rizwanul Fattah (2020). In Germany for example biofuel production and availability is mostly policy driven (Michalopoulos, 2020). This is the main reason why 5 or 10 percent of ethanol is blend into petrol available at gas stations and not further (Michalopoulos, 2020).

However, a well-known problem of the usage of second generation feedstock is the need of hydrolysis, which is known for its economic problem for high cost of enzymes and therefore is considered impractical for commercial purposes (Aditiya et al., 2016).

2.3 Opportunities, Risks and Prospects of Biofuels

As mentioned previously, for second generation biofuels the production is still not done often as it is much easier and cheaper for most countries to purchase fossil fuel or produce bioethanol with first generation production methods (myBiodiesel, 2021). Also, for smaller amounts of blend in biofuels, still first generation feedstock are primarily used.

Since biofuels need biomass for production, further problems can occur. These facts lead to food security concerns and still debates are ongoing. In Brazil it is common to deforest the rainforests in order to produce for example soybeans. That is why soybean cultivation in Brazil for feed and biodiesel threatens the Amazonian rainforest more than other reasons.

Furthermore, are the fruits of oil palms from Indonesia used for global biodiesel production (also called green gold). The cheapest vegetable oil source in the global market is palm oil, because of this it is well-suited as a biodiesel feedstock. But this oil is only this cheap because of the low wages in Indonesia. That is why environmental (deforestation) and social justice concerns limit palm oils market potential. Speaking of cheap oils, biofuels are commonly more expensive than their fossil counterparts. That is another reason why biodiesel is still produced in relatively small quantities in comparison to ethanol and petrol diesel.

A lot of organizations and companies are trying to develop cheap and reliable second or third generation biofuels. That is why lignocellulosic waste streams are in the focus of research. For example, the German Center for Aerospace (DLR) is developing together with European partners a new way to produce synthetic biofuels out of Kraft Lignin in molten salts as catalysts.

2.4 Electricity

The way how electricity is produced depends on region and country (Shittu and Santos, 2021). Electricity is mostly produced by fossil resources such as coal, oil and natural gas (Kåberger, 2018). However, capacities of renewable energies are increasing in order to produce environmentally friendly electricity (Burger, 2020). Until the year 2050 Europe want to produce its energy in a renewable way (Pleßmann and Blechinger, 2017). Like shown in Figure 4 Germany for example produces already 55.8% electricity out of renewable resources for the first half of 2020 (Burger, 2020)

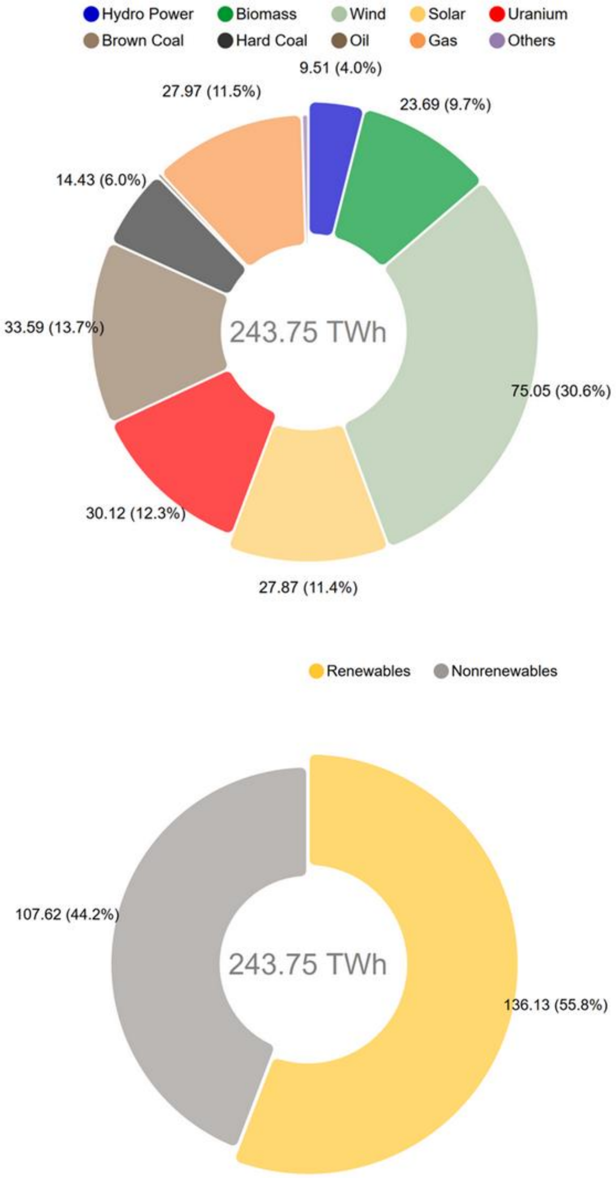


Figure 4: German electricity mix of first half of 2020 (Burger, 2020)

Figure 4 shows the net electricity supplied to the public grid by power plants (Burger, 2020). The biggest part of the electricity is produced by wind with 30.6% (see. Figure 4).

In comparison to Figure 4 the Swedish electricity is mainly produced with nuclear and hydro power (Cruciani, 2016). As shown in Figure 5 fossil fuels only contributes with 3 TWh (approx. 2%) into the electricity mix.

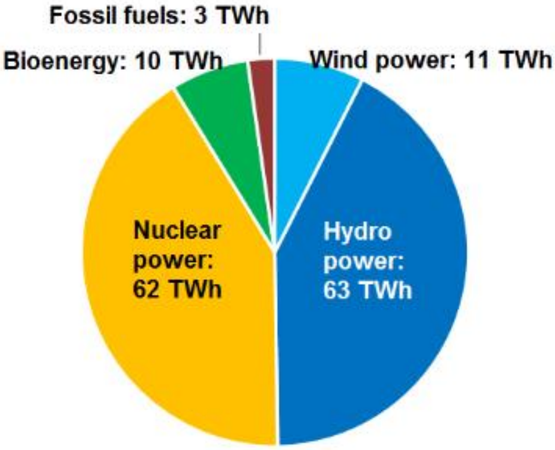


Figure 5: Swedish electricity mix by source (Cruciani, 2016)

Electricity as a fuel is discussed heavily by NGOs in for example Germany. As there is a discussion ongoing about the environmental problems occur with winning essential resources for the necessary batteries in countries like Argentina, Bolivia, Chile and China (Katawala, 2018).

2.4.1 State of the art production

For CO_2-neutral electricity production Pleßmann and Blechinger (2017) suggest to use a combination of solar, wind, biomass and hydro power. Actually renewable energies as well as nuclear power is producing very little to none greenhouse gases (Pleßmann and Blechinger, 2017). Therefore, electricity is a promising solution as an alternative fuel in order to fight climate change.

2.4.2 Availability

Since electricity is available in most countries, its availability as a fuel is also very promising (Ritchie and Roser, 2020). Furthermore, it is also very easy to upgrade a “own one-family-house” in order to charge an electric car. Additionally, more and more car companies are providing cheaper e-cars and governments are substitute the purchase of those (MEED, 2019). Since more and more infrastructure is built by i.e., Tesla and other manufactures. Therefore, a lot of parking lots now are electrified. In for example Germany 633,424 electric cars are driving on the highways every day (IEA, 2021). Though, in comparison to roughly 47.7 million of total registered cars it is still a very small number (Koptyung, 2020).

2.5 Hydrogen

Another type of alternative fuel is hydrogen. Hydrogen is generating power by converting the chemical energy to mechanical energy with the help of catalysts. This happens mostly as shown in Figure 6, in a fuel cell to power electric motor where hydrogen react with oxygen (Reis, 2017).

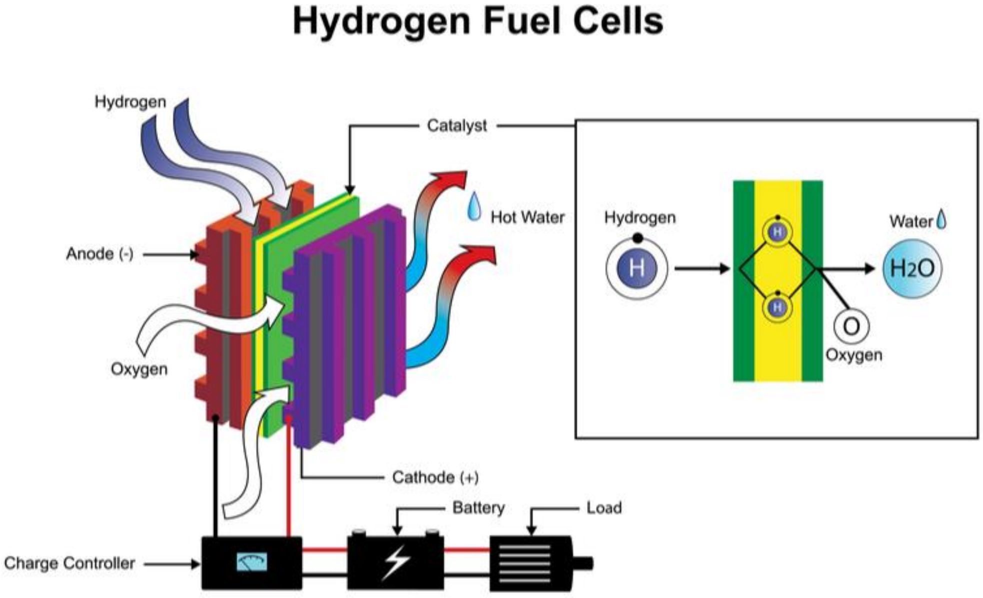


Figure 6 schematics of a modern hydrogen fuel cell (MEED, 2019)

A significant advantage of this fuel is that in the end only hot water and electricity is generated (see. Figure 6) (MEED, 2019). But first the hydrogen has to be produced. Therefore the state of the art production of hydrogen is mostly produced by steam methane reforming (98% as of 2019) (MEED, 2019). This way of production emits carbon monoxide (MEED, 2019), which effects its carbon dioxide footprint. As source for hydrogen production it is possible to use renewable feedstocks, but the production of hydrogen is currently expensive (Romm, 2014). Various low-cost technologies are nowadays under development. For example the research laboratory NREL and the company of Xcel Energy lunched an research project to produce H_2 from wind power via proton exchange membrane electrolyzers and one alkaline electrolyzer with quantities significant enough, to be a competitor to hydrogen production using natural gas (Harrison, 2009).

2.5.1 Availability

Warrick (2021) describes in his article that there were only two models of hydrogen cars commercially available for the year 2021 and only in selected markets. Both are from Asian car manufacturers Toyota and Hyundai. The Toyota Mirai was the first mass produced hydrogen fueled fuel cell electric vehicle (Warrick, 2021). Nearly every company that was testing hydrogen fueled cars have decided to produce battery electric cars instead. The German car producer “Volkswagen” made it clear that the technology has no future in the automotive sector. because with the energy one hydrogen car consumes you could run about three battery electric cars (Warrick, 2021). In the end of year 2020, there were only 31,225 passenger hydrogen powered cars on the globe (IEA, 2021).

2.6 Summary of alternate fuels

For fighting climate change, alternate fuels (electricity and hydrogen) and especially biofuels will play an important role in the future, since there is the need to reduce greenhouse gas emissions and therefore reduce usage of fossil fuels. Fossil fuels are expected to account for approx. 80% of the world’s energy requirement in 2030 with oil still remaining as the dominant energy provider. As a substitute for fossil fuels, biomass is hence projected to be one of the most important source of renewable energy (Jensen et al., 2011). But, with more biofuels also more biomass is needed. As previously mentioned this can leads to problems like deforestation of the Amazonas rainforest or the rainforests in Indonesia and competition to food production.

Furthermore, new solar and wind power is already cheap enough to become less expensive than oil- and some gas-based power. However, *“when coal and nuclear power plants will need major investments for example repairs or upgrades then also renewables possibly prove a better option”* so Kåberger (2018) as the costs to run those power plants would rise. But, with more electric cars the electricity consumption in the transport sector will increase. Therefore, it is important to look at country specific energy mixes as well as possible other environmental impacts, such as the destruction of landscapes or higher water usage for the winning of resources, in order to have local environmental footprints of those electric cars.

Not only for electric cars renewable power is needed but also for hydrogen production a lot of electricity is required. As previously mentioned is also important to have the local energy mixes in mind as they provide electricity based on fossil fuels or renewables. Further, hydrogen fueled cars are less efficient compared to electric cars (MEED, 2019). However, a hydrogen fuel cell, can convert hydrogen with air to produce electricity up to 60% efficiency (MEED, 2019). Therefore, modern hydrogen fuel cells compare favorably with internal combustion engine technology, which only convert hydrogen with approx. 25% efficiency.

3. Methodology

3.1 ABC-Salt

In the framework (see. Figure 7) of the EU-project ABC-Salt process variants will be modeled, analyzed and techno-economically as well as ecologically valuated at DLR. The goal is to produce synthetic fuels based on biomass. The process is based on liquification with molten salts, and subsequent hydropyrolysis developed by project partners. In the end the product is stabilized with hydrodeoxygenation. The biomass used in this project is a lignocellulose-containing waste stream.

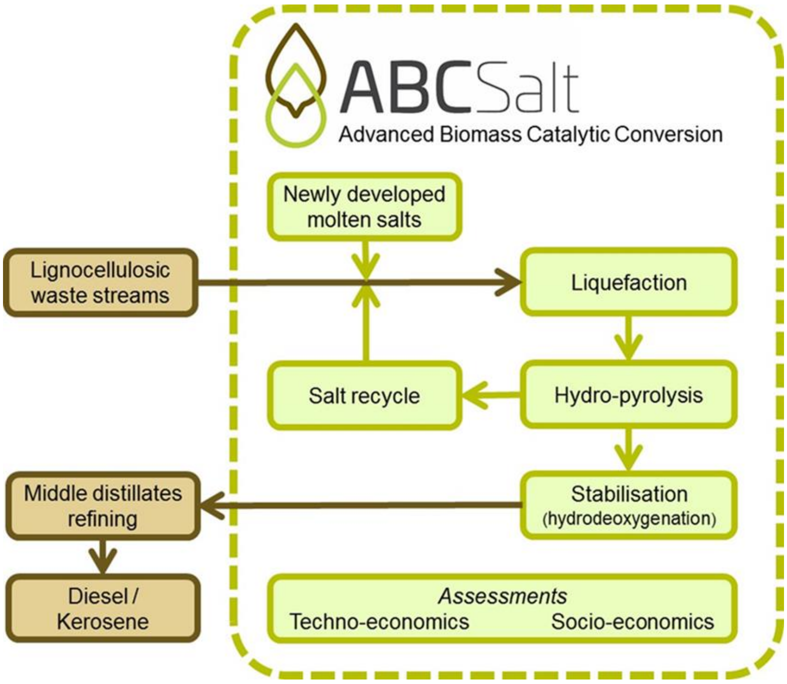


Figure 7: framework of the ABC-Salt Processes

3.1.1 Kraft lignin as input

One of the lignocellulosic waste streams is kraft lignin from a Swedish pulp mill modeled by the project partner RISE in Sweden. The dry kraft lignin contains 8% moisture. However, there are different possible approaches, or scenarios possible. The cases that will be investigated during this LCA are shown in Table 1.

Table 1: LCA cases of this study

Case	description	approach
kraft lignin powder		
base case	unintegrated char and gas phase	Bernier (2013) with data from RISE
integrated	fully integrated char and gas phase	Bernier (2013) with data from RISE
kraft lignin from SBSK		
economic, base case	economic allocation, unintegrated char and gas phase	Culbertson (2016) with data from RISE
energetic, base case	energetic allocation, unintegrated char and gas phase	Culbertson (2016) with data from RISE
economic, integrated	economic allocation, fully integrated char and gas phase	Culbertson (2016) with data from RISE
energetic, integrated	energetic allocation, fully integrated char and gas phase	Culbertson (2016) with data from RISE

3.1.2 Molten Salts

The ABC-Salt project partners newly developed molten salts with catalytic characteristics. The molten salts work as a catalyst as well as a heat carrier. The molten salt chosen for the ABC-Salt process concept contains ZnCl2; NaCl and KCl. For the LCA several biomass-salt-ratios have been tested. For NaCl and KCl ecoinvent database contains activities to use. For $ZnCl_2$ a new flow must to be created as there was no activity implemented in ecoinvent 3.6.

As this salts work as catalysts, can be assumed that they are inert in these processes and 98% of them are recycled. Only 2 wt% of the original mass is needed to be replaced by new molten salts. The use of salts is the most important change, in comparison to other pyrolysis production ways.

3.1.3 Liquefaction

The liquefaction model is based on experimental results from University of Groningen (RUG) (extruder experiments). Some minor chemical reactions take place there, forming water and propylene as a result. Afterwards the remaining components go further to the hydropyrolysis.

3.1.4 Hydropyrolysis

Hydropyrolysis is a combination of a pyrolytic, i.e., thermal, degradation of the chemical structure with simultaneous hydrogenation. By providing hydrogen, the radicals occurring as a result of homolytic cleavage should be saturated as much as possible and thus repolymerization reactions should be suppressed (Michels et al., 2014). The hydropyrolysis produces oil, gas and char as outputs. The products gas and char are going back to the pulp mill as they are burned to produce heat and electricity. Therefore, the consumption of natural gas can be prohibited. The salt is separated and recycled to the liquefaction.

3.1.5 Hydrodeoxygenation

The gaseous oil products from the hydropyrolysis enter the hydrodeoxygenation step. For the phenolic components, it is assumed that the backbone is kept intact during the reaction, while the ring is saturated forming aliphatic, cyclic hydrocarbons, whereas the -OH groups are separated, forming water. Methoxy-groups are assumed to form methane and water. The aliphatic feed components are assumed to pass the reactor as inert.

3.1.6 Classification of ABC-Salt

In this part of the study, the ABC-Salt project is compared to other similar processes as well as to fossil fuel as reference. The processes were compared in availability, production scale and GWP. For the LCA, as a functional unit, 1 MJ of fuel was used. For similar processes it is possible to look at conventional fast pyrolysis and Fischer-Tropsch synthesis (FTS). The FTS for example is a known synthesis process for over 70 years. It is known for clean transportation fuels as well as chemicals production (Schulz, 1999). With FTS it is possible to produce a variety of products. Mainly it is used for gasoline, diesel, waxes and chemicals production (Schulz, 1999). In industry CO and H2 enter the reactor together with a hydrocarbon liquid. Further, cobalt catalysts are used for high quality diesel production (Schulz, 1999). All components together are put in a fixed bed reactor with temperatures of approx. 220-240°C. Mainly diesel and waxes are the desired products (Schulz, 1999). A simple pyrolysis on the other hand can be also used to produce bio-oils or bio-diesel blends. Therefore, for example woody biomass or vegetable oils are used in a fast pyrolysis (Garcia-Perez et al., 2010). According to Garcia-Perez (2010), the production of crude bio-oils through pyrolysis has been the subject of decades of research, with only very little progress to produce additives or transportation fuels from these oils. But, the produced bio-oil has been employed as a fuel to produce electricity in modified gas turbines and diesel engines (Garcia-Perez et al., 2010).

Possibly the main differences of ABC-Salt to similar processes are the usage of molten salts as catalysts and heat exchanger. Furthermore, the ABC-Salt process is still only in lab scale available, while FTS is already in wide use (Schulz, 1999). Further, developed fast pyrolysis oils still cannot be used as transportation fuels yet, but research is still ongoing (Garcia-Perez et al., 2010).

The first approach was already defined by the DLR and the kraft lignin input flow is based on the data from the paper of Bernier (2013). The first LCA shows a total of approx. 300 g CO_2-eq. per MJ product. For easier reading g CO_2-eq. per MJ product is expressed as g CO_2-eq.. For comparison a fossil fuel reference is inserted, which emits 94 g CO_2-eq. (see. in Figure 8 "RED II fossil fuel"). EU guidelines demand a reduction of 65% of greenhouse gases for allowing the renewable fuel to get on the market. It is shown in Figure 8 with the red colored dashed line "RED II 65% limit". Additionally, the biomass was divided into its individual flows, to show where the greenhouse gases come from.

total: 296,65 g CO_2-eq. (Biomass: 273,21 g CO_2-eq.)

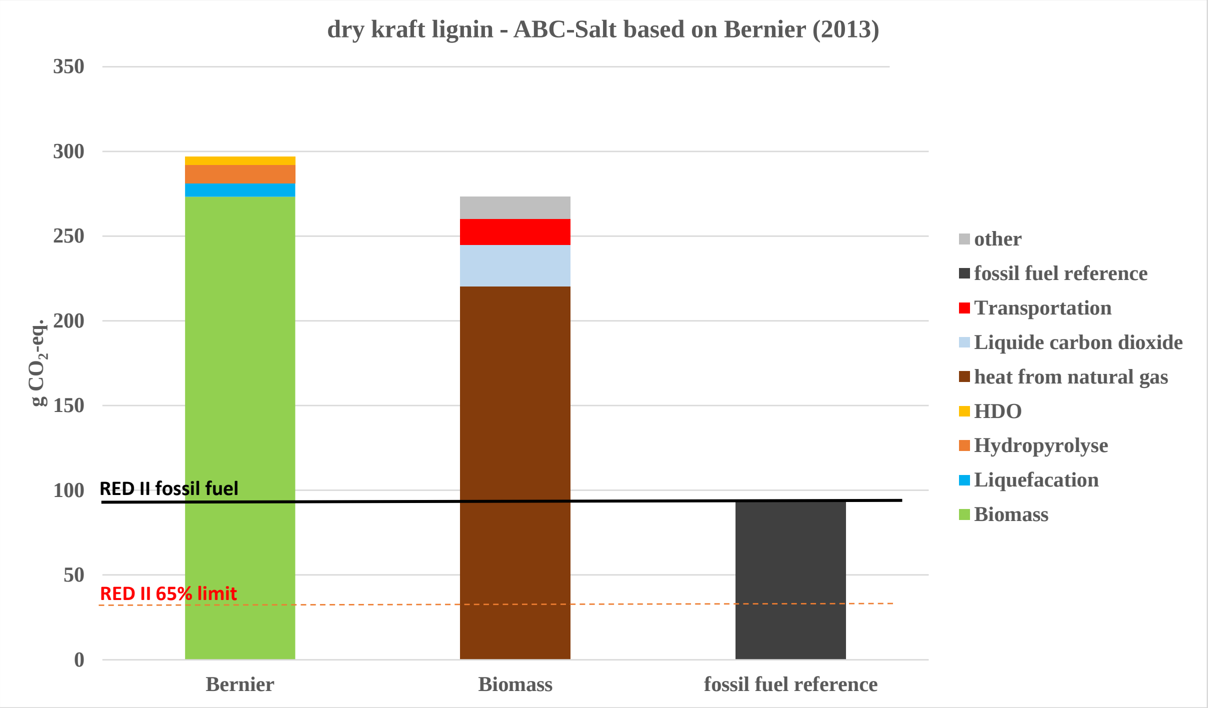


Figure 8: ABC-Salt base case GHG emissions with fossil fuel as reference for Kraft Lignin based on Bernier (2013)

For the classification of the current ABC-Salt process a short comparison to an LCA about pyrolysis is conducted. This LCA was done by Hsu (2012). The LCA suited well for comparison because for its production way as well as the data was reported in 1 MJ of fuel by Hsu (2012). The LCA of Hsu (2012) is performed in the Simapro software with the support of the ecoinvent 2.2 database. Forest residues are processed to bio-oil by pyrolysis with subsequent hydroprocessing in order to produce transportation fuels (see results in Table 2).

Table 2: GHG results for pyrolysis and gasification biofuels [a] (Hsu, 2012)

Case	GHG (g/MJ)
pyrolysis gasoline	39
pyrolysis diesel	39
pyrolysis gasoline with biomass-derived electricity(estimated)	25
pyrolysis diesel with biomass-derived electricity (estimated)	25
ethanol via gasification	10

a Reported per 1 MJ of fuel produced;
diesels lower heating value is not adjusted for greater engine efficiency.

Hsu (2012) was reporting his GHG emission in kg per MJ. For better comparison with this study, it was converted to g per MJ. For pyrolysis diesel as well as pyrolysis gasoline 39 g of CO_2-eq. were recorded. Furthermore, he showed more scenarios in Table 2. Here it is possible to see that those fuels can have GHG emissions from 10 g to 39 g. The first attempt of ABC-Salt process was about 297.65 g CO_2-equivalents. So, the ABC-Salt process is, before updated data is implemented, up to 10 times worse than diesel via pyrolysis.

Furthermore, if the ABC-Salt process is compared to commercial FTS fuels. FTS syndiesel produces about 654 g CO_2-eq. per liter (Searcy and Flynn, 2008). This equals about 20 g CO_2-eq. per MJ. It was assumed that the FTS syndiesel has the same LHV and density than biodiesel (BDBe, 2022)

For the GHG emissions it is possible to say that the ABC-Salt process is in its current form of data quality not a promising solution to reduce GHG emissions. Additionally, it is possible to say that pyrolysis as well as the ABC-Salt process are only available in lab scale. No pilot or commercial plants are actively built or planned currently. On the other hand, FTS is for 70 years commercially available and used. This classification is the reason why further data exchange was provided between RISE and DLR. Therefore, following parts of this study will focus on the LCA with updated data provided by RISE.

3.2. Aspen plus

Aspen Plus is a process simulation software, developed for the chemical industry (Aspen-Technology-Inc, 2022). With Aspen Plus it is possible to do integrated process modeling, cost estimation or energy management just to name a few of it possible capabilities (Aspen-Technology-Inc, 2022).

3.2.1 General process description and workflow

The Aspen Plus simulation was done by Sandra Adelung (DLR) and described in internal communications (Deliverable 2.6). In the first step, elementary balances and mass balances are created in Excel to ensure the mass balance is complete. The results of these calculations are then transferred to the process simulation (Aspen Plus V10). Figure 9 shows the general configuration of the base case V5.5 flowchart. After internal discussions with RISE, it was concluded that the lignin drying process takes place in the pulp mill and is therefore no longer included in the simulation. The dried lignin is mixed with the molten salt (salt, feed) to have 25 wt% lignin in the salt (based on autoclave experiments at RUG) and fed to the liquefaction section. All products from the liquefaction process are fed to the "hydropyrolysis" unit with the addition of hydrogen. Charcoal, salt and steam are the products of this step, which are then separated (ideal separation). The salt is recycled assuming a 2 wt% loss (98 wt% recovered, internal communication). The charcoal stream is then fully routed back to the pulp mill to provide a sufficient amount of thermal energy (25.6 MJ/kg) for the entire process configuration and additional energy that can be sold. The valuable vapor products from hydropyrolysis are further processed in a hydrodeoxygenation (HDO) step. Additional hydrogen is added there to reduce the amount of oxygen in the desired products. The three product fractions are finally separated in a 3-phase flash (1 bar, 25 °C). In the end, the HDO yields a gas phase, an aqueous phase (mainly water) and an oil phase (fuel). This oil phase is currently to be classified in the laboratory as to whether it has the properties of transport fuel. The gas phase goes back to the pulp mill for the same reason as the charcoal, while the gas can provide 61 MJ/kg of energy. The modeling of the various sections is presented in detail in the following sub-chapters.

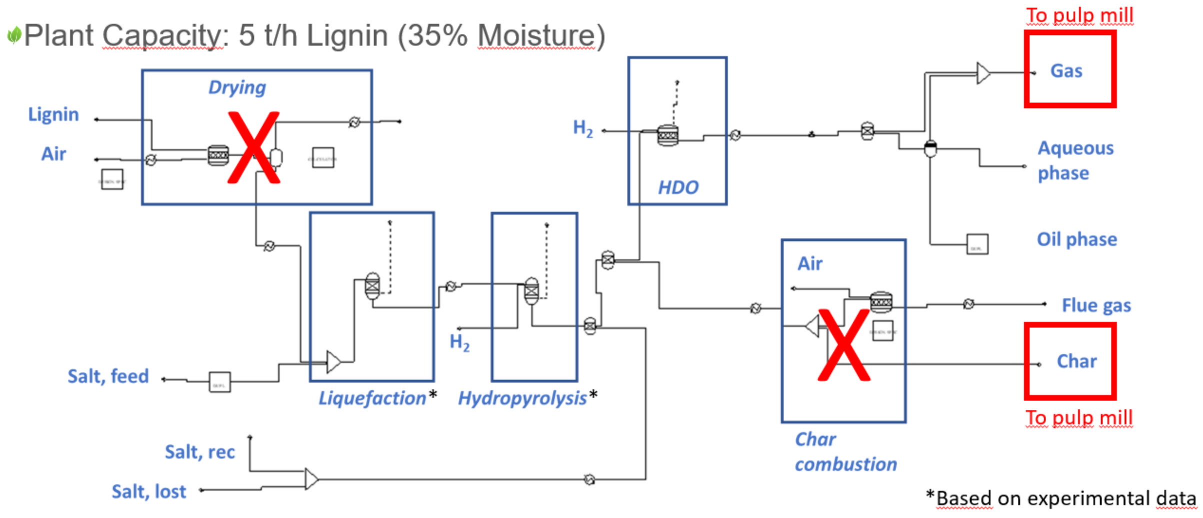
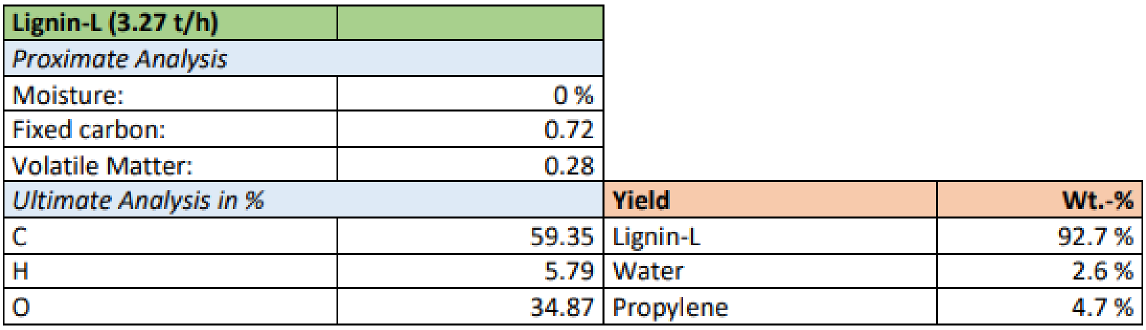


Figure 9:Flowsheet of pulp mill integration based on model V5

3.2.2 Liquefaction

As mentioned, the liquefaction model (see Figure 10) is based on the experimental results of RUG. Some minor chemical reactions take place, with water and propylene being formed as a result. Then the remaining components (coal and liquefied lignin) are combined in a non-conventional component Lignin-L (for specifications see Table 3, left). The C/H/O composition of lignin-L is calculated from the yields of the various components by closing the elemental balance. The liquefaction is modeled in an isothermal yield reactor at 1 bar and 230 °C. Yields by mass are shown in Table 3 on the right. In addition, it is important to note that the extruder experiments were performed with 10 wt% lignin in molten salt. However, since the hydropyrolysis is performed with 25 wt% lignin in molten salt, the liquefaction model is adjusted accordingly (25 wt% lignin-D in molten salt).

Table 3: Specification Lignin-L and liquefaction product yields



Lignin-L (3.27 t/h)			
Proximate Analysis			
Moisture:	0 %		
Fixed carbon:	0.72		
Volatile Matter:	0.28		
Ultimate Analysis in %		**Yield**	**Wt.-%**
C	59.35	Lignin-L	92.7 %
H	5.79	Water	2.6 %
O	34.87	Propylene	4.7 %

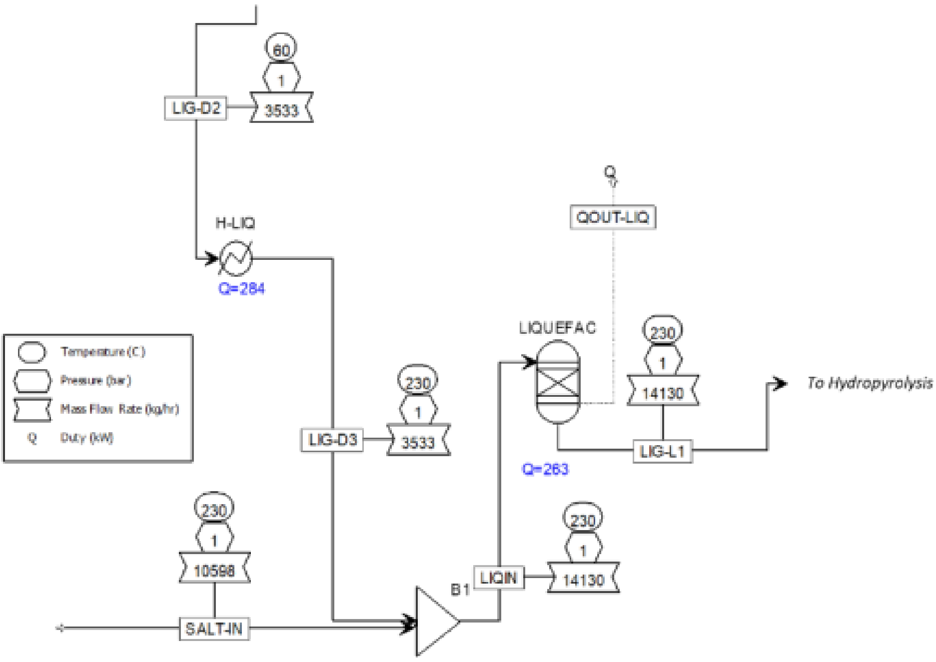
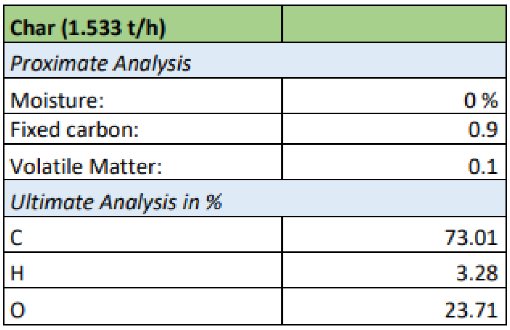


Figure 10: Flowsheet liquefaction section

3.2.3 Hydropyrolysis

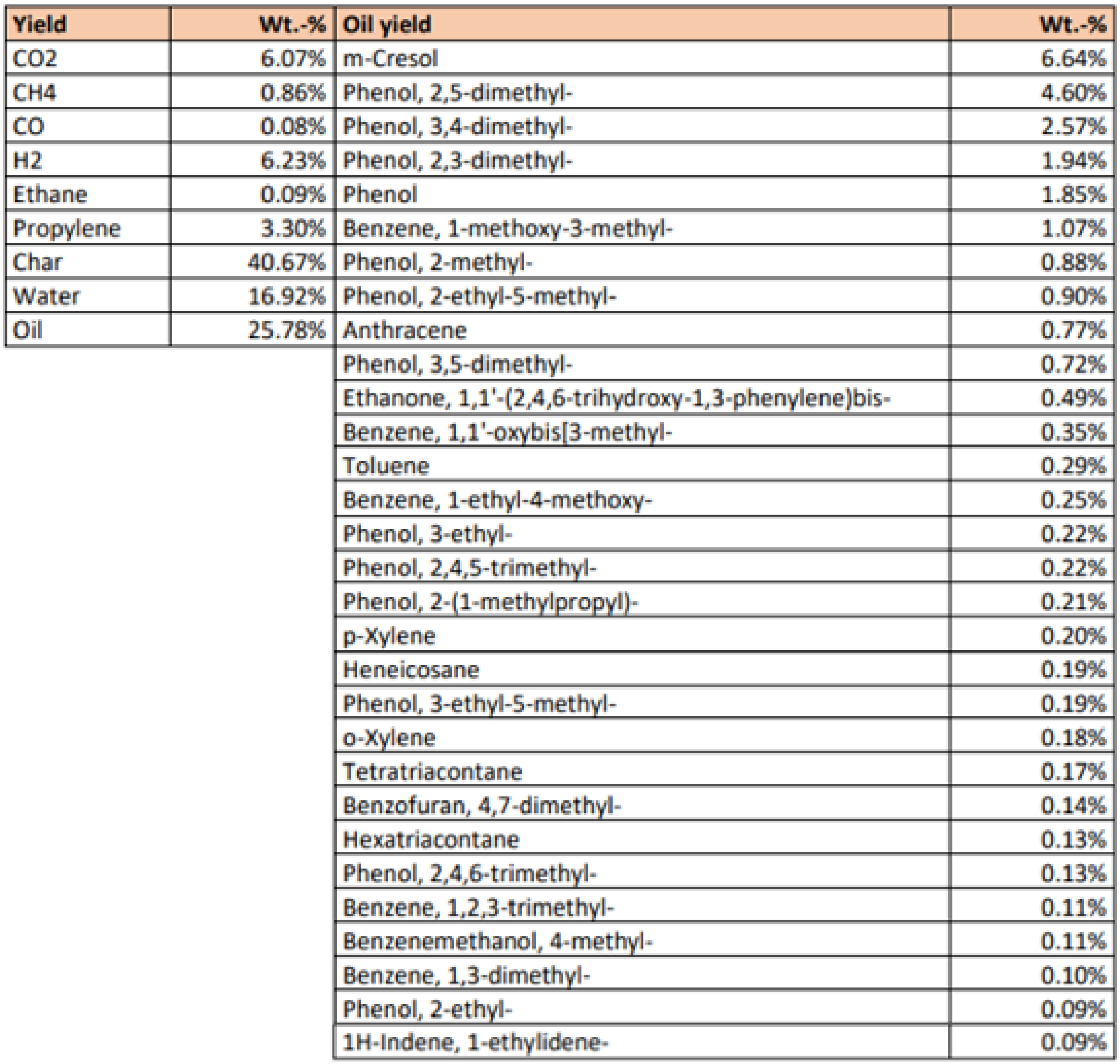
All liquefaction products are then fed into the hydropyrolysis reactor (see Figure 11). No information could be obtained from the experiments about how much hydrogen is needed for the reaction. Since hydrogen is added, it was estimated that 0.067t of H2 would be needed to process 1t of lignin (internal communication). Therefore, 236.7 kg H2/h are fed into the reactor. The hydropyrolysis yields for the simulation are based on autoclave experiments performed by RUG. The amount of oil, water and coal was measured in the experiments. Furthermore, the oil was analyzed, which gives a good estimate of the composition of the oil phase. Since nitrogen is not included in the simulation at this point in time, nitrogen-containing components have been replaced by corresponding hydrocarbons. Therefore, 29 components provide information for 95% by weight of the oil phase. They are assumed to represent the total oil fraction (see Table 5). The approximate gas composition was also provided by RUG. The gas composition is measured after a corresponding running time. From this, the overall yields of the gas components are calculated after 100 minutes in the stream (see Table 5 for results). At that time, no data for the respective coal composition was available from the RUG autoclave experiments. Coal composition (C and O) was therefore calculated by closing the elemental balance. Experimental results from UGENT for Lignoboost pyrolysis are used to calculate the amount of hydrogen incorporated in coal. Their char analysis shows 3.3 wt% H in char. To match the amount of H in coal, the amount of unreacted hydrogen is adjusted. This gives a yield of 6.23 wt% H 2 exiting the reactor. The reaction is modeled with an isothermal yield reactor (25 bar, 400 °C). See Table 4 for the char specification and yields in this stage. In a next step, char and salt are ideally separated from the other products. The remaining fraction then proceeds to the hydrodeoxygenation section.

Table 4: Specification char



Char (1.533 t/h)	
Proximate Analysis	
Moisture:	0 %
Fixed carbon:	0.9
Volatile Matter:	0.1
Ultimate Analysis in %	
C	73.01
H	3.28
O	23.71

Table 5: Hydropyrolysis yields



Yield	**Wt.-%**	**Oil yield**	**Wt.-%**
CO2	6.07%	m-Cresol	6.64%
CH4	0.86%	Phenol, 2,5-dimethyl-	4.60%
CO	0.08%	Phenol, 3,4-dimethyl-	2.57%
H2	6.23%	Phenol, 2,3-dimethyl-	1.94%
Ethane	0.09%	Phenol	1.85%
Propylene	3.30%	Benzene, 1-methoxy-3-methyl-	1.07%
Char	40.67%	Phenol, 2-methyl-	0.88%
Water	16.92%	Phenol, 2-ethyl-5-methyl-	0.90%
Oil	25.78%	Anthracene	0.77%
		Phenol, 3,5-dimethyl-	0.72%
		Ethanone, 1,1'-(2,4,6-trihydroxy-1,3-phenylene)bis-	0.49%
		Benzene, 1,1'-oxybis[3-methyl-	0.35%
		Toluene	0.29%
		Benzene, 1-ethyl-4-methoxy-	0.25%
		Phenol, 3-ethyl-	0.22%
		Phenol, 2,4,5-trimethyl-	0.22%
		Phenol, 2-(1-methylpropyl)-	0.21%
		p-Xylene	0.20%
		Heneicosane	0.19%
		Phenol, 3-ethyl-5-methyl-	0.19%
		o-Xylene	0.18%
		Tetratriacontane	0.17%
		Benzofuran, 4,7-dimethyl-	0.14%
		Hexatriacontane	0.13%
		Phenol, 2,4,6-trimethyl-	0.13%
		Benzene, 1,2,3-trimethyl-	0.11%
		Benzenemethanol, 4-methyl-	0.11%
		Benzene, 1,3-dimethyl-	0.10%
		Phenol, 2-ethyl-	0.09%
		1H-Indene, 1-ethylidene-	0.09%

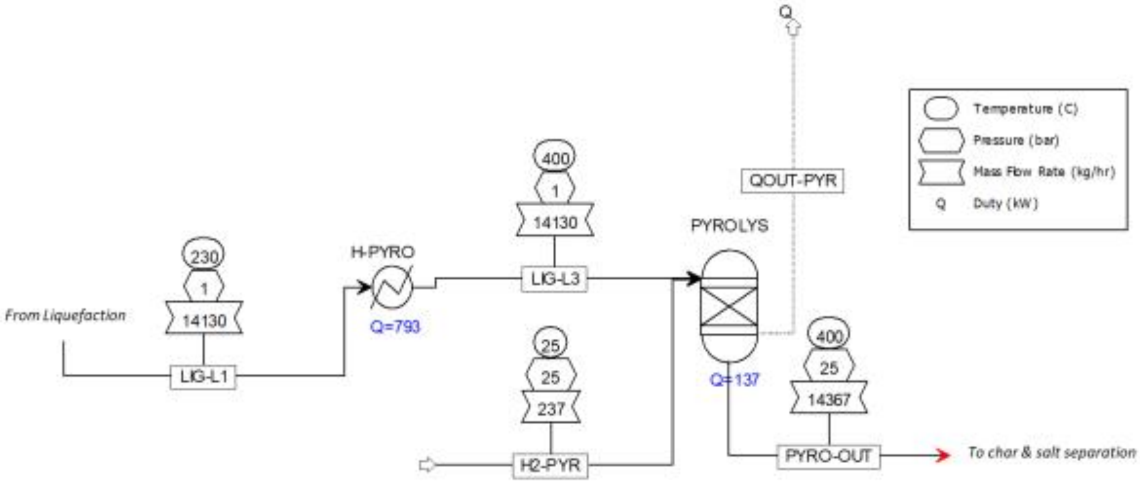
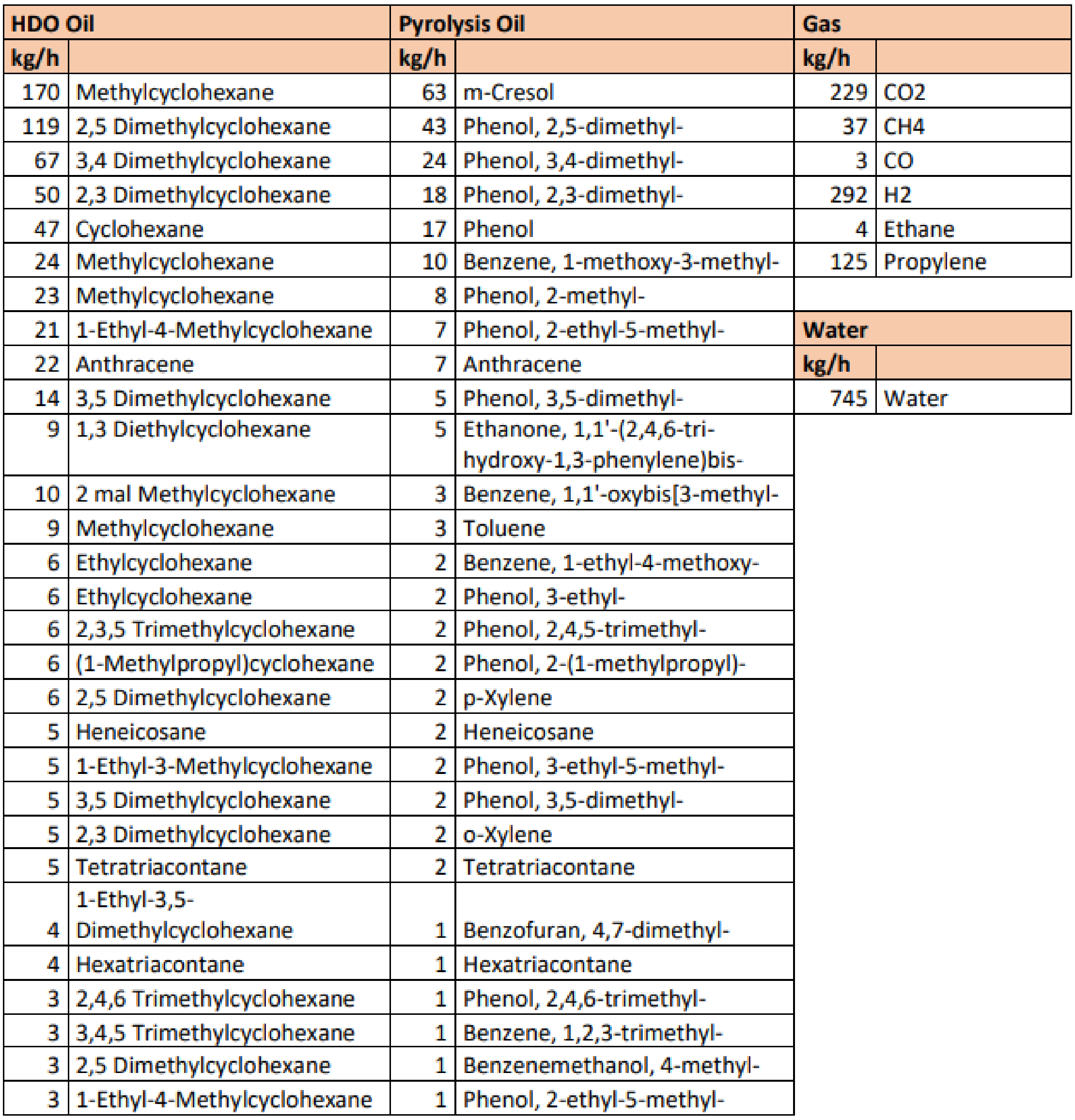


Figure 11:Flowsheet hydropyrolysis section

3.2.4 Hydrodeoxygenation

The vapor products from hydropyrolysis enter the hydrodeoxygenation step (see Figure 12). At this time, no experimental data was available for the HDO of the actual products. Therefore, it was assumed that the molecules are subject to an idealized (complete) HDO. The conversion was set at 75% for each reaction. The HDO is modeled in an isothermal stoichiometric reactor (50 bar, 400 °C). For the phenolic components, it is believed that the backbone remains intact during the reaction while the ring becomes saturated, forming aliphatic, cyclic hydrocarbons, while the -OH groups are separated, forming water. It is believed that methoxy groups form methane and water. The aliphatic feed components are believed to pass through the reactor as inert. The required minimum amount of hydrogen can be calculated from the stoichiometry of the reactions to 0.05 t H2/h. However, the amount of hydrogen actually added to the HDO is taken from the internal communication at 0.106 t H2/h. With the excess hydrogen from the hydropyrolysis, almost 7 times the amount of hydrogen that is stoichiometrically required for the reaction gets into the HDO reactor (conservative approach). The product composition leaving the HDO is shown in Table 6.

Table 6: Hydrodeoxygenation products



HDO Oil		**Pyrolysis Oil**		**Gas**	
kg/h		**kg/h**		**kg/h**	
170	Methylcyclohexane	63	m-Cresol	229	CO2
119	2,5 Dimethylcyclohexane	43	Phenol, 2,5-dimethyl-	37	CH4
67	3,4 Dimethylcyclohexane	24	Phenol, 3,4-dimethyl-	3	CO
50	2,3 Dimethylcyclohexane	18	Phenol, 2,3-dimethyl-	292	H2
47	Cyclohexane	17	Phenol	4	Ethane
24	Methylcyclohexane	10	Benzene, 1-methoxy-3-methyl-	125	Propylene
23	Methylcyclohexane	8	Phenol, 2-methyl-		
21	1-Ethyl-4-Methylcyclohexane	7	Phenol, 2-ethyl-5-methyl-	**Water**	
22	Anthracene	7	Anthracene	**kg/h**	
14	3,5 Dimethylcyclohexane	5	Phenol, 3,5-dimethyl-	745	Water
9	1,3 Diethylcyclohexane	5	Ethanone, 1,1'-(2,4,6-tri-hydroxy-1,3-phenylene)bis-		
10	2 mal Methylcyclohexane	3	Benzene, 1,1'-oxybis[3-methyl-		
9	Methylcyclohexane	3	Toluene		
6	Ethylcyclohexane	2	Benzene, 1-ethyl-4-methoxy-		
6	Ethylcyclohexane	2	Phenol, 3-ethyl-		
6	2,3,5 Trimethylcyclohexane	2	Phenol, 2,4,5-trimethyl-		
6	(1-Methylpropyl)cyclohexane	2	Phenol, 2-(1-methylpropyl)-		
6	2,5 Dimethylcyclohexane	2	p-Xylene		
5	Heneicosane	2	Heneicosane		
5	1-Ethyl-3-Methylcyclohexane	2	Phenol, 3-ethyl-5-methyl-		
5	3,5 Dimethylcyclohexane	2	Phenol, 3,5-dimethyl-		
5	2,3 Dimethylcyclohexane	2	o-Xylene		
5	Tetratriacontane	2	Tetratriacontane		
4	1-Ethyl-3,5-Dimethylcyclohexane	1	Benzofuran, 4,7-dimethyl-		
4	Hexatriacontane	1	Hexatriacontane		
3	2,4,6 Trimethylcyclohexane	1	Phenol, 2,4,6-trimethyl-		
3	3,4,5 Trimethylcyclohexane	1	Benzene, 1,2,3-trimethyl-		
3	2,5 Dimethylcyclohexane	1	Benzenemethanol, 4-methyl-		
3	1-Ethyl-4-Methylcyclohexane	1	Phenol, 2-ethyl-5-methyl-		

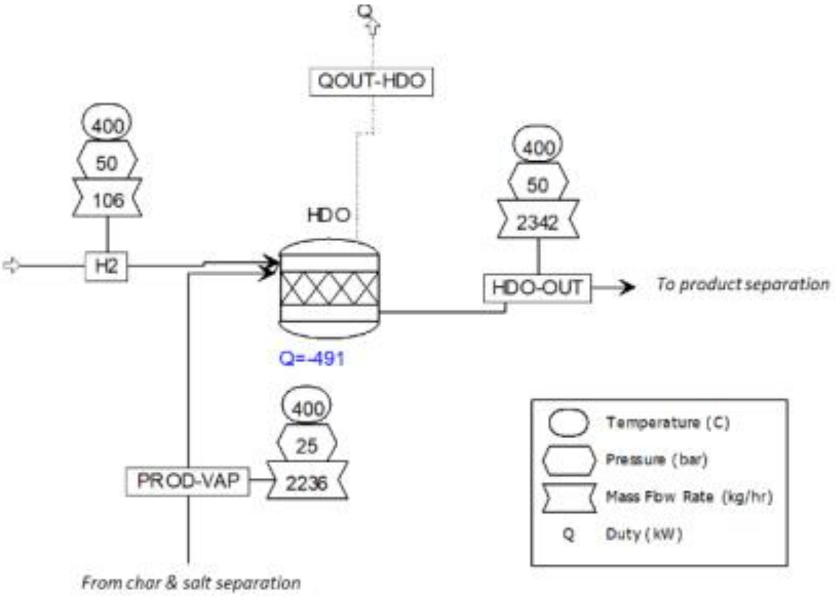


Figure 12: Flowsheet hydrodeoxygenation section

Additionally, the implementation of lignin into pulp mill or a scenario without was discussed in several meetings with the project partner RISE and lead to the different scenarios of this study.

3.3 Inventory

In the following Tables all inputs and products as well of the used flows of the LCA are shown. Those are shown in an inventory. The general inventory for 1 MJ of ABC-Salt product is shown in Table 7. Therefore, 992,5 g of biomass is needed. For the liquefaction process 0,64 g of KCl, 1,53 g of NaCl and 3,78 g of ZnCl are needed and 5,96 g of waste produced. For Hydropyrolysis only 6,65 g additional hydrogen is needed. In the end further 2,98 g of H2 are used together with 2,06E-05 m3 of wastewater is produced in the HDO. One megajoule of product is equivalent to 249 g.

Table 7: Inventory for 1 MJ of ABC-Salt fuel

Inventory for 1 MJ ABC-Salt product

inputs

materials	**units**	**value**
biomass supply		
dry kraft lignin	g	992.50
liquefacation		
KCl	g	0.64
NaCl	g	1.53
ZnCl2	g	3.78
hydropyrolysis		
H2	g	6.65
HDO		
H2	g	2.98
outputs		
waste		
solid waste	g	5.96
wastewater	m^3	2.06E-05
products		
1 MJ of fuel	g	249.00

Table 8: inventory of dry kraft lignin for the integrated and the base case scenario of the Bernier (2013) approach

Inventory 1 kg dry kraft lignin (base case)

inputs

materials	**units**	**value**
technosphere		
CO2, liquid	g	180.00
sulfuric acid	g	170.00
sodium hydroxide	g	140.00
ash	g	220.00
tap water	g	4200.00
medium voltage	kWh	2.77
outputs		
products		
dry kraft lignin	kg	1.00

Inventory 1 kg dry kraft lignin (integrated)

inputs

materials	**units**	**value**
technosphere		
CO2, liquid	g	180.00
sulfuric acid	g	170.00
sodium hydroxide	g	140.00
ash	g	220.00
tap water	g	4200.00
outputs		
products		
medium voltage	kWh	0.19
dry kraft lignin	kg	1.00

For all cases liquefaction, hydropyrolysis and HDO are the same. The main differences of the different approaches are for the biomass supply. For all cases the kraft lignin and its inputs as well as outputs are showed in more detail for each scenario in tables 8 and 9.

For the Bernier (2013) approach of kraft lignin recovery, 180 g of liquid CO_2 is needed at the precipitation step, liquid CO_2 is injected into the black liquor for decreasing its pH. Further, 170 g of sulfuric acid and additional 140 g of sodium hydroxide are used for washing. The process of washing is done with tap water and sulfuric acid, some of which is neutralized by the remaining traces of black liquor. Therefore, some additional sodium hydroxide must be included somehow in order to replace the sodium entrained at the washing step. Furthermore, 4.200 g of tap water and 220 g of ash are also required (see. Table 8). The difference between the base case and the integrated scenario are localized for the electricity needed. For the base case the char and gas of the ABC-Salt process are not integrated into the pulp mill. Therefore, external electricity is needed for providing heat and energy. Furthermore, 2,77 kWh are required for the production of 1 kg of dry kraft lignin. It is needed for filtration and substituting heat which is required for the processes. In comparison to the integrated scenario, were the char and gas are going back to the pulp mill, in order to produce the required energy, the ABC-Salt process is producing 0,19 kWh of medium voltage electricity.

For the Culbertson (2016) approach the inventory is similar to the Bernier approach. In both approaches the main difference is power supply. For both scenarios more power is produced as consumed and therefore sold. With integration of the ABC-Salt process into the pulp mill more power (+3,11 kWh) is produced and sold. Furthermore, the inputs are split into technosphere and biosphere (see. Table 9). During the LignoBoost process 200 g of liquid CO_2 is needed. Furthermore, 685.4 g of sulfuric acid and 858.5 g of sodium hydroxide are used during all processes. At the bleach plant 373.4 g of hydrogen peroxide, 29.6 g of methanol and 589.6 g of sodium chlorite are required as well as liquid oxygen, sulfur dioxide and magnesium sulfate (see. Table 9). In the beginning 54.17 kg of softwood (pine) is needed in order to produce 1 kg of dry kraft lignin and its byproducts like tall oil, pulp and turpentine (see. Table 9).

Table 9: inventory of Dry Kraft Lignin for the integrated and the base case scenario of the Culbertson (2016) approach

Inventory 1 kg Dry Kraft Lignin SBSK (base case)		
Inputs		
materials	**units**	**value**
technosphere		
CO2, liquid	g	200.00
sulfuric acid	g	685.40
sodium hydroxide	g	858.50
hydrogen peroxide	g	373.40
lime	g	223.30
methanol	g	29.60
sodium chlorite	g	388.60
sulfur dioxide	g	53.40
oxygen, liquid	g	693.40
magnesium sulfate	g	61.40
bark	kg	2.00
wood	kg	54.17
transport	tkm	5.06
biosphere		
water	m3	0.58
water, natural	m3	0.64
CO2, non-fossile	kg	68.59
SO2	g	46.00
outputs		
waste		
solid waste	kg	1.31
products		
turpentine	g	53.40
tall oil	kg	1.07
wood pulp	kg	24.12
medium voltage	kWh	23.60
Dry Kraft Lignin	kg	1.00

Inventory 1 kg Dry Kraft Lignin SBSK (integrated)		
Inputs		
materials	**units**	**value**
technosphere		
CO2, liquid	g	200.00
sulfuric acid	g	685.40
sodium hydroxide	g	858.50
hydrogen peroxide	g	373.40
lime	g	223.30
methanol	g	29.60
sodium chlorite	g	388.60
sulfur dioxide	g	53.40
oxygen, liquid	g	693.40
magnesium sulfate	g	61.40
bark	kg	2.00
wood	kg	54.17
transport	tkm	5.06
biosphere		
water	m3	0.58
water, natural	m3	0.64
CO2, non-fossile	kg	68.59
SO2	g	46.00
outputs		
waste		
solid waste	kg	1.31
products		
turpentine	g	53.40
tall oil	kg	1.07
wood pulp	kg	24.12
medium voltage	kWh	26.72
Dry Kraft Lignin	kg	1.00

3.4 Brightway2 and Activity Browser

The LCA program brightway2 (bw2) which is based on the programming language python was used because implementation of external data was easier and the calculation speed was much faster than its competitors like openLCA. For this Julia Weyand created a code which ultimately takes the Aspen Plus data and processes those data via TEPET. Activity Browser (AB) is a GUI based on bw2 which allows to create or edit flows and maps the LCA or the data calculated from the impact categories. These can be displayed numerically, graphically or as a Sankey diagram.

3.5 Techno-Economic Process Evaluation Tool (TEPET)

TEPET is an Excel based program developed by DLR to evaluate and calculate in detail techno-economic and ecological problems. TEPET takes data from the process simulation of Aspen Plus and lets the user connect the energy and mass flows to appropriate LCA processes and biosphere flows to form a life cycle inventory (LCI) (see. Figure 13). The LCI gets exported into bw2 when the LCA is conducted for a selected number of impact categories. The background information i.e., the ecoinvent database are then combined with the process information so that the streams form links and are included in the calculation for environmental impacts.

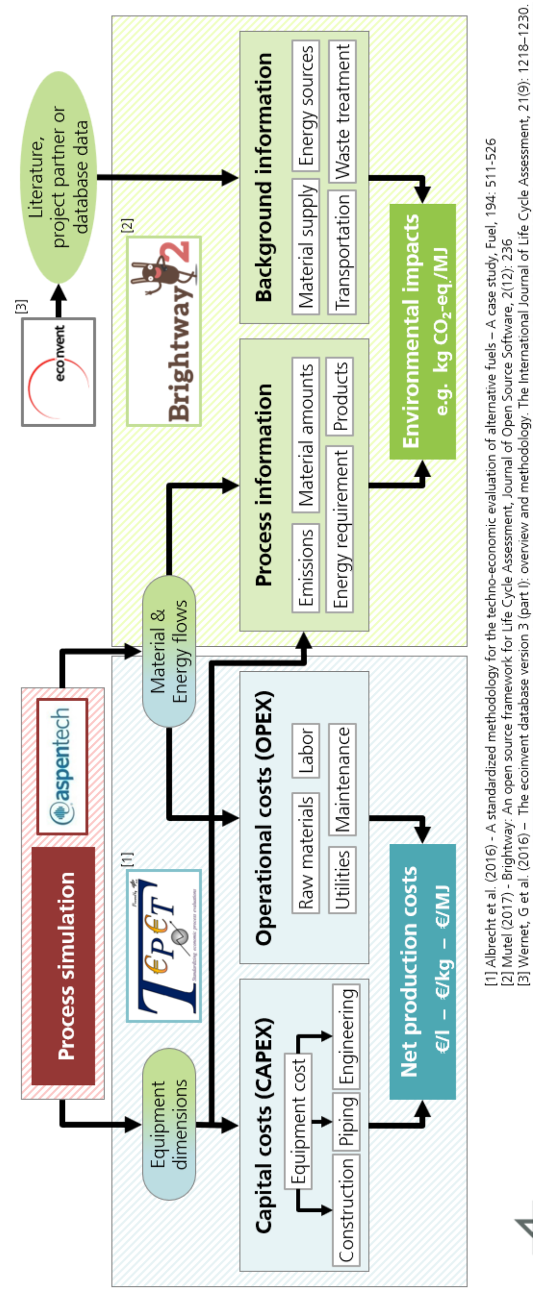


Figure 13: schematic flowsheet of TEPET (internal communication with DLR)

3.6 Goal and scope

The goal of this LCA is to summarize and analyze all relevant environmental impacts. These can be traced back to the necessary work steps for the production of the ABC-Salt product in Europe. All energy and material flows are to be determined at the LCA in order to make the environmental impacts assessable and to compare it with a fossil fuel reference. That’s why a cradle-to-gate approach was used.

3.7 System boundaries

For an LCA it is an important part to define the system boundaries. For this part of an LCA in Europe the DIN EN ISO 14040,2006-11 standards exist.

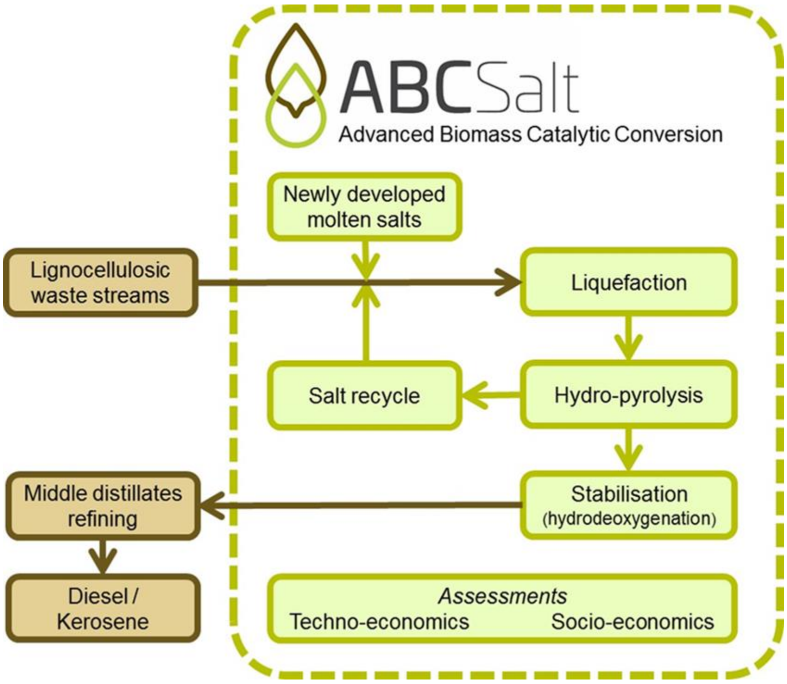


Figure 14: System boundaries of ABC-Salt

Therefore, in Figure 14 the important processes are shown. The system boundaries are set as a cradle-to-gate approach. Therefore, the used resources as well as the desired products and by-products are considered. The dried lignocellulosic waste stream of a pulp mill goes into the ABC-Salt plant, where they are mixed with molten salts ($ZnCL2$; $NaCl$; KCl) and comes to the liquefaction section. After the liquefication the intermediate products are going into the hydropyrolysis reactor, where additional hydrogen is added. The char and gas products are going back to the pulp mill for heat production. This is done to provide the pulp mill and the

ABC-Salt plant with the needed energy. The oil is then stabilized with HDO. In the end the middle distillates are refined and Diesel as well as Kerosene is produced.

3.8 Impact categories

For impact categories (IC) the calculation method of Environmental footprint v3.0 (EF v3.0) – ILCD 2.0 2018 was used. It was decided to use this impact categories because for the ReCiPe 2016 method its characterization factors (CF) were not verified before implementation in bw2. Furthermore, CML was implemented later and was therefore not considered. EF v3.0 was the newest of ILCDs methods with updated CF. However, it was also decided to use the EF v3.0 methods as those are recommended by the European Commission and this is an LCA for Europe. Furthermore, normalization factors are available for this as the results are normalized in the end.

The impact categories decided for are described below. With this approach, the relevant environmental impacts of the ABC-Salt process can be analyzed and evaluated. The summary and analysis of all product relevant processes can be traced back to the manufacturing process of ABC-Salt in Sweden. Therefore, there is no need to adjust the objectives or the scope of the study. All uncertainties of the characterization factors and methodologies are widely documented and discussed in extensive stakeholder debates. These discussions are not repeated here.

3.8.1 Climate change

The only method with a wide consensus for global warming potential (GWP) characterization at midpoint level are the ones of IPCC's. EF v3.0 selected this method as representative for all midpoint methods currently used in LCA (ILCD, 2011). Furthermore, at midpoint level, GWP's from the Intergovernmental Panel on Climate Change is recommended. According to ILCD (2011) those GWP's are the most up-to-date ones and scientifically robust. This method produces characterization factors based on radiative forcing and time which the greenhouse gases (GHG) are present in the atmosphere. The emissions lead to an increased atmospheric concentration of greenhouse gases (ppb). In doing so, the radiative forcing capacity (w/m2) is increased and ultimately this leads to an increase in the global average temperature (°C). The GWP expresses the possible increase in infrared radiation that occurs over time (100 years at midpoint level) as a result of the emission of 1 kg of GHG. Those GHG are presented in the

LCA as kg CO_2-equivalents (ILCD, 2011). This refers to the environmental impact of releasing 1 kg of CO_2 over the same period (Huijbregts et al., 2016).

3.8.2 Ozone depletion

This impact category is an indicator of emissions to air that cause the destruction of the stratospheric ozone layer. The unit of ozone depletion is kg CFC-11-equivalents (ILCD, 2011). According to ILCD report (2011) all LCIA methodologies do use ozone depletion potentials (ODP) developed by WMO and have an impact category “Ozone Layer Depletion”. EF v3.0 uses the WMO characterization model as it has high scores in nearly all criteria and sub criteria. Furthermore, the factors are widely discussed and therefore accepted as the preferred choice as a default method for the calculation of midpoint characterization factors (ILCD, 2011).

3.8.3 Particulate matter

As ILCD report is recommending RiskPoll and (Greco et al., 2007). EF v3.0 is using a combination of both as a basis for calculating intake fractions (ILCD, 2011). Both are simplified models for example RiskPoll is a model that has been set up with several projects to reflect all the factors that have an influence on intake and subsequent damages. Furthermore, the calculated effects are based on epidemiologic studies. This impact category is measured in “disease incidence”.

3.8.4 Photochemical ozone formation

ILCD (2011) describes that LOTOS-EUROS model, same as used in the ReCiPe method, is recommended for photochemical ozone formation. It calculates the area- and time of integrated ozone concentration increase, in perspective of Europe without giving priority to inhabited regions, before applying these as CF at midpoint level. Furthermore, ILCD also mentions that the model should be improved for some of the Factors like NMVOC, CH4, CO and NOx. During this study factors for CO and CH4 are still missing.

3.8.5 Ionizing radiation

The EF v3.0 is using the method developed by Frischknecht et al., 2000 for mid- and endpoint perspective. According to the report of ILCD the ionizing radiation is affecting the human health related to releases of radioactive materials into the environment. The approach of (Frischknecht et al., 2000) is described as the only method usable for a quantitative approach, as it meets some general requirements for. Furthermore, the fate and exposure model is based on the ExternE work by (Dreicer et al., 1995). He described the routine of French nuclear fuel cycles, including 14 atmospheric and liquid discharges. Furthermore, for 3 additional radionuclides Data from (UNSCEAR, 2000) was used. The impact category is depicting its impacts as kBq U235-equivalents.

3.8.6 Acidification

For the impact categories of EF v3.0 the midpoint methods of AE (Accumulated Exceedence) (Jyri Seppälä et al., 2006) was used by ILCD (2011). Furthermore, ILCD described that AE is to be recommended as default method for midpoint evaluation of acidification. Therefore, the most up-to-date factors are used. However, the method is accepted both from stakeholder as well as it meets the science-based criteria, as AE based calculations are currently used for policy purposes and by the UNECE Convention on "Long-range Transboundary Air Pollution (LRTAP)". For the Acidification category of EF v3.0 atmospheric and soil fate factors which are looked at different emission scenarios and separated between non-sensitive and sensitive areas. Its impacts are shown as mol H+ equivalents.

3.8.7 Eutrophication, terrestrial

For this impact category is also the AE (Accumulated Exceedence) preferred by the ILCD as recommended model for midpoint evaluation. As previously mentioned, the method meets all the science-based expectations, as well as a good acceptance of the stakeholders. It is depicted as mol N equivalents.

3.8.8 Eutrophication, marine

According to the ILCD (2011) recommendation, most of the impact categories which look at aquatic eutrophication do have "*weak*" characterization models, ignoring some of potent removal processes for N and P. ILCD (2011) recommends using the CARMEN model. ReCiPe and EDIP2003 are both using this method. However, ReCiPe uses a more up-to-date model than EDIP2003. ReCiPe eventually adopts a more consistent framework with focus on the nutrient concentration increasing aquatic compartments to the limiting nutrient. Therefore, the ReCiPe approach is recommended as default method at midpoint level. For eutrophication of freshwater and marine the midpoint method of Struijs (ReCiPe 2016) is recommended (ILCD, 2011). It splits the emissions in P-emissions which are consider in freshwater eutrophication and for marine eutrophication only N is considered. The increase in dissolved inorganic nitrogen in seawater is the indicator for this impact category. This indicator is combined with the midpoint factor "marine eutrophication potential" (MEP) and expressed in kg N-equivalents. It presents the effects of eutrophication due to nitrogen and phosphorus emissions in water (Huijbregts et al., 2016). Environmental impacts associated with marine eutrophication due to nutrient enrichment indicate a plenty of ecosystem impacts, including “benthic anoxia”. This can lead to the onset of hypoxic water and, in excess, to anoxia and “dead zones”, which is one of the most serious and widespread causes of marine ecosystem disturbance (Huijbregts et al., 2016).

3.8.9 Eutrophication, freshwater

EF v3.0 is orientating on this method. Huijbregts (2016) describes his ReCiPe 2016 midpoint eutrophication of freshwater as following described. Freshwater eutrophication occurs due to the release of nutrients such as phosphorus or nitrogen into soil or freshwater bodies and the subsequent increase in nutrient levels. The environmental impacts resulting from freshwater eutrophication are numerous. According to Huijbregts (2016) they follow a series of ecological impacts that are accounted for by the increase in nutrient emissions to freshwater. This leads to increased nutrient uptake by autotrophic organisms i.e., cyanobacteria and algae, as well as heterotrophic species such as fish and invertebrates. This subsequently leads to a relative loss of species (Huijbregts et al., 2016). Freshwater eutrophication is calculated using the midpoint factor "freshwater eutrophication potential" (FEP) and expressed as kg P-eq. specified.

3.8.10 Ecotoxicity freshwater

For ecotoxicity of freshwater EF v3.0 uses the USEtox as default method for the midpoint evaluation. Its results reflect the common and agreed recommendations from a consortium of experts. As there is no available method recommended by the ILCD (2011) to address marine and terrestrial ecotoxicity, it is therefore not looked at. However, chemicals that doesn’t remain over time in freshwater and may have terrestrial or marine effects are not yet addressed by USEtox. Ecotoxicity freshwater is shown as CTUe (ILCD, 2011).

3.8.11 Water use

For water use the Swiss Ecoscarcity (water) method is preferred by ILCD (2011) for a midpoint evaluation. It takes into account the impact of water depletion. Actually, the environmental model of this method is a very rudimentary one, as it relates water use directly to local scarcity of water. This approach enables further differentiation where water extraction causes different levels of impact. Water use is therefore expressed as “m3 world equivalents” (ILCD, 2011).

3.8.12 Homan toxicity

The same model is used for human toxicity as for ecotoxicity. In the ILCD report the use of USEtox as multimedia model is recommended for combining chemical fate and exposure with toxicological data. Some characterization factors (e.g. for "metals", "dissociating substances" and "amphiphiles" - detergents) are classified as preliminary according to expert opinion, since the factors for these substance groups are considered to have higher uncertainty compared to others in current practice (ILCD, 2011).

3.8.13 Land use

In the Land use category EF v3.0 uses one indicator which describes soil quality developed by Milà i Canals et al. (2007). This method unfortunately does not register biodiversity impacts. However, this method is chosen as the most accurate of the existing approaches, although its scope is very limited in its extent (ILCD, 2011).

3.8.14 Resource depletion

As a midpoint indicator, exergy is considered the most mature method. With bio-based products, the exergy of the absorbed solar radiation is used. This impact path does not describe the degradation processes, but the consumption of exergy (ILCD, 2011). This does not depend on resource scarcity (i.e. the exergy value remains equal even if the last bit of a resource is used up). According to ILCD (2011) this method do not address the question if losses of exergy from solar energy are as important as the exergy losses in the Earth's mineral stock or not. All these exergy consumption types are simply added without weighting them (ILCD, 2011).

3.8.15 Resource use

In the CML method, the Abiotic Depletion Potential (ADP) is expressed in kg of antimony equivalents. Furthermore, it is multiplied with the amount of a given resource extracted. The CML method is used by EF v3.0 and recommended in the ILCD report as it captures scarcity by including both the extraction and the reserves of a certain resource. ILCD (2011) describes that CF are recorded for *“metals, fossil fuels and, in the case of reserve base and economic reserves, mineral compounds”*.

3.9 Allocation methods

For allocation methods economically and energetically were selected, as a mass allocation would not make any sense as there is electricity produced. All the allocation results are presented in Table 10.

Table 10: allocation methods used for base case and integrated scenarios.

a: 403€/t for base case and 247€/t for integrated. b:23,602 kWh for base case and 26,718 kWh for integrated

products	economic, base case	economic, integrated	energetic, base case	energetic, integrated
kraft Lignin[a]	2.34%	1.43%	5.56%	5.42%
electricity, medium voltage[b]	6.85%	7.75%	19.41%	21.42%
tall oil soap	0.55%	0.55%	2.86%	2.78%
wood pulp	89.66%	89.66%	71.63%	69.84%
turpentine	0.61%	0.61%	0.54%	0.53%

Furthermore, the results are calculated with data from 2014. Therefore, an average exchange rate of 0.753941 was implemented (reisebuch, 2021). This was done to be able to compare the results with those of Culbertson (2016). For the energetic allocation the LHV of all products are registered. For kraft lignin a LHV of 24.35 MJ/kg was found (Echresh et al., 2019). Additionally, 11.685 MJ/kg is considered for the tall oil soap (Tran and Vakkilainnen, 2007) and an conversion of 3.6 MJ for 1 kWh (convertlive, 2021). In addition to those, also the LHV for turpentine (44.5 MJ/kg) (O.Arpa et al., 2010) and wood pulp (13 MJ/kg) (López et al., 2012) was required. Those data are also expressed in Table 19 (see. appendix A). For the economic allocation the same data is used for tall oil soap (117$/t) and wood pulp (850$/t) as in Culbertson’s paper. Furthermore, the changing prices of the Kraft Lignin (for integrated: 247€/t and unintegrated: 403€/t), in dependence of the electricity amount sold, was provided by RISE. The same was for the price of electricity that can be sold in Sweden (0,05€/kWh). The last price that was determined was for turpentine with 1,960.25€/t (ECSA-chemicals, 2020).

4. Results

After implementing all required flows and data from RISE and RUG into bw2, the software was able to calculate the desired quantities regarding the impact categories. Therefore, the impact categories described earlier were looked at. Furthermore, in Table 11 and 12 the normalized results of the different scenarios are compared to each other and also to normalized fossil diesel (Sala et al., 2017). All results pictured in Tables 11 and 12 are globally normalized per person based on the Normalization Factors (NF) for EF by Sala et al. (2017). For calculation the results of the LCA were divided by the NF of Sala et al. (2017). For the Culbertson approach the results are also allocated economically and energetically based on the information depicted in Table 10.

Table 11: Normalized LCA results of the base case and the integrated scenario of the Bernier (2013) approach

EF v3.0 no LT Bernier 1 MJ fuel

impact category	**unit**	**fossil diesel**	**Base case (Bernier)**	**integrated (Bernier)**
Climate change	kg CO_2-eq.	5.51E-02	4.36E-02	3.21E-02
Ozone depletion	kg CFC-11-eq.	4.57E-03	4.23E-03	8.03E-03
Particulate matter	disease incidence	3.59E-02	3.44E-02	2.41E-02
Photochemical ozone formation	kg NMVOC-Eq	4.11E-02	3.30E-02	2.72E-02
Ionising radiations	kBq U235-Eq	6.87E-03	8.13E-02	5.00E-03
Acidification – freshwater and terrestrial	mol H+-Eq	3.05E-02	6.00E-02	5.35E-02
Eutrophication – terrestrial	mol N-Eq	3.44E-02	2.45E-02	1.85E-02
Eutrophication – marine	kg N-eq.	1.96E-02	1.25E-02	5.79E-03
Eutrophication – freshwater	kg P-eq	8.82E-04	7.05E-03	9.72E-03
Ecotoxicity freshwater	CTUe	7.03E-03	5.88E-01	1.82E+00
Water use	m3 world eq. deprived	7.91E-04	5.56E-02	2.06E-02
Human toxicity – cancer effect	CTUh	1.99E-02	1.61E-02	5.07E-03
Human toxicity – non-cancer effect	CTUh	2.18E-02	5.59E-02	2.32E-02
Land use	dimensionless	1.93E-04	6.73E-03	9.77E-04
Resource depletion – fossil	MJ, net calorific value	9.96E-02	2.85E-01	1.40E-01
Resource use – minerals and metals	kg Sb-Eq	5.40E-03	1.20E+01	1.19E+01

Table 12: Normalized LCA results of the base case and the integrated scenario of the Culbertson (2016) approach

EF v3.0 no LT Culbertson 1 MJ fuel normalized per person

impact category	**unit**	**fossil diesel**	**economic, base case**	**energetic, base case**
Climate change	kg CO_2-eq.	5.51E-02	5.46E-03	2.87E-02
Ozone depletion	kg CFC-11-eq.	4.57E-03	4.25E-04	2.24E-03
Particulate matter	disease incidence	3.59E-02	5.67E-03	2.98E-02
Photochemical ozone formation	kg NMVOC-Eq	4.11E-02	5.08E-03	2.67E-02
Ionising radiations	kBq U235-Eq	6.87E-03	8.71E-04	4.58E-03
Acidification – freshwater and terrestrial	mol H+-Eq	3.05E-02	1.08E-02	5.67E-02
Eutrophication – terrestrial	mol N-Eq	3.44E-02	2.91E-03	1.53E-02
Eutrophication – marine	kg N-eq.	1.96E-02	7.15E-03	3.76E-02
Eutrophication – freshwater	kg P-eq	8.82E-04	6.42E-03	3.38E-02
Ecotoxicity freshwater	CTUe	7.03E-03	9.08E-02	4.78E-01
Water use	m3 world eq. deprived	7.91E-04	3.20E-03	1.68E-02
Human toxicity – cancer effect	CTUh	1.99E-02	7.63E-04	4.01E-03
Human toxicity – non-cancer effect	CTUh	2.18E-02	1.48E-03	7.79E-03
Land use	dimensionless	1.93E-04	2.89E-02	1.52E-01
Resource depletion – fossil	MJ, net calorific value	9.96E-02	1.00E-02	5.28E-02
Resource use – minerals and metals	kg Sb-Eq	5.40E-03	1.37E-01	7.18E-01

EF v3.0 no LT Culbertson 1 MJ fuel normalized per person

impact category	**unit**	**fossil diesel**	**economic, integrated**	**energetic, integrated**
Climate change	kg CO_2-eq.	5.51E-02	5.46E-03	2.87E-02
Ozone depletion	kg CFC-11-eq.	4.57E-03	4.25E-04	2.24E-03
Particulate matter	disease incidence	3.59E-02	5.67E-03	2.98E-02
Photochemical ozone formation	kg NMVOC-Eq	4.11E-02	5.08E-03	2.67E-02
Ionising radiations	kBq U235-Eq	6.87E-03	8.71E-04	4.58E-03
Acidification – freshwater and terrestrial	mol H+-Eq	3.05E-02	1.08E-02	5.67E-02
Eutrophication – terrestrial	mol N-Eq	3.44E-02	2.91E-03	1.53E-02
Eutrophication – marine	kg N-eq.	1.96E-02	7.15E-03	3.76E-02
Eutrophication – freshwater	kg P-eq	8.82E-04	6.42E-03	3.38E-02
Ecotoxicity freshwater	CTUe	7.03E-03	9.08E-02	4.78E-01
Water use	m3 world eq. deprived	7.91E-04	3.20E-03	1.68E-02
Human toxicity – cancer effect	CTUh	1.99E-02	7.63E-04	4.01E-03
Human toxicity – non-cancer effect	CTUh	2.18E-02	1.48E-03	7.79E-03
Land use	dimensionless	1.93E-04	2.89E-02	1.52E-01
Resource depletion – fossil	MJ, net calorific value	9.96E-02	1.00E-02	5.28E-02
Resource use – minerals and metals	kg Sb-Eq	5.40E-03	1.37E-01	7.18E-01

For easier comparison the impact categories are presented as radar charts. In the Figures 15, 16 and 17 the emissions of the Bernier approach were presented. As previously mentioned, the global NF for EF per person of Sala et al. (2017) were used. Those are implemented in the appendix (see. Table 20). Not only are those scenarios compared to each other but also with a fossil fuel reference (RED II fossil fuel) and the guideline of 65% of GHG reduction (RED II 65% limit) (described later). In the end it is important to say, that because of the “65% RED II” limit a special focus is therefore on the greenhouse gases and the climate change impact category.

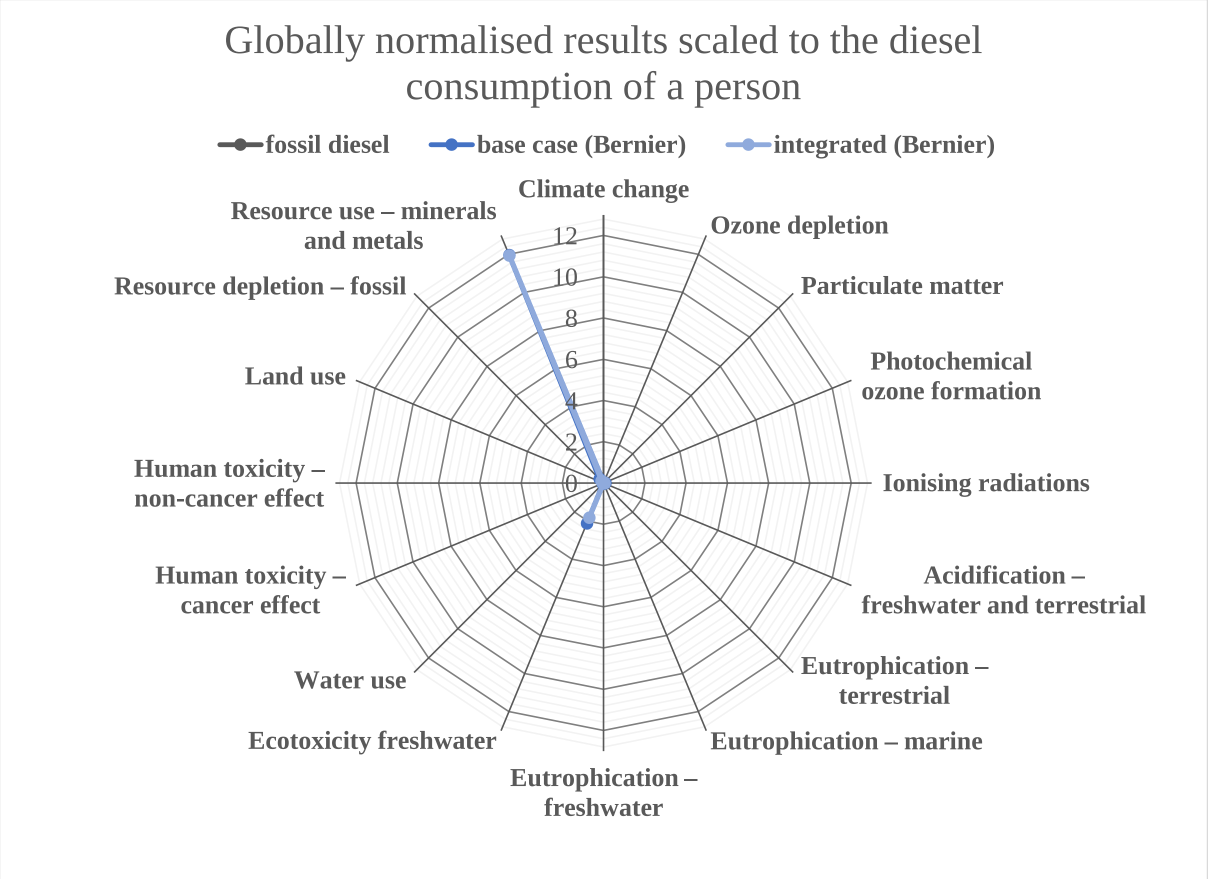


Figure 15: Normalized results for all impact categories of Bernier approach

Compared to fossil diesel there are some categories were the ABC-Salt fuel surpass the diesel by far. First, these impact categories where therefore looked at. Resource use – minerals and metals and ecotoxicity freshwater have very big impacts because of the salts and the energy mix of Sweden used in this study. Commonly as mentioned the energy mix of Sweden uses nearly 50% of nuclear power. Therefore, the winning of uranium has big impacts on Resource use. Additionally, the Salts potassium chloride and zinc chloride have also major impacts on the category of freshwater ecotoxicity.

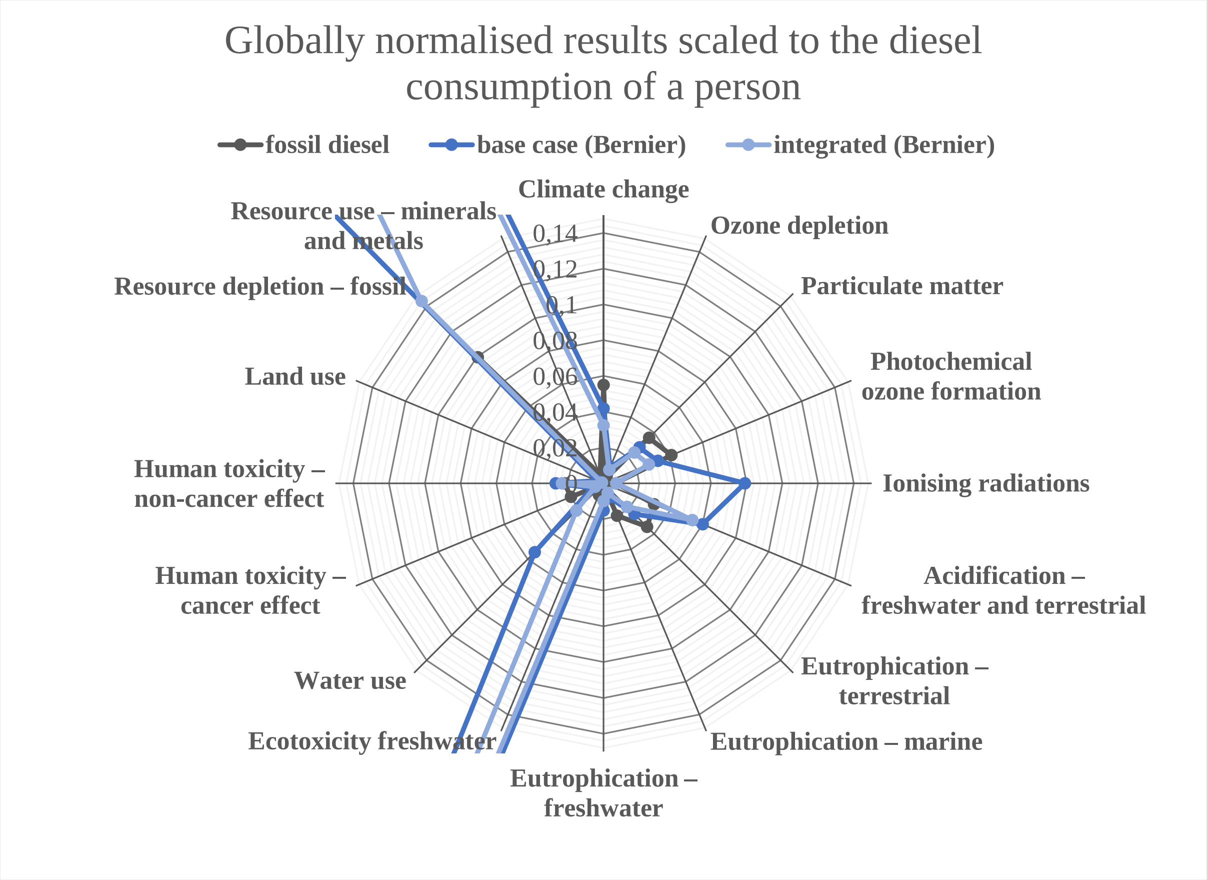


Figure 16: Normalized results for all impact categories of Bernier approach (zoomed in)

Furthermore, zoomed in, in the same radar chart it is possible to see that the different scenarios are quite similar. However, the base case has some bigger deviations for water use and ionizing radiations. Unlike for the first two impact categories (resource use and ecotoxicity) the hydrogen production is impacting the most for integrated and the selling of electricity is credited about 22% because no uranium mining is needed. For the unintegrated scenario the uranium mining is impacting this category the most. Furthermore, both ABC-Salt scenarios have a higher impact on acidification than its fossil counterpart. But on the other hand, in comparison to the ABC-Salt scenarios fossil diesel is worse in climate change, eutrophication, human toxicity with cancer effects and the impact category particulate matter (see. Figure 17 or also Table 11).

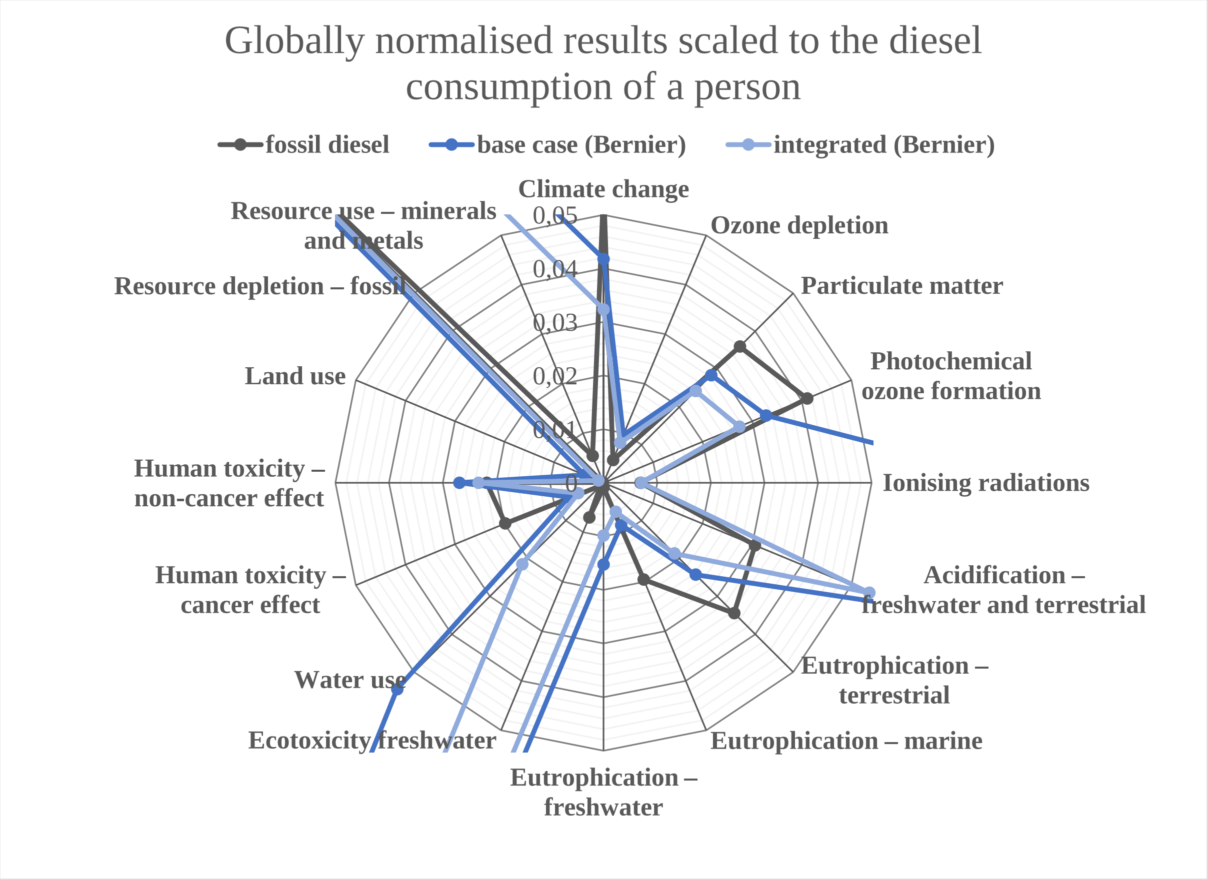


Figure 17: Normalized results for all impact categories of Bernier approach (zoomed in further)

If further zoom is applied the similarities of the scenarios become clearer. In the end it is possible to say that the fossil diesel has bigger impacts on climate change, particulate matter, photochemical ozone formation, eutrophication both terrestrial and marine and as mentioned human toxicity with cancer effects. On the other hand, the base case is significantly worse in ionizing radiations and acidification, in addition to ecotoxicity and resource use (see. Figure 17).

As the results of the base case and integrated scenario of the Culbertson approach are nearly the same (see. Figure 25), it was decided to show only the base case as radar chart. As same as for Figures 15, 16 and 17 the emissions were also normalized globally per person. Also, the same normalization factors (NF) were used (Sala et al., 2017).

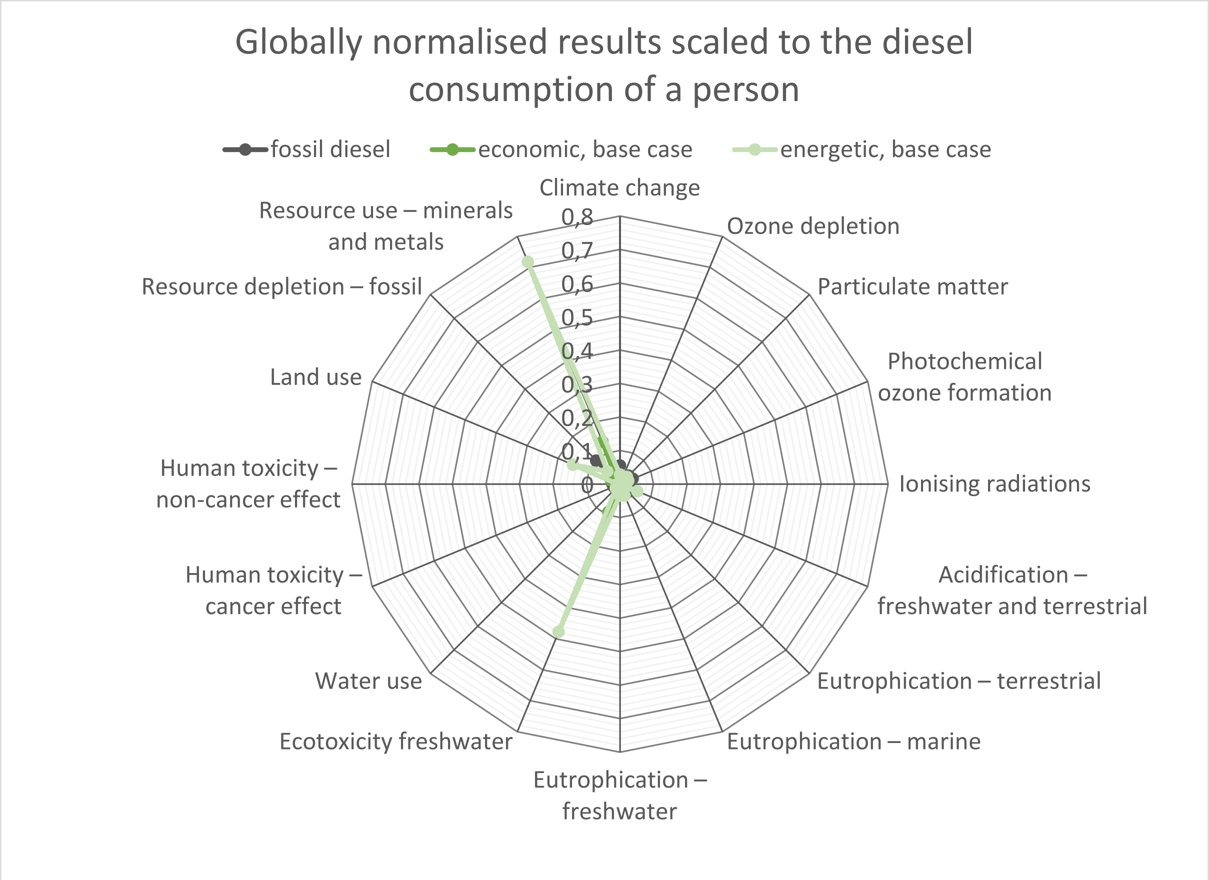


Figure 18: Normalized results for all impact categories of Culbertson approach

As similar to the Bernier approach, the impact categories like Resource use – minerals and metals, ecotoxicity freshwater surpass the fossil diesel by far. Additionally, land use was also looked at in more detail as the Culbertson approach takes the cultivation of softwood as it is the main driver of this impact category into account. As previously mentioned, the energy mix of Sweden uses some amount of nuclear power. Therefore, the winning of uranium has big impacts on Resource use. Additionally, the salts potassium chloride and zinc chloride have same as for the Bernier approach the biggest impacts on the category of freshwater ecotoxicity.

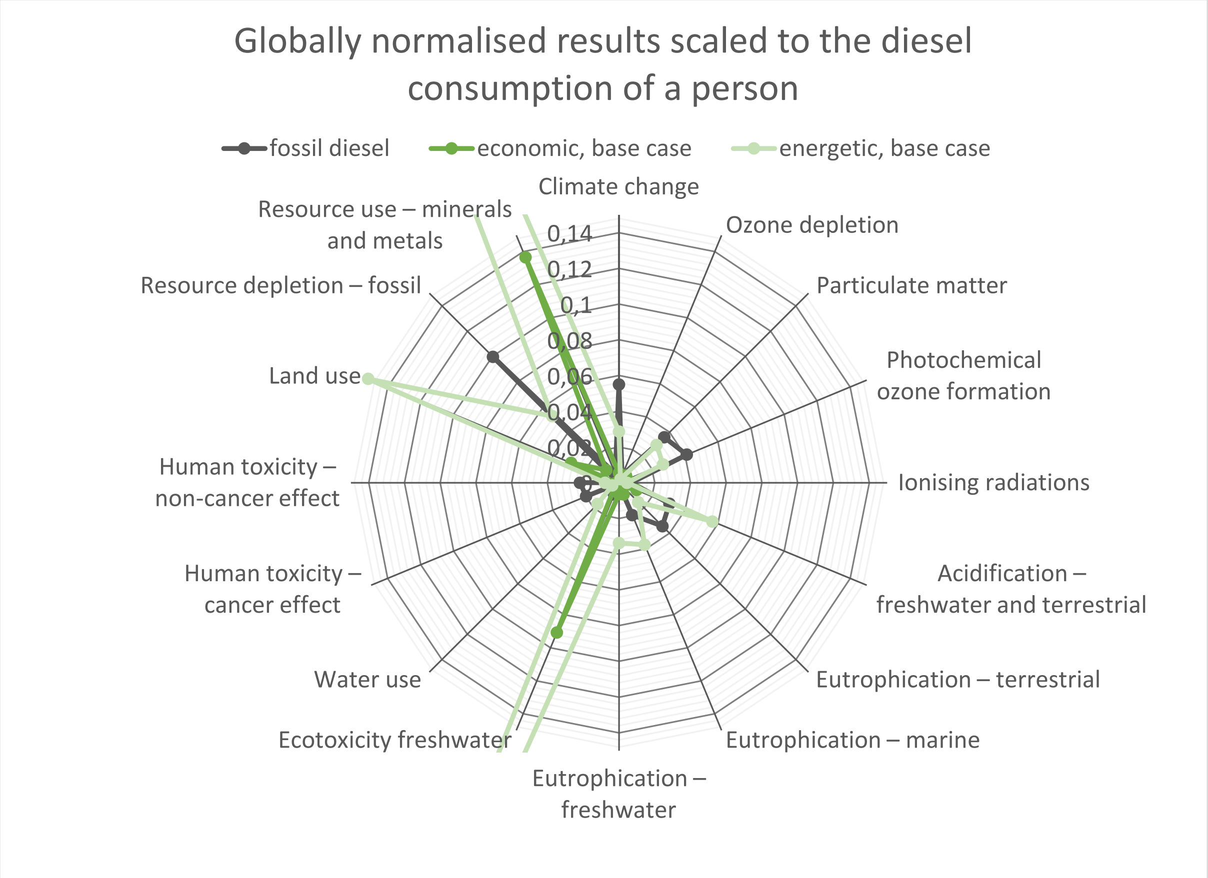


Figure 19: Normalized results for all impact categories of Culbertson approach (zoomed in)

In Figure 19 it is possible to see that both allocations can have high differences. This is because of the number of environmental burdens allocated. That is why the economic allocation of the base case has a significant less impact on the categories of land use, resource use and ecotoxicity as the energetic one in comparison, but still more of an impact as the fossil diesel (see. Figure 19). Again, this is because of the uranium mining, the growing of softwood and the salt used during the ABC-Salt process. Furthermore, it must be acknowledged that both allocation methods also can outcompete the fossil diesel in quit a lot of impact categories such as climate change, particulate matter, photochemical ozone formation, terrestrial eutrophication, both of the human toxicity categories and resource depletion. This can be observed also in the next Figure (Figure 20), where it was further zoomed in.

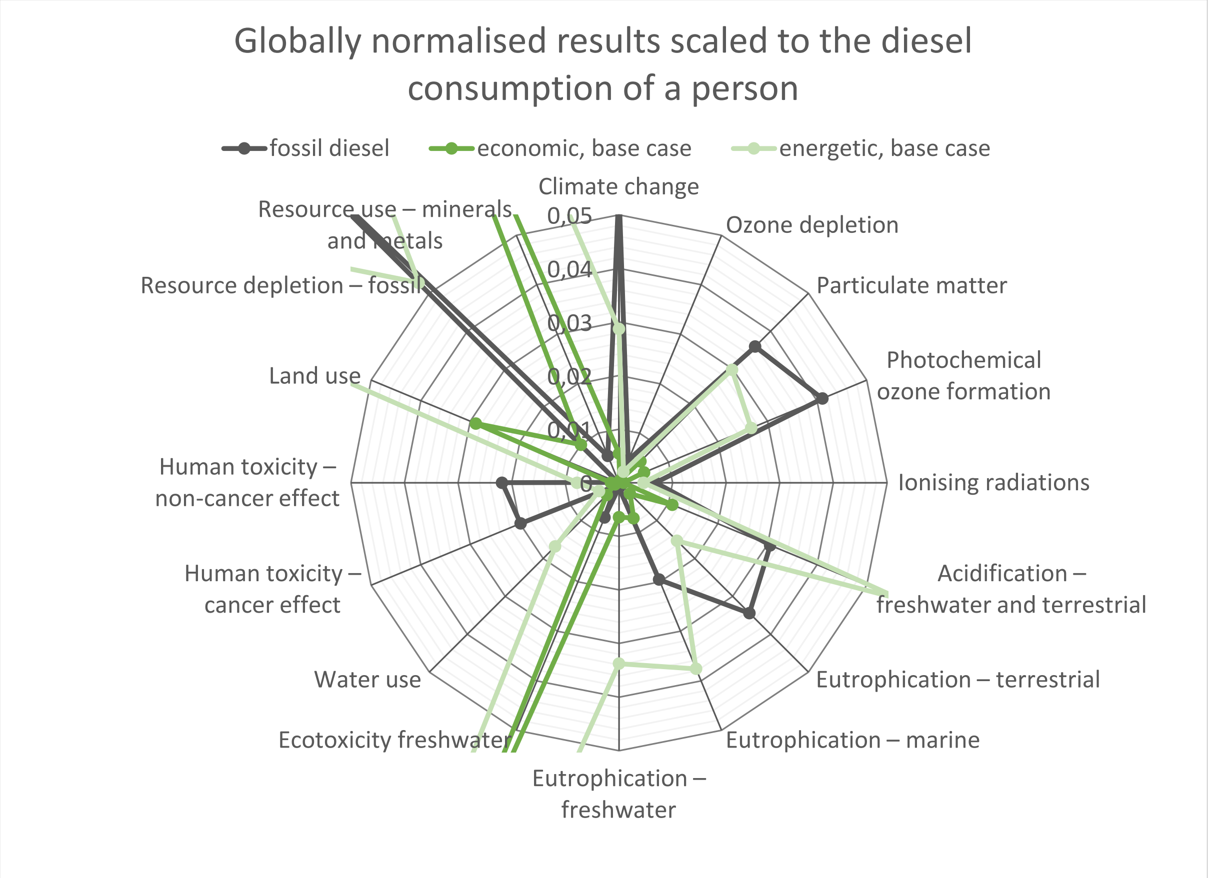


Figure 20: Normalized results for all impact categories of Culbertson approach (zoomed in further)

In this radar chart it is possible to observe the high differences of the different allocation methods. For acidification for example the energetic approach is worse compared to fossil diesel. On the other hand, the economic allocation has less impact than both, fossil diesel and the energetic allocation for this impact category. To sum-up the economic allocation of the Culbertson approach has less impacts on following impact categories as fossil diesel: climate change, ozone depletion, particulate matter, photochemical ozone formation, ionizing radiations, acidification, eutrophication marine and terrestrial, both human tox., resource depletion. But the economic allocation of the base case is worse for eutrophication freshwater, resource use, land use and ecotoxicity. Furthermore, the energetic allocation method has less environmental burdens for climate change, ozone depletion, particulate matter photochemical ozone formation, ionizing radiations, terrestrial eutrophication, both of the human toxicity categories as well as resource depletion. In the end the energetic scenario is worse for acidification, marine and freshwater eutrophication, water, land and resource use.

In general, in Figure 20, it is possible to see that both the economic and the energetic allocation follow the same pattern, only the number of emissions which are assigned to differs. In this study the economic allocation has less emissions compared to the energetic method. This is because sales account over 89% for the wood pulp. The kraft lignin gets 2.34% of the emissions produced by the pulp mill (ABC-Salt) for economic allocation and 5.56% of emissions for the energetic method.

4.1 Bernier approach

For the impact category of climate change the base case is compared to the fossil fuel reference for a functional unit (FU) of 1 MJ fuel. For this amount of fuel, the ABC-Salt fuel is emitting less CO_2-eq. into the environment than common petrol fuels. With 65.53 g of CO_2-eq.per MJ product it is a reduction compared with its fossil counterpart of 30.29%. The second biggest part of GHG emissions are emitted by the hydropyrolysis process (16.4%) because of the necessary hydrogen production. Additionally, the liquefaction is emitting about 8.06 g CO_2-eq. or 12.3% mostly because of the zinc chloride production. The HDO only produces 4.8 g of GHG also because of the hydrogen used. In the end the biggest part of the GHG emissions is from Biomass supply with 41.94 g of CO_2-eq. per MJ product. That is why it was pictured in more detail in Figure 21.

Base Case – Kraft Lignin without ABC-Salt integration (RER) – SE electricity mix

total: 65.53 g CO2-eq. (Biomass: 41.94 g CO2-eq.)

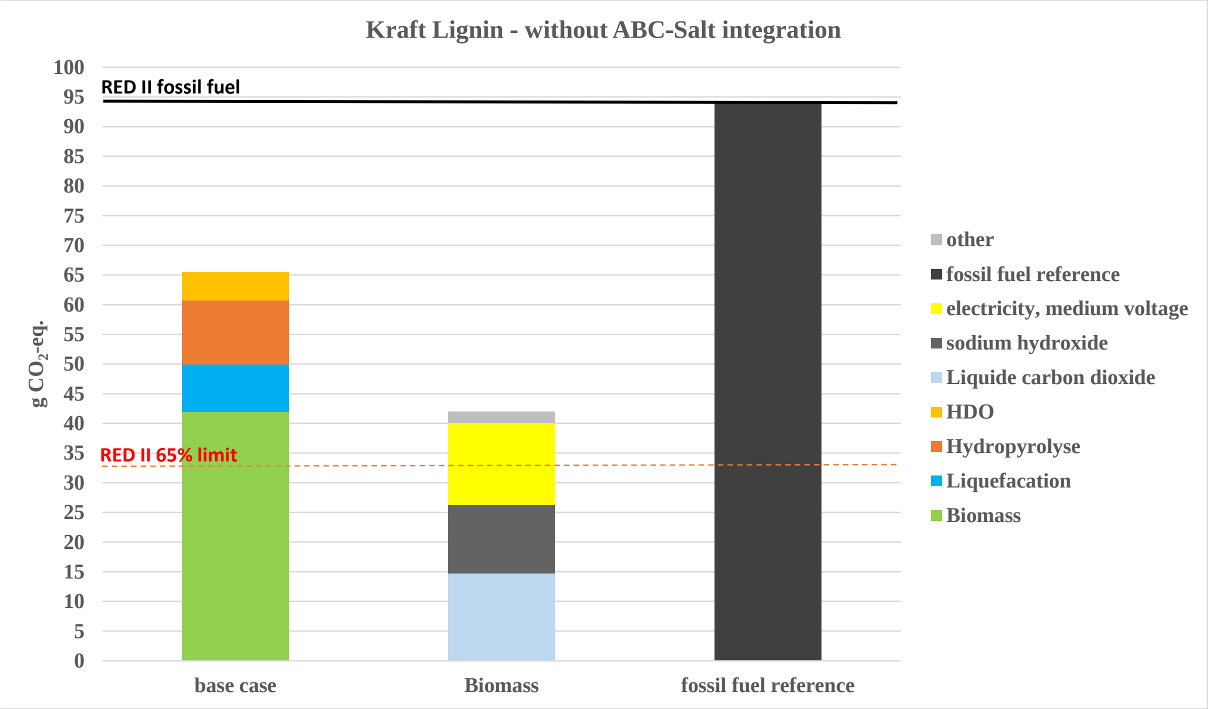


Figure 21: ABC-Salt base case results in comparison with the fossil fuel reference and the biomass supply showed in detail

The Kraft Lignin as biggest contributor of GHG is because of the amount of electricity as well as liquid carbon dioxide used for producing it. The electricity used are about 32.9% or 13.8 g CO_2-eq. and the liquid CO_2 count about 35% or 14.68 g CO_2-eq. per MJ product. Furthermore, the sodium hydroxide is emitting about 27.6%. This equals the amount of approx. 11.57 g of greenhouse gases. The produced electricity by char and gas in the integrated scenario is fully allocated to the Lignin.

Second Case – Kraft Lignin integrated ABC-Salt process (RER)

total: 50.77 g CO_2-eq. (Biomass: 27.16 g CO_2-eq.)

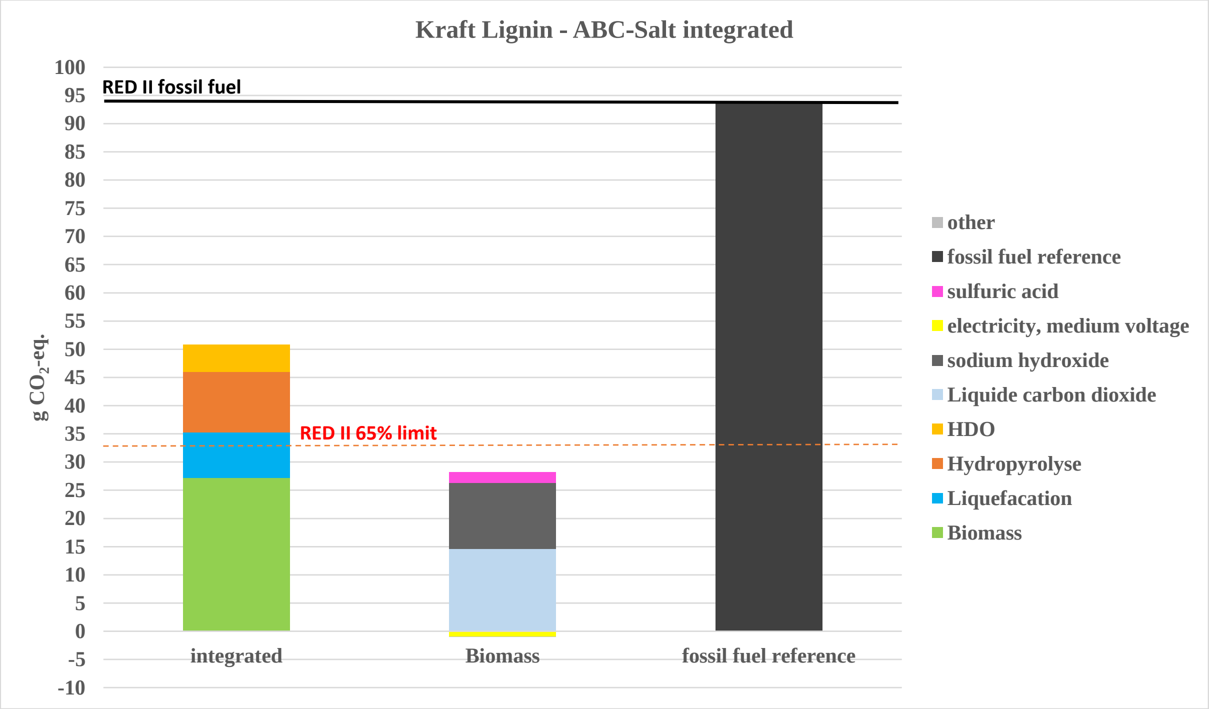


Figure 22: integrated ABC-Salt results in comparison with the fossil fuel reference and the biomass supply showed in detail

Additionally, the integrated scenario of Bernier approach was also compared to the fossil fuel reference. Overall emissions of the integrated ABC-Salt fuel are 50.77 g of CO_2-eq. per MJ fuel. Compared to the GHG emissions of the base case a further reduction of emissions is noticed. As the main difference of both scenarios is the electricity flow as a small amount of it is sold (0.19 kWh) for the integrated scenario. Therefore, 3.43% of the GHG are compensated by the amount of electricity produced. This equals a reduction of 0.93 g of CO_2-eq. per MJ fuel. Still the RED II 65% limit was not achieved.

ABC-Salt comparison of Bernier (2013) and RISE

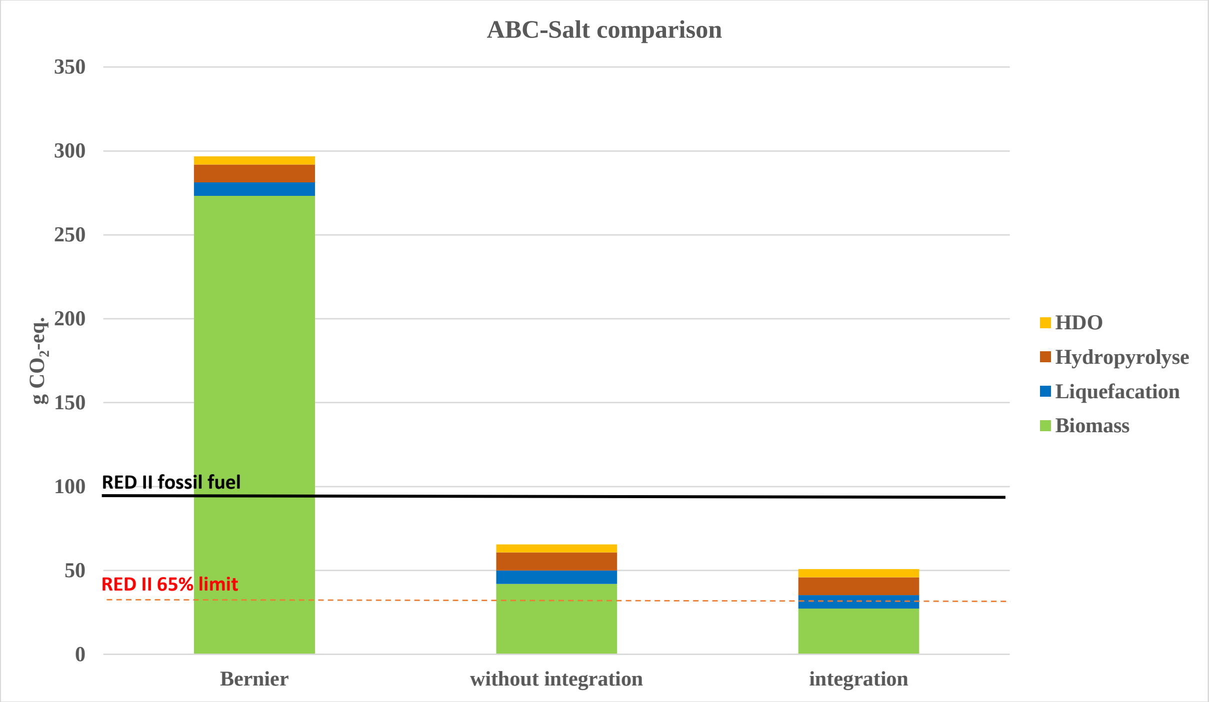


Figure 23: Comparison of Bernier's LCA and the scenarios of this study, based on Bernier's paper

In the end the results from the data of RISE are compared to the original approach of Bernier (2013). Furthermore, a high reduction of GHG emission is observed for both cases of this study compared to Bernier (see. Figure 23). The total emissions of Bernier are about 296.65 g CO_2-eq. per MJ fuel and nearly 6 times higher than those of the integrated scenario. This is mainly because Bernier uses heat from natural gas for his kraft lignin production (see. Figure 24) as the biomass supply is the main driver of this impact category.

Furthermore, he uses also more liquid carbon dioxide. The heat from natural gas emitting approx. 220.21 g of CO_2-eq. per MJ of fuel and 24.45 g of GHG are emitted by the liquid carbon dioxide. Additionally, 15.33 g or 5.61% of the environmental burdens are from transportation. In comparison to the RED II lines the case with data from Bernier is even worse than the fossil fuel reference.

Comparison Biomass of Bernier (2013) and RISE

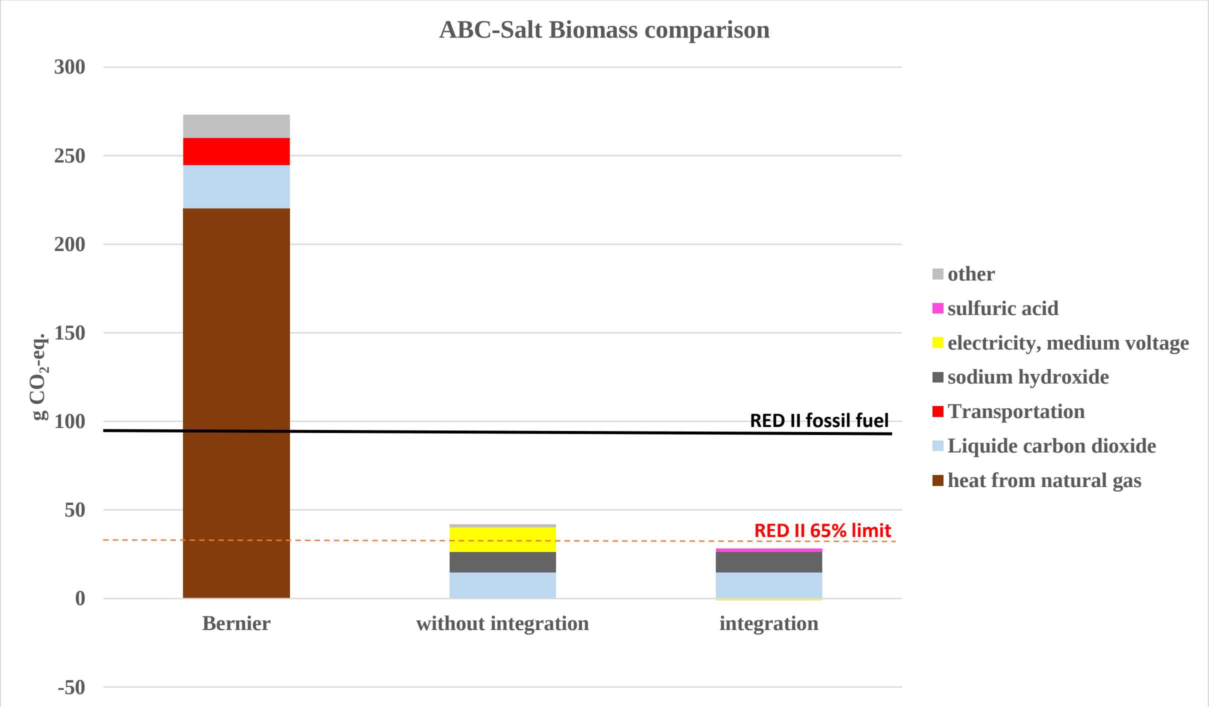


Figure 24: Comparison of the biomass supply and where the emissions are coming from, based on Bernier's paper

4.2 Culbertson approach

The second approach was the one described by Culbertson (2016). Therefore, the second base case was compared to Culbertson's data and the integrated scenario in Figure 25. As mentioned earlier, there was similar data in the end for integrated and the base case that was neglectable for this study (see. Table 13 and Figure 26). It was therefore decided only to present the results of the base case for the Culbertson approach. The different allocation methods are expressed in Figure 27 as the biomass was allocated as mentioned in Table 10. The data of Culbertson was recalculated with the ecoinvent 3.6 database, greenhouse gases of his economically allocated approach reached 893.41 g CO_2-eq. per MJ of product. The ABC-Salt approach was very similar as 809.77 g of total CO_2-eq. are calculated for both of the scenarios (without allocation).

ABC-Salt comparison of Culbertson (2016) and RISE

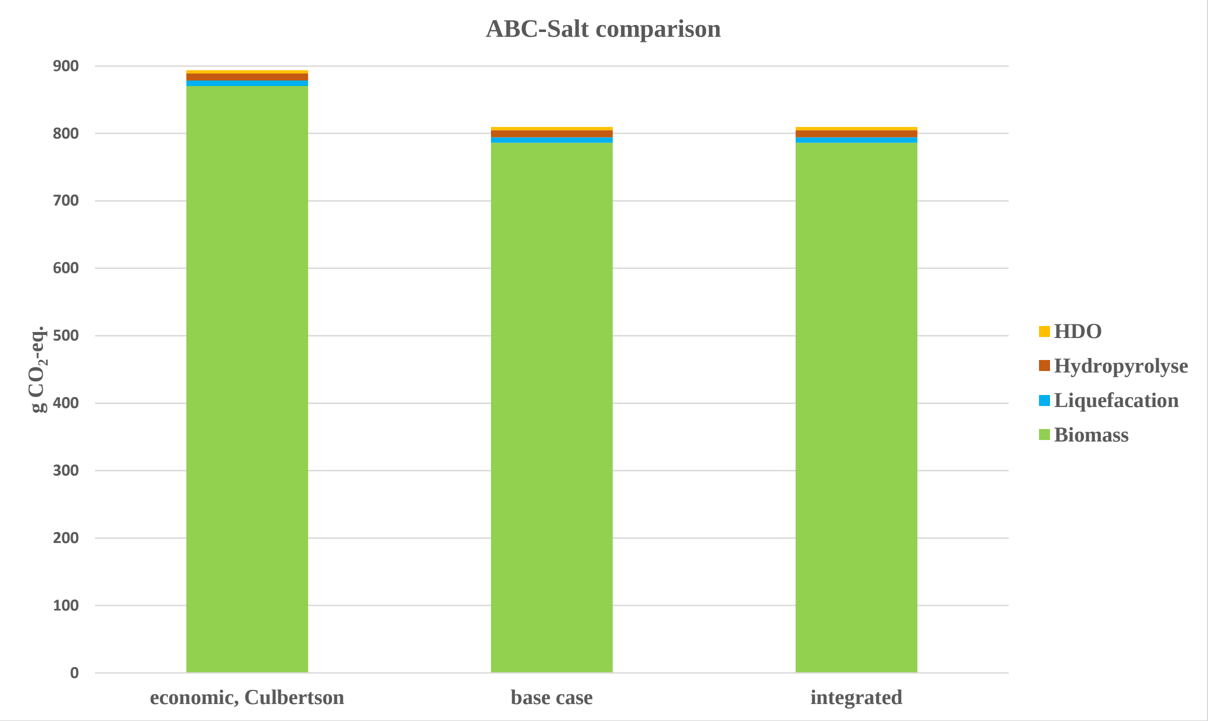


Figure 25: Comparison of Culbertson's LCA and the scenarios of this study, based on his paper

But as allocation was used in this study the different scenarios and its allocated emissions were looked in detail as pictured in Figure 26. In this Figure it is possible to see that both scenarios are very similar to each other. Because the integrated case was very similar to the base case in the energetic allocations, therefore only the base case was looked at more in detail in the following Figures. Furthermore, the economic allocation of the integrated scenario had a little bit less GHG allocated to the kraft lignin than the base case (see. Table 13).

Table 13: GHG emission in g/MJ allocated for each ABC-Salt scenario compared to data based on Culbertson.

	economic, Culbertson	economic, base case	energetic, base case	economic, integrated	energetic, integrated	fossil fuel reference
Biomass	870.41	786.29	786.29	786.29	786.20	0
Liquefacation	8.03	8.03	8.03	8.03	8.03	0
Hydropyrolyse	10.69	10.69	10.69	10.69	10.69	0
HDO	4.79	4.79	4.79	4.79	4.79	0
Products						
Kraft Lignin	175.95	18.38	43.74	11.27	42.64	0
electricity, medium voltage	0	53.82	152.62	60.92	168.43	0
oil soap	84.03	4.30	22.46	4.30	21.89	0
SBSK wood pulp	610.44	705.00	563.21	704.93	549.08	0
Turpentine	0	4.77	4.27	4.77	4.16	0
other	0	0	0	0	0	0
fossil fuel reference	0	0	0	0	0	94

In order to compare the input of the kraft lignin also the other products had to been locked at shown in Table 13. As the amount of electricity produced is getting higher for the integrated scenario, also the price of the kraft lignin was going down (internal communication with RISE).

Therefore, the kraft lignin got about 7.11 g CO_2-eq. less emissions allocated to the economic allocation (integrated) and 1.1 g CO_2-eq. for the energetic one. But in general, less GHG for both allocation methods compared to the base case. Furthermore, the electricity is getting more GHG emissions allocated to. Approximately +15.81 g of CO_2-eq. for the energetic method and +7.10 g CO_2-eq. per MJ fuel for the economic allocation. Pulp, turpentine, and oil soap stay more or less the same for both economic allocations.

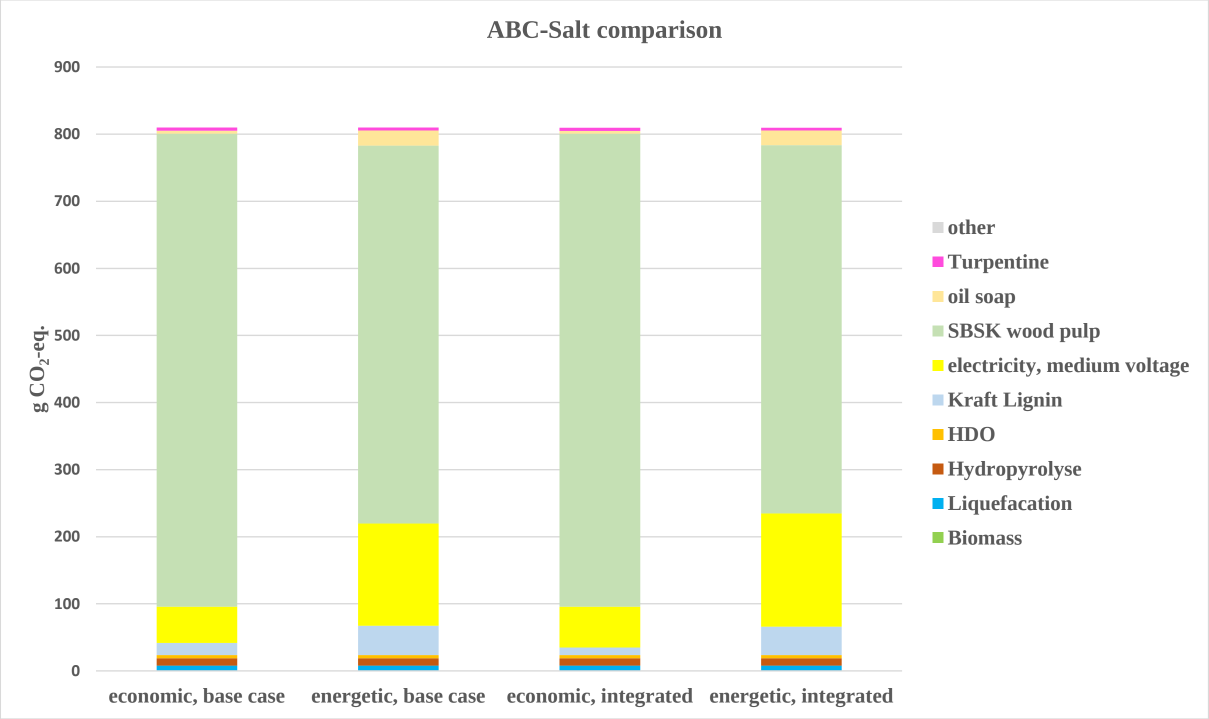


Figure 26: Comparison of the scenarios and their allocations of this study based on Culbertson approach

The graphs are too similar to compare as previously mentioned. The only small notable differences are between the economic and the energetic scenarios, as there the amount of GHG is a little bit more allocated to electricity. This is why the data of the integrated scenario and its allocations are only provided in the Table 12 and are not discussed. Furthermore, see in Table 19 how the allocations are calculated.

Base Case – Kraft Lignin extraction of SBSK, without ABC-Salt integration

Culbertson total: 893.93 (biomass: 870.41 gCO2-eq)

ABC-Salt total: 809.77 g CO_2-eq. (biomass: 786.29 g CO_2-eq.)

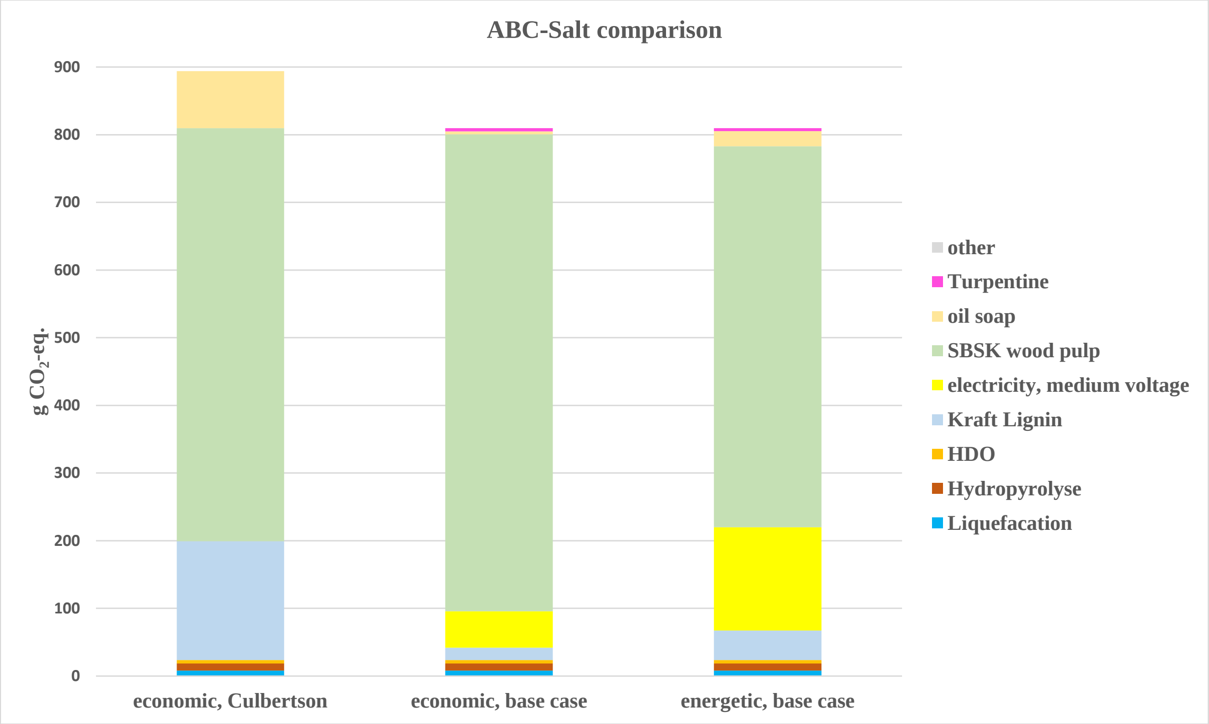


Figure 27: Comparison of the biomass supply and where the emissions are coming from, based on Culbertson's paper

If the allocations are compared the Culbertson scenario based on the data of the paper had higher GHG emission allocated to the kraft lignin and to the oil soap than both the economic and the energetic scenario of the base case scenario based on the Culbertson approach with the data from RISE. Furthermore, Culbertson does not produce any electricity and therefore none was sold. That is why no electricity is found in his allocation. Notable is also that the wood pulp is for all cases and scenarios the product with the highest GHG allocated to it.

allocations:

economic: total 41.90 g CO_2-eq. (Biomass: 18.38 g CO_2-eq.)

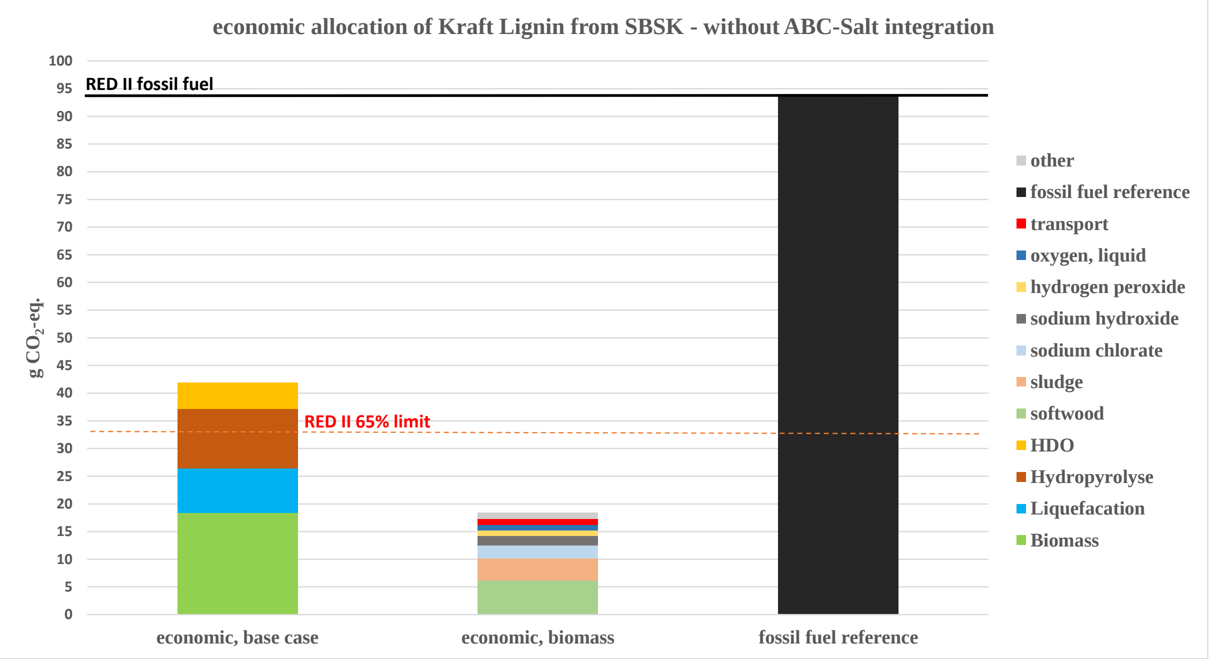


Figure 28: Economic allocation of kraft lignin from SBSK – base case compared to a fossil fuel reference

In general, Figure 28 shows that with the economic allocation the ABC-Salt fuel is near the RED II 65% limit of the EU, but still about 9 g CO_2-eq. above this limit. The biomass is split into softwood with the highest amount of GHG allocated to (about 6.41 g CO_2-eq.) on second place the treatment of sludge with a part of 21.9 percent. Additionally, 2.39 g of GHG are coming from the use of sodium chlorate. All the other flows like sodium hydroxide, hydrogen peroxide, liquid oxygen transport and the cut-off (2.5%) combined are emitting about 5.83 g of CO_2-equivalents. This is respectively of about 31% of the GHG emitted by the biomass supply.

energetic: total 67.25 g CO_2-eq. (Biomass: 43.74 g CO_2-eq.)

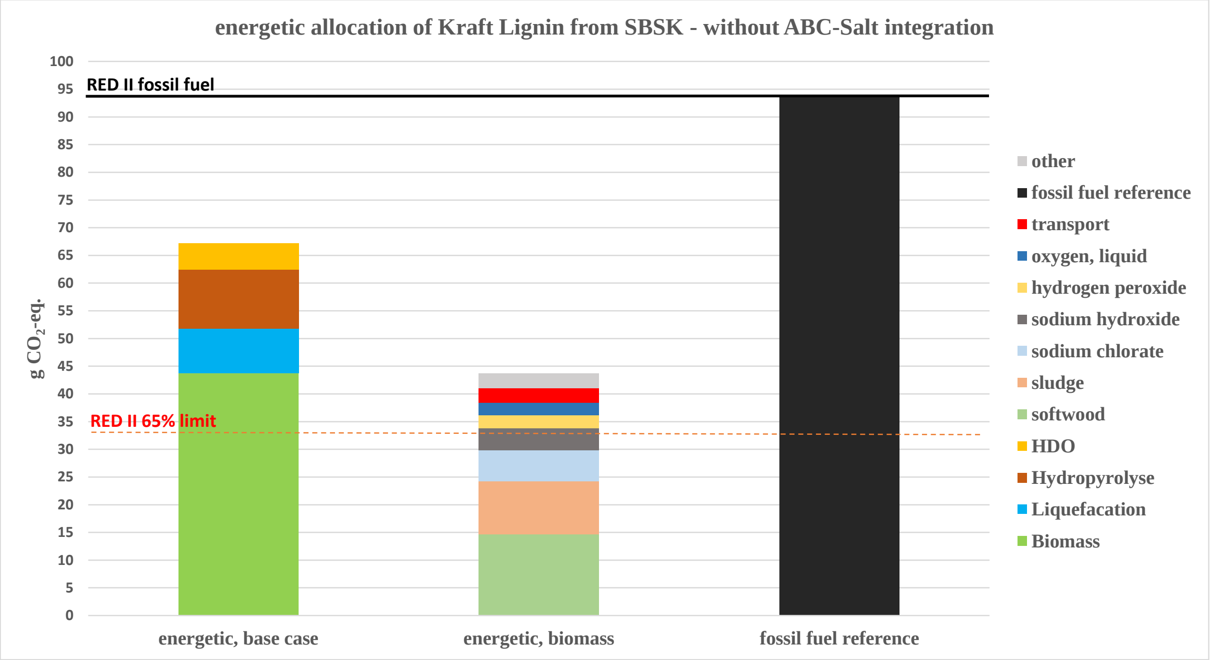


Figure 29: Energetic allocation of kraft lignin from SBSK – base case compared to a fossil fuel reference

The data of the energetic allocation are further looked in detail since the biomass supply is based on the kraft lignin the amount of input flows is shown accordingly in Figure 29. In this figure the energetic allocation of the ABC-Salt fuel is depicted. In contrast to the economic allocation already the biomass of the energetic method is over the RED II 65% limit. The softwood counts 14.61 g of CO_2-equivalents. Furthermore, following flows are presented in Figure 29: Sludge 9.58 g; sodium chlorate 5.69 g; sodium hydroxide 3.95; hydrogen peroxide 2.37 g; liquid oxygen 2.29 g; and transport about 2.54 g CO_2-eq. per MJ fuel. Furthermore, because of the 2.5% cut-off, 2.71 g CO_2-eq. per MJ fuel are from other unspecified flows.

ABC-Salt comparison of fossil fuel reference and RISE

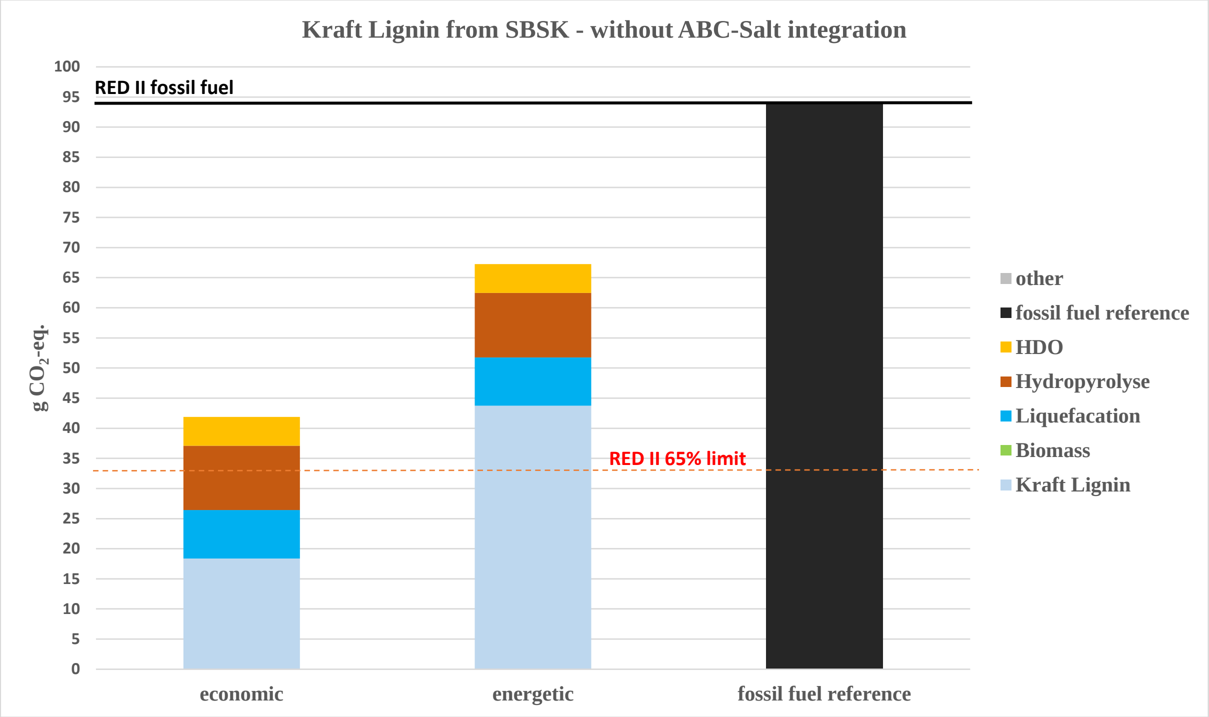


Figure 30: Comparision of the allocated GHG emission of the base case scenario with a fossil fuel reference

In the end the in Figure 30 allocated scenarios of the ABC-Salt fuel (base case) are compared to the fossil fuel reference. Both have, as mentioned in Table 12, less impact on the climate change than the fossil fuel, but both cannot reach the RED II 65% limit. Therefore, the impact of a higher oil yield was also considered. For this scenario the integrated case of the Bernier approach was used because this one represents roughly the middle of all scenarios and thus reflects a good average.

Table 14: yields in % based on data from internal communication with RUG. a: based on internal communicated formula provided by Sridharan (2021).

Source	Liquid Yield	Char Yield	Gas Yield	Organic Yield	Water Yield
Sridharan (RUG)	42.7	46.9	10.4	25.8	16.9
Solver (EA)[a]	38.3	40.6	21.1	30.0	8.3
Solver (EA)[a]	61.1	24.4	14.5	48.3	12.8
Solver (EA)[a]	70.9	19.5	9.6	64.6	6.3
Solver (EA)[a]	87.8	5.0	7.1	86.8	1.0

In the end of this study, as mentioned, the Bernier approach was adapted to different organic yields in order to have a look how and when a GHG reduction of 65% is achieved. The percentages in Table 14 were implemented in the excel sheet of the Aspen Plus simulation to get all the necessary data. Therefore, following table of char and gas yields was calculated (see. Table 15).

Table 15: char and gas yields based on the change of the oil yield

oil yield	char	gas	unit
25%	1.5328	0.7170	t/h
30%	1.2953	0.7953	t/h
48%	0.6847	0.5465	t/h
65%	0.5000	0.3619	t/h

As there was data missing from the project partners regarding the efficiency of the turbines used for electricity production, therefore for calculation the rule of three was applied. Furthermore, additional data was provided by RISE: Gas = 4.68 MW for 0.717 t and Char = 4.32 MW for 1.53 t

The results of this calculation are presented in Table 16.

Table 16: power produced by char and gas in MWh per t of lignin

oil yield	char	gas	unit
25%	1.2238	1.3258	MWh/t
30%	1.0361	0.6362	MWh/t
48%	0.5477	0.4372	MWh/t
65%	0.3999	0.2894	MWh/t

The calculated power values where than adjusted for 1 MJ of fuel and implemented into the LCA. Therefore, following GHG emission occur (see. Figure 31). With a higher oil yield, significant reductions in GHG emissions can be observed despite the fact that less char and less gas go back to the pulp mill (see Figure 31). The LCA with the Bernier approach is already below the RED II limit from around 48% of an oil yield, which is why this can be seen as a magical barrier up to which the oil yield must increase without adapting the basic framework conditions.

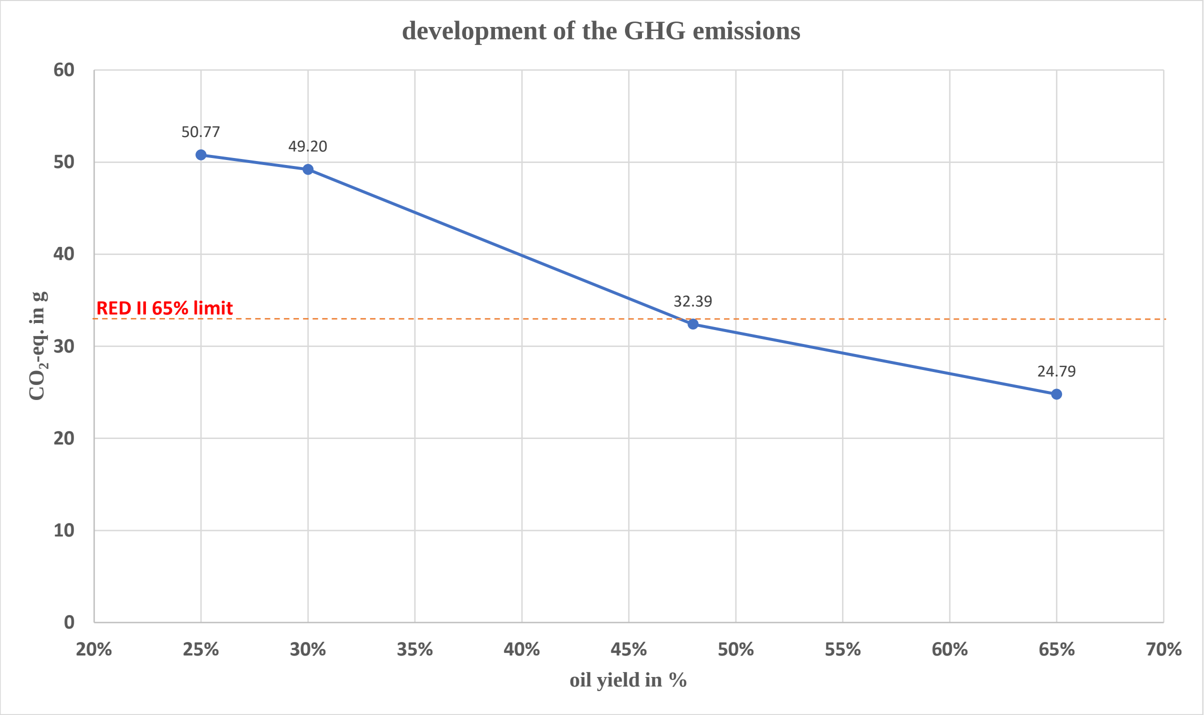


Figure 31: development of the GHG emissions with increasing oil yield

First of all, it must be mentioned that the product of the ABC-Salt process is still no fully usable fuel and therefore still needed to be classified by the project partners. The data used in this study is a mixture of experimental data, literature data and assumptions and calculations. Furthermore, there is currently no coherent real process or pilot plant, so the values here should also be viewed with caution because scale-up effects are very difficult to take into account. So far there is little data on molten salts to compare it with other literature. So, this study had to trust the data of the project partners and errors of their formulas or calculations cannot be ruled out. The liquefaction, hydropyrolysis and HDO are based on the values and data shared by project partners. Furthermore, there were sufficient literature sources on kraft lignin from pulp mills to be able to implement allocation methods using the data from the project partners. Furthermore, it is recommended to read the papers of Bernier (2013) and Culbertson (2016) on whose paper this study is based, or the scenarios are depicted. The calculations are done with the help of TEPET, which are based on the calculations of aspen plus. Those calculations should also be viewed with caution. Since a connected pilot plant was simulated using aspen, an attempt was made to model it on the basis of primary data. Due to a lack of primary information from the project partners regarding the composition of the "fuel", some assumptions were made here on the basis of secondary literature (see tables 5 & 6).

Compared to the LCA of Hsu (2012), 39 g of greenhouse gases emitted, the ABC-Salt fuel is still higher than all of the pyrolysis fuels. This could by because of the feedstock Hsu (2012) used for his LCA as it contributes only a small amount of GHG. Furthermore, compared to synfuels using Fischer Tropsch synthesis (20g per MJ), is even further below the results of ABC-Salt. However, a direct comparison with the two similar processes is quite difficult to regard as perfect, since, for example, the influence of the FTS synfuel was created by Simapro and an older ecoinvent database (2.2). Apart from that, however, the following conclusions can be drawn based on the calculations in bw2.

The calculated GHG emissions are going down a bit for the ABC-Salt product but at the expense of other impact categories. This is partly due to the salts and the Swedish electricity mix, which each have a high impact on, for example, ecotoxicity or resource use. This is mainly due to the mining of uranium and the unintentional release of zinc chloride and potassium chlorite into the environment also during resource winning. It is noticeable that in the Bernier approach the category land use was hardly taken into account respectively the cultivation of the softwood was neglected. Therefore, hardly any influence on this category was recorded here, which does not correspond to the expectations beforehand this study. At Culbertson approach, however, this addition was considered. For human tox. – cancer effects it can be argued that both approaches (Culbertson and Bernier) have lesser effects on human health. Roughly speaking, the results of the impact category climate change do not fall below 65% in most scenarios, but a good reduction in greenhouse gases can still be observed. For climate change an average reduction of 42,13% can be observed. Therefore, it was checked how much oil yield is necessary to get below 65% threshold. With a higher yield, the emissions per MJ of fuel are reduced and the 65% mark is cracked from an oil yield of 48%. This roughly corresponds to the average of all scenarios.

Conclusion and outlook

On basis of this study, it can be concluded that with a better oil yield, there will probably also be a better reduction of greenhouse gases and thus compliance with the RED II limit of 65%. With a reduction in GHG emissions through ABC-Salt product, this could succeed if the 65% limit is observed. For the ABC-Salt product the biggest impact was the kraft lignin supply. With a better way of production or rather a more efficient way of kraft lignin production could do the trick. However, a GHG reduction of about 65% seems achievable, since the previous LCA calculations show a lower number of CO_2-equivalents than with the fossil fuel reference and therefore indicates that in future with higher oil yields a reduction of 65% can be achieved. In order to fight climate change and stay below the 2°C mark, some trade-offs must be considered, such as increasing land use, ecotoxicity and acidification. Furthermore, the high use of nuclear power in Sweden also increases the resource use of mineral and metals.

Considering the actual situation, it looks as if e-cars will prevail on the market, but due to the limited availability of resources needed there is no realistic possibility of replacing all fossil fuel cars by electric ones. Biofuels or synfuels i.e., by FTS or pyrolysis must therefore be researched further and produced in a climate-neutral manner. In the future, the ABC-Salt product should be classified and analyzed in detail, by the project partners. Furthermore, an attempt must be made to increase the oil yield in order to reduce further GHG emissions. In addition, an improved Aspen Plus simulation would be recommended as a basis for the LCA in the future. A coherent pilot plant would also be helpful to rule out any scale-up effects and to test the properties of the resulting product. Furthermore, a refining of the product may have to be considered if it does not achieve transport fuel quality.

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Appendix A

Table 17: Inventory of 1kg of dry kraft lignin (data based on Bernier, 2013)

Inventory 1 kg dry kraft lignin (Bernier)		
inputs		
materials	**units**	**value**
technosphere		
CO2, liquid	g	300.00
sulfuric acid	g	230.00
sodium hydroxide	g	107.00
lime	g	0.23
tap water	g	4850.00
heat, natural gas	MJ	31.50
medium voltage	kWh	0.01
transport	tkm	0.934
outputs		
products		
dry kraft lignin	kg	1.00

Table 18: Inventory of 1kg of dry kraft lignin (data based on Culbertson, 2016)

Inventory 1 kg dry kraft lignin SBSK (Culbertson)		
inputs		
materials	**units**	**value**
technosphere		
CO2, liquid	g	284.50
sulfuric acid	g	303.70
sodium hydroxide	g	259.30
hydrogen peroxide	g	126.70
lime	g	427.40
methanol	g	38.86
sodium chlorite	g	388.60
wood	kg	23.99
transport	tkm	3.08
power	kWh	11.52
heat natural gas	MJ	22.16
biosphere		
water, resource	m3	1.81
CO2, fossile	kg	2.78
CO2, non-fossile	kg	37.87
SO2	g	27.35
water	m3	1.77
outputs		
waste		
sludge	kg	1.12
products		
tall oil	g	257.50
wood pulp	kg	9.04
power	kWh	11.50
dry kraft lignin	kg	1.00

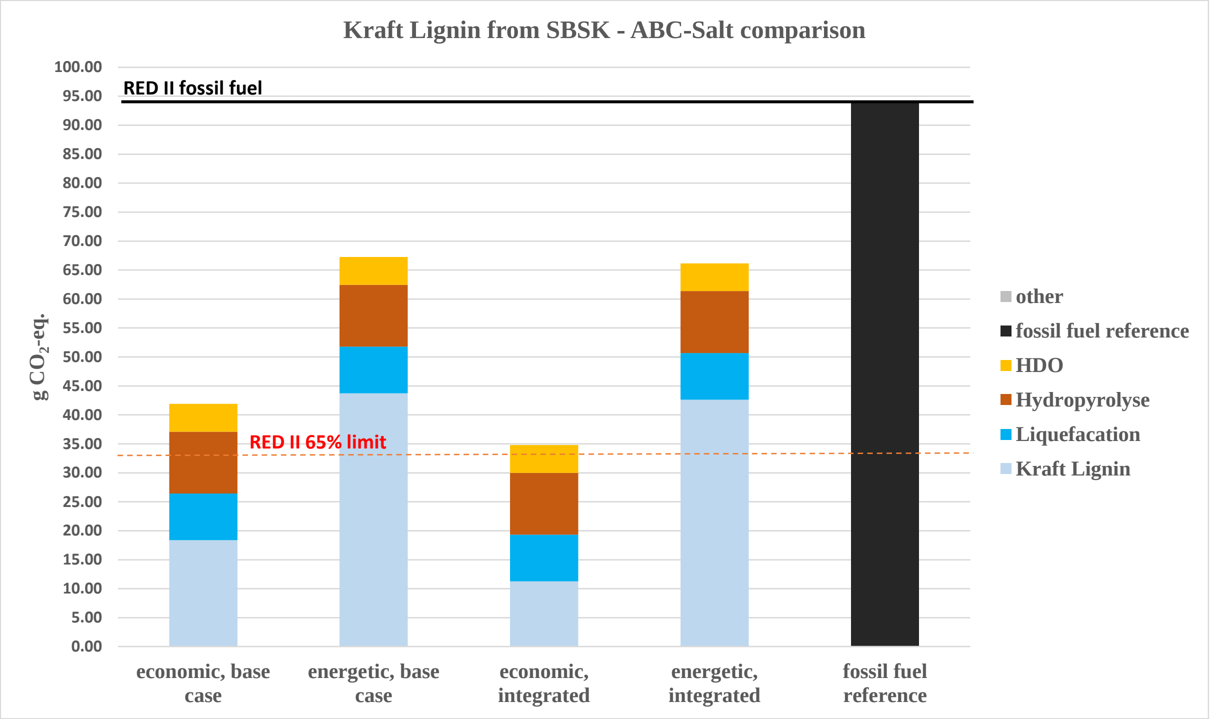


Figure 32: Comparison of all allocated scenarios of the Culbertson approach with a fossil fuel reference

Table 19: Data for allocation of the Culbertson approach

Process from Culbertson (2016)

kraft lignin extraction; from southern bleached softwood kraft, elemental chlorine free (ECF) bleached process; at mill; base case

products	amount	unit	price $/t	price €/t	lower heating value (LHV)	unit	value €	value MJ	economic	energetic
kraft Lignin	1.00	t	534.52	403.00	24.35	MJ/kg	403.00	24,350.00	2.34%	5.56%
electricity, medium voltage	23602	kWh	0.066	0.05	3.6	MJ	1,180.10	84,967.20	6.85%	19.41%
tall oil soap, kraft unrefined, at mill	1.07	t	117.00	88.21	11.685	MJ/kg	94.39	12,502.95	0.55%	2.86%
wood pulp; southern bleached softwood kraft (ECF), bleached	24.12	t	850.00	640.85	13	MJ/kg	15,457.30	313,560.00	89.66%	71.63%
turpentine	0.0534	t	2600.00	1960.25	44.5	MJ/kg	104.68	2,376.30	0.61%	0.54%
total			4101.59	3092.36	97.14	MJ/kg	17,239.46	437,756.45	100.00%	100.00%

Process from Culbertson (2016)

kraft lignin extraction; from southern bleached softwood kraft, elemental chlorine free (ECF) bleached process; at mill; integrated

products	amount	unit	price $/t	price €/t	lower heating value (LHV)	unit	value €	value MJ	economic	energetic
kraft Lignin	1.00	t	327.61	247.00	24.35	MJ/kg	247.00	24,350.00	1.43%	5.42%
electricity, medium voltage	26718	kWh	0.066	0.05	3.6	MJ	1,335.90	96,184.80	7.75%	21.42%
tall oil soap, kraft unrefined, at mill	1.07	t	117.00	88.21	11.685	MJ/kg	94.39	12,502.95	0.55%	2.78%
wood pulp; southern bleached softwood kraft (ECF), bleached	24.12	t	850.00	640.85	13	MJ/kg	15,457.30	313,560.00	89.66%	69.84%
turpentine	0.0534	t	2600.00	1960.25	44.5	MJ/kg	104.68	2,376.30	0.61%	0.53%
total			3894.68	2936.36	97.14	MJ/kg	17,239.26	448,974.05	100.00%	100.00%

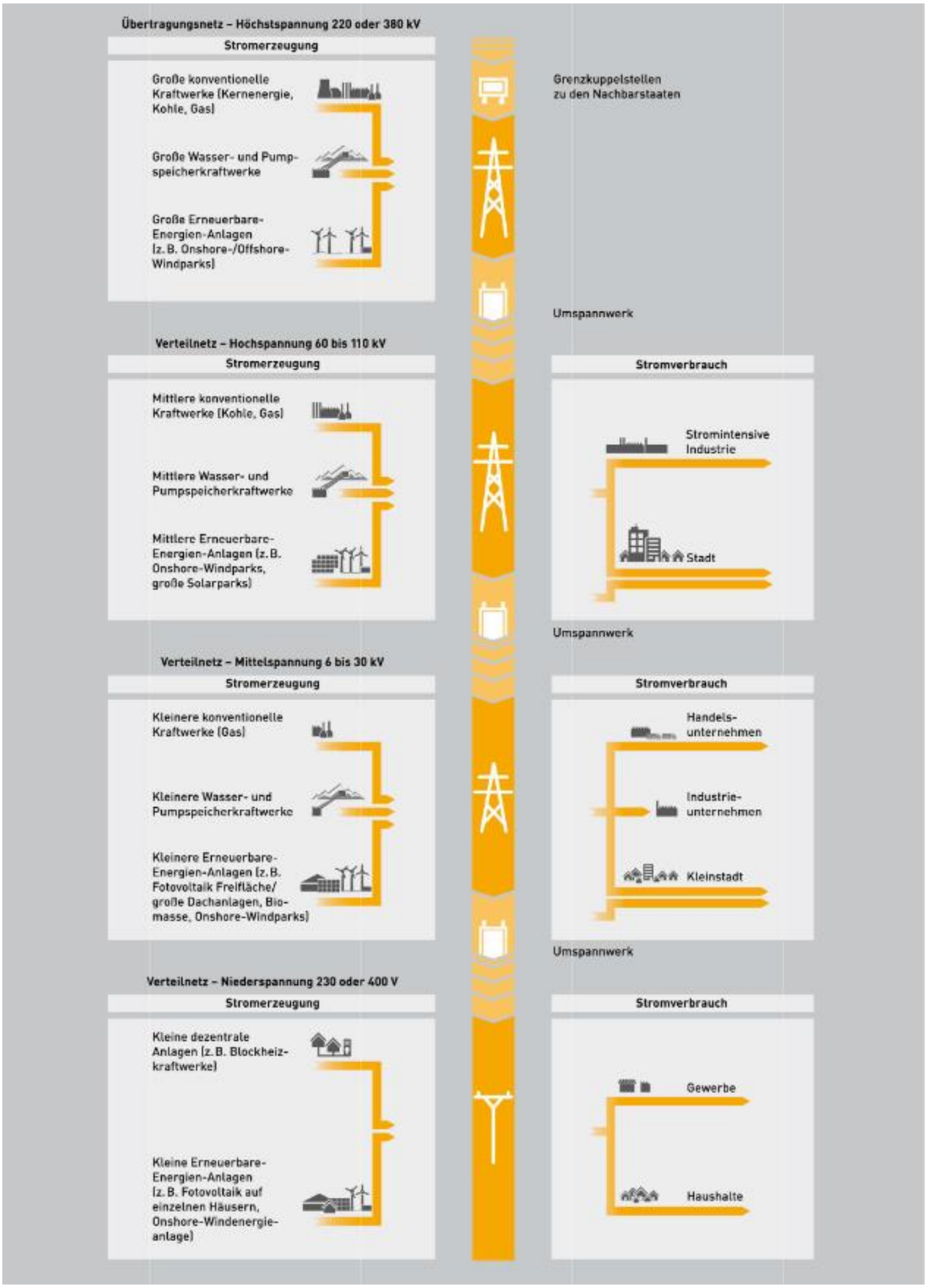
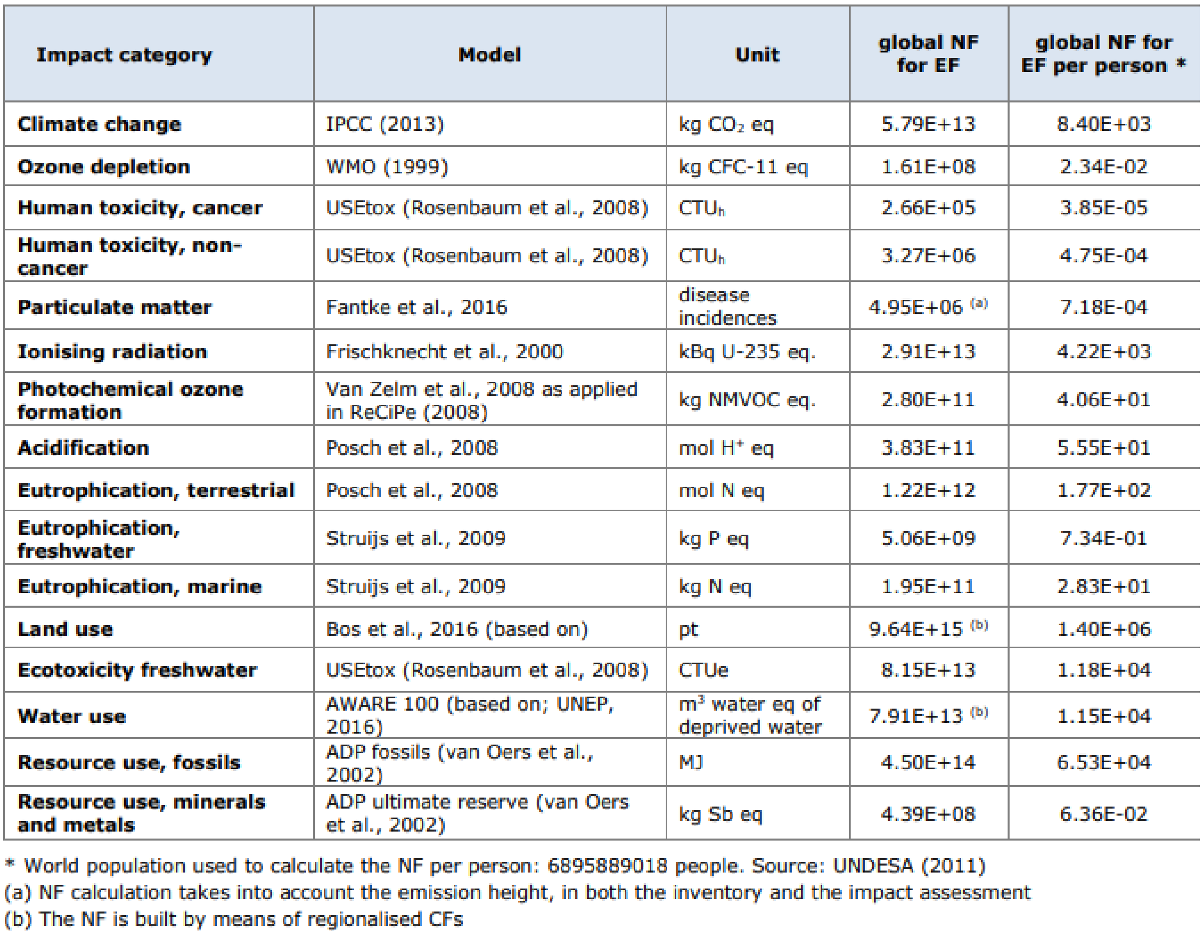


Figure 33: Structure of a general electricity grid in Germany

Table 20: Global normalization factors for emissions and resource extraction in 2012 based on EF 2017 method (Source: Sala et al. 2017)



Impact category	Model	Unit	global NF for EF	global NF for EF per person *
Climate change	IPCC (2013)	kg CO_2 eq	5.79E+13	8.40E+03
Ozone depletion	WMO (1999)	kg CFC-11 eq	1.61E+08	2.34E-02
Human toxicity, cancer	USEtox (Rosenbaum et al., 2008)	CTU_h	2.66E+05	3.85E-05
Human toxicity, non-cancer	USEtox (Rosenbaum et al., 2008)	CTU_h	3.27E+06	4.75E-04
Particulate matter	Fantke et al., 2016	disease incidences	4.95E+06 (a)	7.18E-04
Ionising radiation	Frischknecht et al., 2000	kBq U-235 eq.	2.91E+13	4.22E+03
Photochemical ozone formation	Van Zelm et al., 2008 as applied in ReCiPe (2008)	kg NMVOC eq.	2.80E+11	4.06E+01
Acidification	Posch et al., 2008	mol H^+ eq	3.83E+11	5.55E+01
Eutrophication, terrestrial	Posch et al., 2008	mol N eq	1.22E+12	1.77E+02
Eutrophication, freshwater	Struijs et al., 2009	kg P eq	5.06E+09	7.34E-01
Eutrophication, marine	Struijs et al., 2009	kg N eq	1.95E+11	2.83E+01
Land use	Bos et al., 2016 (based on)	pt	9.64E+15 (b)	1.40E+06
Ecotoxicity freshwater	USEtox (Rosenbaum et al., 2008)	CTUe	8.15E+13	1.18E+04
Water use	AWARE 100 (based on; UNEP, 2016)	m^3 water eq of deprived water	7.91E+13 (b)	1.15E+04
Resource use, fossils	ADP fossils (van Oers et al., 2002)	MJ	4.50E+14	6.53E+04
Resource use, minerals and metals	ADP ultimate reserve (van Oers et al., 2002)	kg Sb eq	4.39E+08	6.36E-02

* World population used to calculate the NF per person: 6895889018 people. Source: UNDESA (2011)
(a) NF calculation takes into account the emission height, in both the inventory and the impact assessment
(b) The NF is built by means of regionalised CFs

Appendix B

Biomass supply:

untransformed dry kraft lignin powder (Bernier approach)

Activity:

kraft lignin production; pulp mill; marginal approach | cut-off

Geography:

RER

Description:

Bernier (2013) - Life cycle assessment of kraft lignin for polymer applications

Base Case with data from RISE implemented

carbon dioxide, liquid

Activity:

market for carbon dioxide, liquid | cut-off

Geography:

RER

Description:

Special transport modelling for liquid gases: No ship transport and normal transport modelling for chemicals reduced by 90%.

Sulfuric acid

Activity:

market for sulfuric acid | cut-off

Geography:

RER

Description:

The transport amounts are based on eurostat transport statistics for 2016 (http://ec.europa.eu/eurostat/data/database, extracted on the 2018-06-01). See exchange comments for additional details.
A regional market for Europe [RER] is motivated by the low share (in the range of 1.3%-2.9% of total trade quantities between 2010-2016) of import quantities to EU28 from outside (excluding Norway and Switzerland) the Union. In addition, the export quantities exceeded the import quantities (the ratio export/import was in the range of 43-76 in the same period). Source: Eurostat database, EU trade since 1988 by HS6 (DS-016893), HS6-code: 280700 - SULPHURIC ACID; OLEUM,

Assessed on: 2017-11-15.

This dataset represents the supply of 1 kg of sulfuric acid from activities that produce it within the geography RER.

sodium hydroxide, without water, in 50% solution state

Activity:

chlor-alkali electrolysis, membrane cell | cut-off

Geography:

RER

Description:

This dataset is mainly based on a document concerning the best available techniques in the chlor-alkali manufacturing industry (European Commission 2001).
Althaus H.-J., Chudacoff M., Hischier R., Jungbluth N., Osses M. and Primas A. (2007) Life Cycle Inventories of Chemicals. Final report ecoinvent data v2.0 No. 8. Swiss Centre for Life Cycle Inventories, Dübendorf, CH.
References:
European Commission (2001) Integrated Pollution Prevention and Control (IPPC) - Reference Document on Best Available Techniques in the Chlor-Alkali Manufacturing Industry. Institute for Prospective Technological Studies, Sevilla.
Sodium hydroxide is a white odorless pellet or solid that is very soluble. Sodium hydroxide is used for the synthesis of other chemicals, and is used in the metal industry, the pulp and paper sector, the textile industry and in other various sectors.
Euro Chlor (2013) An Eco-profile and Environmental Product Declaration of the European Chlor-Alkali Industry, Chlorine (The chlor-alkali process).
Chlorine is largely used in the synthesis of chlorinated organic compounds. PVC and isocyanates are the main drivers of chlor-alkali production in the EU-27 and EFTA countries (Euro Chlor 2013). These products are used in a wide range of applications, such as construction materials, plastics, clothing and pesticides.
This dataset represents the production of chlorine and sodium hydroxide (NaOH) by means of chlor-alkali electrolysis using a membrane cell. The chlor-alkali process is the main technology

for the production of chlorine and sodium hydroxide. In this process, chlorine and sodium hydroxide are produced by electrolysis of a salt solution using either a mercury cell, diaphragm cell or membrane cell.

Geography: European average values.

Technology: In the membrane cell process, the anode and cathode compartments are separated by a perfluoropolymer cation-exchange membrane that selectively transmits sodium ions but suppresses the migration of hydroxyl ions (OH-) from the catholyte into the anolyte. Saturated brine flows through the anode compartment, where chlorine gas is produced at the anode. The electric field in the electrolysis cell causes hydrated sodium ions to migrate through the membrane into the cathode compartment. The cathode compartment is fed with diluted sodium hydroxide solution. Water is electrolysed at the cathode releasing gaseous hydrogen and hydroxyl ions, which combine with the sodium ions and thus increase the concentration of sodium hydroxide in the catholyte. Typically, the outlet concentration of sodium hydroxide is around 32 wt.-%. A part of the product stream is diluted with demineralised water to about 30 wt.-% and used as catholyte inlet. In some units, a more diluted 23 wt.-% NaOH solution is produced. In these cases, the inlet concentration is adjusted to 20-21 wt.-%. Usually the NaOH solution is evaporated to the marketable concentration of 50 wt.-% using steam. Depleted brine leaving the anode compartment is saturated with chlorine and is therefore sent to a dechlorination unit to recover the dissolved chlorine before it is resaturated with salt for recirculation. The advantages of the membrane cell technique are the very high purity of the sodium hydroxide solution produced and the comparably low energy demand. Disadvantages comprise the high requirements on brine purity, the need for sodium hydroxide evaporation to increase concentration, and the comparably high oxygen content in the produced chlorine. In general, multiple cell elements are combined into a single unit, called electrolyser, of whom the design can be either monopolar or bipolar. In a monopolar electrolyser, the anodes and cathodes of the cells are connected electrically in parallel, whereas in the bipolar design, they are connected in series. Therefore, monopolar electrolysers require high current and low voltage, whereas bipolar electrolysers require low current and high voltage. Since bipolar systems allow higher current densities inside the cells, investment and operating costs are usually lower than for monopolar systems.

References:

Euro Chlor (2013) An Eco-profile and Environmental Product Declaration of the European Chlor-Alkali Industry, Chlorine (The chlor-alkali process).

tap water

Activity:

market for tap water | cut-off

Geography:

RER

Description:

This dataset is created as a child of global dataset.

[This dataset is meant to replace the following datasets:

- market for tap water, at user, Europe without Switzerland, 2011 - 2011 (10c8e59b-4e34-4a05-acbb-8d2fdfeae1b6)]

ash from paper production sludge

Activity:

treatment of ash from paper production sludge, residual material landfill | cut-off

Geography:

Europe without Switzerland

Description:

Inventoried waste contains 100% composition of paper sludge ash; .

waste composition (wet, in ppm): H_2O n.a.; O 30083; H n.a.; C 9164.7; S 41259; N 6222.5; P 146230; B n.a.; Cl 0.012408; Br n.a.; F 9.6141; I n.a.; Ag n.a.; As 10.215; Ba n.a.; Cd 1.5403; Co 32.145; Cr 98.271; Cu 560.17; Hg 1.0175; Mn 1069.5; Mo 22.403; Ni 60.085; Pb 267.55; Sb n.a.; Se n.a.; Sn 79.568; V n.a.; Zn 865.8; Be n.a.; Sc n.a.; Sr n.a.; Ti n.a.; Tl n.a.; W n.a.; Si 199030; Fe 158420; Ca 221030; Al 50413; K 14897; Mg 29415; Na 90757;

Share of carbon in waste that is biogenic 100%.

Geography: Technology encountered in Switzerland in 2000. It is assumed to be representative for European conditions as well. Landfill includes base seal and leachate collection system.
Technology: Swiss residual material landfill for polluted, inorganic waste. With base seal and leachate collection system. Recultivation after closure.

Time period: Waste composition as given in literature reference, theoretical data or other source. Transfer coefficients from prospective model.

electricity, medium voltage

Activity:

market for electricity, medium voltage | cut-off

Geography

SE

Description:

The shares of electricity technologies on this market are valid for the year 2016. They have been calculated by the data provider and don't necessarily correspond with the production volumes entered in the undefined datasets of the different electricity producers. The shares have been calculated based on statistics from 2016: IEA World Energy Statistics and Balances. OECD iLibrary, eISSN: 1683-4240, DOI: 10.1787/enestats-data-en and ENTSO-E: Physical Energy & Power Flows, https://www.entsoe.eu/data/power-stats/physical-flows/. Further information can be found in a report available on ecoQuery, section 'Files'.
This dataset describes the electricity available on the medium voltage level in (location) for year (year). This is done by showing the transmission of 1kWh electricity at medium voltage.
Technology: - Low voltage level below 1 kV (Households)
and public buildings)
- High voltage level above 24 kV (large scale industry)
Definition of the voltage levels:
- Medium voltage level between 1 kV and 24 kV (medium to small scale industry, service sector
Average technology used to transmit and distribute electricity. Includes underground and overhead lines, as well as air-, vacuum- and SF6-insulated high-to-medium voltage switching stations. Electricity production according to related technology datasets.

Time period: The composition of this market is valid for the year 2014.

kraft lignin from southern bleached softwood kraft; unintegrated (Culbertson approach)

Activity:

kraft lignin extraction; from southern bleached softwood kraft, elemental chlorine free (ECF) bleached process; at mill; unintegrated

Geography:

RER

Description:

Edit: "Data and flows adapted based on data from RISE (internal communication). Further, bark was not mentioned in the paper of Culbertson (2016). Therfore, it was removed of the model. Furthermore, Transport was adjusted because of that, 80 km for Softwood and 160 km for raw material (chemicals) transport. In the end all data was updated to the inventory data of the Paper from Culbertson (2016)."

This unit process represents the gate-to-gate production of 1 air-dried metric tonne of kraft lignin, coproduced with southern bleached softwood kraft pulp (SBSK), high voltage electricity and unrefined tall oil soap. The pulp is derived from pine or loblolly pine in a kraft pulping process at a mill in the southern United States (U.S.). Lignin is extracted via precipitation and acid washing. All flows are production weighted to kraft lignin. The SBSK pulp production technologies are an aggregation of those applied in the southern U.S. in 2013.
Primary data for this unit process were gathered and generated as part of a "Life cycle assessment of lignin extraction in a softwood kraft pulp mill" (Culbertson et al. 2016) over a three year time period from 2013 to 2016 (time of publication). However, the data may be considered representative of common kraft pulping technology, with an average technology maturity age of over 50 years. Any improvements or process efficiencies over time may be considered incremental.
Secondary data were taken from ecoinvent Centre (2010).
Life cycle inventory data were generated from the material and energy balance of a simulated kraft pulp mill, located in the southeastern United States (i.e., States of Mississippi, Oklahoma,

Kentucky, West Virginia, Virginia, Tennessee, North Carolina, South Carolina, Georgia, Alabama, Louisiana, Florida). The user should exercise caution when selecting material flows (both technical and elemental) for the primary foreground system. Users are encouraged to update and modify this LCI using regionally specific material flows, when available. In many cases, the authors for this process (Culbertson et al. 2016) selected material flows for the background system (secondary data) which are not located in the United States.

This unit process is a gate-to-gate model for activities in a kraft pulp mill located in the southeastern U.S. (see "Geography description" field for details). This unit process produces "kraft lignin; from southern bleached softwood kraft, Elemental chlorine free (ECF) bleached process; at mill; 95% air dried metric tons" and three other co-products. Process modeling is based on the operation of a WinGEMS v5.3 (Valmet Automation 2016) kraft pulp mill with an operating capacity of 464,000 ADmt/year (air dry metric tonnes per year) southern bleached softwood kraft pulp and 52,000 ADmt/year kraft lignin. Pulp yields and related inputs and outputs represent aggregated data from three years of operation (2013-2016).

The primary foreground systems included the pulp mill digester and brown-stock washing, evaporation, recovery boiler, and power production. Incremental changes to the process flows relative to the base case were simulated and data exported were used to build the life cycle inventory inputs and outputs. Background systems for the elementary flows into the pulp mill included softwood production and harvesting as well as chemical, fuel, landfill service and electricity production.

A detailed description of the technologies involved in this unit process can be found in Culbertson et al. (2016).

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transport, freight, lorry >32 metric ton, EURO5

Activity:

transport, freight, lorry >32 metric ton, EURO5 | cut-off

Geography:

RER

Description:

16-32t 5.79t 15.79t
This dataset represents the service of 1tkm freight transport in a lorry of the size class >32 metric tons gross vehicle weight (GVW) and Euro V emissions class. The transport datasets refer to the entire transport life cycle i.e. to the construction, operation, maintenance and end of life of vehicle and road infrastructures. Fuel consumption and emissions are for average

European journeys and load factors and not representative of a specific transport scenario. The average load factors are taken from the Tremove model v2.7b (2009) and EcoTransIT (2011) report. These are as follows:

Lorry size class Average load factor GVW

7.5-16t 3.29t 9.29t

Ntziachristos, L., et al. (2013) EMEP/EEA air pollutant emissions inventory guidebook 2009: Exhaust emissions from road transport. European Environment Agency, Copenhagen, DK.

Spielmann, M., et al. (2007) Transport Services. ecoinvent report No. 14., Swiss Centre for Life Cycle Inventories, Dübendorf, CH.

Knörr, W. et al. (2011) Ecological Transport Information Tool for Worldwide Transports (EcoTransIT): Methodology and data update. Berlin, Hannover, Heidelberg, DE.

For road infrastructure the expenditures and environmental interventions due to construction of roads have been allocated based on the gross tonne kilometer performance. Expenditures due to operation of the road infrastructure, as well as land use have been allocated based on the yearly vehicle kilometer performance. The same assumption on vehicle lifetime performance has been transferred from the ecoinvent v2 datasets of 540 000 km/vehicle. The production, maintenance and disposal of the vehicle are as reported in the ecoinvent (2007) report on transport services.

Non-exhaust emissions are accounted for as weight dependent by-products and exist as seperate datasets.

Keller, M. et al. (2010) Handbook emission factors for road transport v3.1, HBEFA. INFRAS, Berne, CH.

Main data sources:

De Ceuster, G., et al. (2009) TREMOVE: Final Report. Model code v2.7b, 2009. European Commission, Brussels.

The lorry size and load factor determines the GVW and therefore also the fuel consumption and amount of both exhaust and non-exhaust emissions. Non-exhaust emissions are those resulting from tyre, brake and road wear.

3.5-7.5t 0.98t 4.98t

Fuel consumption and exhaust emissions are taken from v3.1 of the HBEFA model, using the data for Germany and without applying model weighting. There are a higher number of size categories used in HBEFA than in ecoinvent and so the data are grouped in order to fit the lorry size classes used in ecoinvent. The selective catalytic reduction (SCR) technology is around 3 times more common than that of exhaust gas recovery (EGR) as an emissions reduction measure

and so the emission factors given in the dataset are weighted to reflect this. The data for the HBEFA categories SCR* and VI* were disregarded. The exhaust emissions caused by the burning of fuel are either fuel dependent (fuel type and quantity) or Euro class dependent. The latter reflect the emission regulations to which the vehicle complies. Regulated emissions are CO, NOx, particulate matter (PM) and total hydrocarbons (HC). Data from the Emissions Inventory Guidebook (EMEP/EEA, 2013) were used for specific exhaust emissions not covered by the HBEFA model.
>32t 15.96t 29.96t
Geography: References:
The data for road infrastructure reflect Swiss conditions. Data for vehicle operation, manufacturing and maintenance represents generic European data. Data for the vehicle disposal reflect the Swiss situation. The environmental interventions due to vehicle transport are modelled by linking the environmental interventions due to vehicle operation with impacts due to vehicle manufacturing, vehicle maintenance, vehicle disposal, road construction, operation and maintenance of roads and road disposal. So-called demand factors are used to link the transport service components to the functional unit of one tonne kilometre [tkm] (Spielmann & Scholz 2005).
Spielmann M. and Scholz R. W. (2005) Life Cycle Inventories for Transport Services - Background Data for Freight Transport. In: Int J LCA, 10(1), pp.
Technology: Diesel and diesel engine. Lorry transport is further differentiated with respect to vehicle weight and emission technology standard (EURO-standard).

Technology classifications are based on those used widely within the works of the European Environment Agency, particularly in the Emissions Inventory Guidebook.

sludge from pulp and paper production

Activity:

treatment of sludge from pulp and paper production, sanitary landfill | cut-off

Geography:

Europe without Switzerland

Description:

Inventoried waste contains 100% sludge from pulp and paper production; .
waste composition (wet, in ppm): upper heating value 5.032 MJ/kg; lower heating value 2.645 MJ/kg; H2O 250000; O 427890; H 29257; C 157500; S 3367; N 26559; P 12074; B n.a.; Cl 0.025838; Br n.a.; F 1.9261; I n.a.; Ag n.a.; As 1.4625; Ba n.a.; Cd 0.255; Co 4.7786; Cr 12.75; Cu 84.585; Hg 0.18; Mn 156.56; Mo 2.8282; Ni 8.925; Pb 46.95; Sb n.a.; Se n.a.; Sn 11.862; V n.a.; Zn 131.5; Be n.a.; Sc n.a.; Sr n.a.; Ti n.a.; Tl n.a.; W n.a.; Si 17626; Fe 20951; Ca 29909; Al 5851.4; K 2344.6; Mg 3357.9; Na 12849;
Share of carbon in waste that is biogenic 100%.
Overall degradability of waste during 100 years: 60%.

Technology: Swiss municipal sanitary landfill for biogenic or untreated municipal waste ('reactive organic landfill'). Landfill gas and leachate collection system. Recultivation and monitoring for 150 years after closure.

hydrogen peroxide, without water, in 50% solution state

Activity:

hydrogen peroxide production, product in 50% solution state | cut-off

Geography:

RER

Description:

References:
This dataset represents the production of 1 kg of hydrogen peroxide. Hydrogen peroxide is a colourless liquid with a slightly sharp odour at higher concentrations. Due to its characteristics as a strong oxidising agent, hydrogen peroxide is widely used as a bleaching agent in the paper and the textile industry. Further important uses are e.g. wastewater treatment, disinfection applications or hydrometallurgical processes. In dilute solutions H2O2 acts as a very efficient antiseptic.
This dataset is based on a study performed by EMPA and Boustead Consulting, commissioned by CEFIC, and contains data from 8 European producers of hydrogen peroxide.

Althaus H.-J., Chudacoff M., Hischier R., Jungbluth N., Osses M. and Primas A. (2007) Life Cycle Inventories of Chemicals. ecoinvent report No. 8, v2.0. EMPA Dübendorf, Swiss Centre for Life Cycle Inventories, Dübendorf, CH.

Boustead I. and Fawer M. (1998) Ecoprofile of hydrogen peroxide. Peroxygens - a sector group of CEFIC, Brussels (Belgium), Online-Version under: http://www.cefic.org/sector/peroxy/ecohydro/tc.htm.

Geography: Average data from 8 European producers.

Technology: The most common technique for the production of hydrogen peroxide is the autooxidation (AO) or anthraquinone process. In a first step, hydrogen peroxide is produced by reducing alkylanthraquinone with hydrogen in the presence of a catalyst to the hydrochinone. Then the catalyst is removed and the hydrochinone is oxidised – usually with air – back to the origin quinone and in the same time hydrogen peroxide is produced. The quinones can then be re-hydrolysed again. The whole reaction takes place in a working solution that consists of a mixture of various solvents (i.e. parts are aromatic solvents). The whole process is exothermic. In a second step, hydrogen peroxide is extracted from the working solution and concentrated. Both steps are included in this dataset.

Time period: Time of publications.

lime, hydrated, packed

Activity:

market for lime, hydrated, packed | cut-off

Geography:

RER

Description:

A regional market for Europe [RER] is motivated by the low share (in the range of 0.6%-1.5% of total trade quantities between 2010-2016) of import quantities to EU28 from outside (excluding Norway and Switzerland) the Union. In addition, the export quantities exceeded the import quantities (the ratio export/import was in the range of 26.83-63.54 in the same period).

Source: Eurostat database, EU trade since 1988 by HS6 (DS-016893), HS6-code: 252220 - SLAKED LIME, Assessed on: 2018-02-02.

Geography: Europe

methanol

Activity:

Methanol production | cut-off

Geography:

GLO

Description:

Only a small proportion is used for energy production (2% of production), although this use has great potential.

- Methyl methacrylate (MMA): 3% of production.
- Methyl tert-butyl ether (MTBE): 28% of production.

As of 2000, more than 70% of the methanol produced worldwide is used in chemical syntheses. In order of importance the produced methanol was used as follows:

Althaus H.-J., Chudacoff M., Hischier R., Jungbluth N., Osses M. and Primas A. (2007) Life Cycle Inventories of Chemicals. ecoinvent report No. 8, v2.0. EMPA Dübendorf, Swiss Centre for Life Cycle Inventories, Dübendorf, CH.

This dataset represents the production of methanol using the steam reforming process. The inventory is based on data from literature and reports on plant design or efficiency.

References:

This dataset represents the production of 1 kg of methanol from natural gas. Methanol (CH_3OH) is a clear, colourless, volatile liquid with a faint alcohol-like odour. Methanol is the simplest of the alcohols, having only one carbon atom, and is completely miscible in water. Methanol easily dissolves in other alcohols and chlorinated hydrocarbons, but has limited solubility in diesel fuel, vegetable oils, and aliphatic hydrocarbons.

Commercial production of methanol is based on synthesis gas mixtures (carbon monoxide and hydrogen) derived primarily from natural gas.

- Dimethyl terephthalate (DMT). 2% of production.

- Acetic acid: 10% of production.
- Formaldehyde: 34% of production.

Geography: Data from various plants at different locations.

Technology: Althaus H.-J., Chudacoff M., Hischier R., Jungbluth N., Osses M. and Primas A. (2007) Life Cycle Inventories of Chemicals. ecoinvent report No. 8, v2.0. EMPA Dübendorf, Swiss Centre for Life Cycle Inventories, Dübendorf, CH.

The main resource for methanol production is natural gas, which acts as feedstock and fuel. A natural gas based methanol plant consumes typically 29-37 MJ (LHV) of natural gas per kg of methanol. This gas is needed as feedstock for the produced methanol (20 MJ kg-1 LHV) and also used as fuel for the utilities of the plant.

For an average plant the total carbon efficiency is around 75%, 81% for the synthesis gas preparation and 93% for the methanol synthesis (Le Blanc et al. 1994, p. 114). For steam reformers usually a steam to carbon ratio of 3:1 to 3.5:1 is used.

As methanol production is a highly integrated process with a complicated steam system, heat recovery and often also internal electricity production (out of excess steam), there were only data of the efficiency and energy consumption of the total process available. Therefore the process was not divided into a reforming process, a synthesis process and a purification process for estimating the energy and resource flows. Also the energy and resource flows in the methanol production plants are site specific (dependent on the local availability of resources such as CO_2, O_2, or electricity). In this inventory typical values for a methanol plant using steam-reforming technology were used.

From the converted feed, 1 kg methanol and 0.06 kg hydrogen is yielded. It was assumed that the purged hydrogen was also burned in the furnace. The only emission to air considered from burning hydrogen is NO_X. The energy amount generated is not considered, because the process of the furnace is specified for natural gas as fuel. The NO_X emissions of the hydrogen burning were therefore calculated separately.

References:

Methanol synthesis:

$CH_4 + H_2O \rightarrow CO + 3\,H_2$; $\Delta H = 206$ kJ mol-1

$CO + H_2O \rightarrow CO_2 + H_2$; $\Delta H = -41$ kJ mol-1

$CO + 2\,H_2 \rightarrow CH_3OH$; $\Delta H = -98$ kJ mol-1

The reaction of the steam-reforming route can be formulated for methane, the major constituent of natural gas, as follows:

$CO_2 + 3\,H_2 \rightarrow CH_3OH + H_2O$; $\Delta H = -58$ kJ mol-1

Methanol produced using a low pressure steam reforming process (ICI LPM) accounts for approximately 60% of the world capacity (Synetix 2000a). Besides steam reforming, combined reforming has gained importance due to the production of methanol in large plants at remote locations.

More recently, Lurgi developed another two-step gas production scheme. It is based on catalytic autothermal reforming with an adiabatic performer and has economical advantages for very large methanol plants. At locations where no carbon dioxide is available most of the methanol plants are based on the following gas production technologies, depending on their capacities: steam reforming for capacities up to 2000 t d-1 or combined reforming from 1800 to 2500 t d-1 (Ullmann 2001). For the energy and resource flows in this inventory a modern steam reforming process was taken as average technology. To estimate best and worst case values, also values from combined reforming and autothermal reforming were investigated.

Synthesis gas preparation:

For normal methanol synthesis, reforming is performed in one step in a tubular reactor at 850 – 900 °C in order to leave as little methane as possible in the synthesis gas. For large methanol synthesis plants, Lurgi has introduced a two-step combination (combined reforming process) that gives better results. In the primary tubular reformer, lower temperature (ca. 800 °C) but higher pressure (2.5-4.0 MPa instead of 1.5-2.5 MPa) are applied.

Time period: Time of publications.

sodium chlorate, powder

Activity:

sodium chlorate production, powder | cut-off

Geography:

RER

Description:

References:

Althaus H.-J., Chudacoff M., Hischier R., Jungbluth N., Osses M. and Primas A. (2007) Life Cycle Inventories of Chemicals. ecoinvent report No. 8, v2.0. EMPA Dübendorf, Swiss Centre for Life Cycle Inventories, Dübendorf, CH.

Bowsted and Fawer (1996) Ecoprofile of sodium chlorate. http://www.cefic.be/sector/naclo3/ecoprofile /tc.htm#tc.

This dataset represents the production of sodium chlorate by means of electrolysis of a sodium chloride solution. Sodium chlorate ($NaClO_3$) is a white, hygroscopic, crystalline solid. It is an efficient oxidising agent. Sodium chlorate is used in the manufacture of chlorine dioxide bleach for the pulp and paper industry. Second in importance is its use as an intermediate in the production of other chlorates, mainly potassium chlorate, and of sodium perchlorate for conversion to ammonium perchlorate, which is used as an oxidiser in solid propellants. Sodium chlorate is further used as an oxidising agent in uranium refining and other metallurgical operations, as an additive in agricultural products and dyes, in textile and fur dyeing, metal etching, and in chemical laboratories and throughout the chemical industry as an oxidising agent. The values in this dataset are literature average values, based on Fawer (2002), and a personal comunication on the background information from Bowsted and Fawer (1996) regarding confidential data of European manufacturing plants. This information allows to disclose the data from Bowsted and Fawer (1996) in a suitable manner for this dataset.

Geography: Average values of six European manufacturing plants.

Technology: The concentrated chlorate solution is either submitted to crystallisation or it is used directly, particularly in the production of chlorine dioxide. Sodium chlorate, hydrogen gas (H_2) and heat are formed in the production process. The solution formed is crystallised and the chlorate crystals are separated, washed and dried. The final product contains mostly 99 to 99.9% sodium chlorate. The hydrogen gas and the heat produced can be exported for different uses. The main raw materials are sodium chloride and water. Energy is provided by electrical power.

$NaCl + 3H_2O + 6e^- \rightarrow NaClO_3 + 3H_2$

Sodium chlorate is produced by electrolysis of an aqueous sodium chloride solution. This is achieved according the following overall reaction equation:

Althaus H.-J., Chudacoff M., Hischier R., Jungbluth N., Osses M. and Primas A. (2007) Life Cycle Inventories of Chemicals. ecoinvent report No. 8, v2.0. EMPA Dübendorf, Swiss Centre for Life Cycle Inventories, Dübendorf, CH.

References:

Time period: The period corresponds to the early nineties, estimated to be from 1990 to 1995.

bundle, energy wood, measured as dry mass

Activity:

softwood forestry, pine, sustainable forest management | cut-off

Geography:

SE

Description:

-

bark

Activity:

sawing, softwood | cut-off

Description:

Geography:

Represents average Swiss conditions.

oxygen, liquid

Activity:

air separation, cryogenic | cut-off

Geography:

RER

Description:

Smith A. R. and Klosek J. (2001) A Review of Air Separation Technologies and their Integration with Energy Conversion Processes. In: Fuel Processing Technology, 70(2), pp. 115-134.

This dataset represents the production of liquefied nitrogen, oxygen and argon by cryogenic air separation. The liquefaction process of air represents an average cryogenic air separation process. Cryogenic air separation is currently the most efficient and cost-effective technology for producing large quantities of oxygen, nitrogen, and argon as gaseous or liquid products (Smith & Klosek 2001). The fraction of each output is based on the composition of air (1.4% Argon, 23.1% Oxygen and 75.5% Nitrogen).

This dataset is based on literature data and estimations.

Althaus H.-J., Chudacoff M., Hischier R., Jungbluth N., Osses M. and Primas A. (2007) Life Cycle Inventories of Chemicals. ecoinvent report No. 8, v2.0. EMPA Dübendorf, Swiss Centre for Life Cycle Inventories, Dübendorf, CH.

Argon (Ar) is a monatomic, chemically inert gas composing slightly less than 0.93% by volume of the air. Argon is colourless, odourless, tasteless, non-corrosive, non-flammable, and non-toxic. Argon is the most abundant and most used of the noble gases. Commercial argon is the product of cryogenic air separation. Argon is the most abundant and most used of the noble gases. Its chief use is in metallurgy, where it provides an inert atmosphere in which hot metals can be worked. Because argon is very un-reactive, it prevents chemical reactions of the very hot metal being welded or forged.

Nitrogen (N2) constitutes 78.09% by volume of the air. It is colourless, odourless, and tasteless. Nitrogen is often used as an 'inert' gas due to its non-reactive nature with many materials. Commercial nitrogen is produced by different air separation processes, such as cryogenic liquefaction and distillation, pressure swing adsorption (PSA) and membrane separation. Liquid nitrogen, produced by the cryogenic air separation process, finds wide use as a refrigerant in applications such as cryogenic grinding of plastics and food freezing. Gaseous nitrogen is used in the chemical and petroleum industries for storage tank blanketing and vessel inerting applications, in the food industries to pack oxidisable foods and by the electronics and metals industries for the inert properties.

Oxygen (O2) constitutes 20.95% by volume of the air. Liquid oxygen is pale blue. The principal use of oxygen stems from its strong oxidising properties. Oxygen is produced by air separation processes that use either cryogenic liquefaction and distillation or separation with vacuum swing adsorption (VSA). The major commercial uses of oxygen are in metal manufacturing, metal fabricating, and in health services. Oxygen is also used extensively in the chemical industry and in the pulp and paper industry.

References:

Geography: Data from several producers in Europe, as well as U.S. and Russian producers.

Technology: Cryogenmash (2001) KxAxApx Type Double-Pressure Air Separation Plants. Gen-eral Data. Cryogenic Industries, Moscow, Russia. Retrieved 16.01.2002 from http://www.cryogenmash.ru/production/vru/vru_kgag2_e.htm

Praxair (2002) Gases > Nitrogen > Production of Nitrogen. Praxair Technology Inc. 2002. Retrieved 16.01.2002 from http://www.praxair.com

Smith A. R. and Klosek J. (2001) A Review of Air Separation Technologies and their Integration with Energy Conversion Processes. In: Fuel Processing Technology, 70(2), pp. 115-134.

Barron and Randall F. (1985) Cryogenic Systems. 2 Edition. Oxford University Press, New York

Cryogenic distillation accounts for approximately 85% of nitrogen and over 95% of oxygen production. It is the preferred supply mode for high volume and high purity requirements (Praxair 2002). Cryogenic air separation is currently the most efficient and cost-effective technology for producing large quantities of oxygen, nitrogen, and argon as gaseous or liquid products (Smith & Klosek 2001). Besides the air needed as a resource the major input for the liquefying process is the electricity to compress the inlet air, which normally comprises 95% of the utility costs of a cryogenic air separation plant. In some plants the amount of processed air (in Nm3) can be up to 5 times larger than the derived liquid products (Cryogenmash 2001). In these plants, the waste gas stream is naturally also much larger (in order to obtain the mass balance). As output of the cryogenic air separation there are three products: liquid oxygen, liquid nitrogen and liquid crude argon. The assumed process includes no gaseous co-products. In reality gaseous products are also processed if there is a demand at the production site. The investigated cryogenic air separation process leads to liquid products in the following quality:

Commercial argon is the product of cryogenic air separation, where liquefaction and distillation processes are used to produce a low-purity crude argon product.

Numerous configurations of heat exchange and distillation equipment can separate air into the required product streams. These process alternatives are selected based on the purity and number of product streams, required trade-offs between capital costs and power consumption, and the degree of integration between the air separate unit and other facility units. This process requires very complicated heat integration techniques because the only heat sink for cooling or condensation is another cryogenic stream in the process.

Since the boiling point of argon is between that of oxygen and nitrogen, it acts as an impurity in the product streams. If argon were collected and separated from the oxygen product, an oxygen purity of less than 95% by volume would result (Barron & Randall 1985). On the other

hand, if argon were collected with the nitrogen product, the purity of nitrogen would not exceed 98.7% by volume. To achieve higher purities of oxygen and nitrogen the elimination of argon is necessary.
An air pre-treatment section downstream of the air compression (0.7 MPa) and after cooling removes process contaminants, including water, carbon dioxide, and hydrocarbons. The air is then cooled to cryogenic temperatures and distilled into oxygen, nitrogen, and, optionally, argon streams. Alternate compressing and expanding the recycled air can liquefy most of it.

- Liquid oxygen: min. 99.6 wt-%
- Liquid argon, crude: 96-98 wt-%
- Liquid nitrogen: min. 99.9995 wt-%

The main components of air are nitrogen and oxygen, but it also contains smaller amounts of water vapour, argon, carbon dioxide and very small amounts of other gases (e.g. noble gases). The purification and liquefaction of various components of air, in particular oxygen, nitrogen and argon, is an important industrial process, and it is called cryogenic air separation.

Image: https://db3.ecoinvent.org/images/b1f86554-243f-4c79-b3a2-e6a9efa3a7ef

magnesium sulfate

Activity:

magnesium sulfate production | cut-off

Geography:

RER

Description:

The functional unit represent 1 kg of magnesium sulphate. Large uncertainty of the process data due to weak data on the production process.
[This dataset was already contained in the ecoinvent database version 2. It was not individually updated during the transfer to ecoinvent version 3. Life Cycle Impact Assessment results may still have changed, as they are affected by changes in the supply chain, i.e. in other datasets. This dataset was generated following the ecoinvent quality guidelines for version 2. It may have been subject to central changes described in the ecoinvent version 3 change report (http://www.ecoinvent.org/database/ecoinvent-version-3/reports-of-changes/), and the results

of the central updates were reviewed extensively. The changes added e.g. consistent water flows and other information throughout the database. The documentation of this dataset can be found in the ecoinvent reports of version 2, which are still available via the ecoinvent website. The change report linked above covers all central changes that were made during the conversion process.]
Geography: Data are used here as European average.

Technology: Data approximated with data from lime mining, crushing and milling.

carbon dioxide, liquid

Activity:

market for carbon dioxide, liquid | cut-off

Geography:

RER

Description:

Special transport modelling for liquid gases: No ship transport and normal transport modelling for chemicals reduced by 90%.

Sulfuric acid

Activity:

market for sulfuric acid | cut-off

Geography:

RER

Description:

The transport amounts are based on eurostat transport statistics for 2016 (http://ec.europa.eu/eurostat/data/database, extracted on the 2018-06-01). See exchange comments for additional details.

A regional market for Europe [RER] is motivated by the low share (in the range of 1.3%-2.9% of total trade quantities between 2010-2016) of import quantities to EU28 from outside (excluding Norway and Switzerland) the Union. In addition, the export quantities exceeded the import quantities (the ratio export/import was in the range of 43-76 in the same period). Source: Eurostat database, EU trade since 1988 by HS6 (DS-016893), HS6-code: 280700 - SULPHURIC ACID; OLEUM,

Assessed on: 2017-11-15.

This dataset represents the supply of 1 kg of sulfuric acid from activities that produce it within the geography RER.

sodium hydroxide, without water, in 50% solution state

Activity:

chlor-alkali electrolysis, membrane cell | cut-off

Geography:

RER

Description:

This dataset is mainly based on a document concerning the best available techniques in the chlor-alkali manufacturing industry (European Commission 2001).
Althaus H.-J., Chudacoff M., Hischier R., Jungbluth N., Osses M. and Primas A. (2007) Life Cycle Inventories of Chemicals. Final report ecoinvent data v2.0 No. 8. Swiss Centre for Life Cycle Inventories, Dübendorf, CH.
References:
European Commission (2001) Integrated Pollution Prevention and Control (IPPC) - Reference Document on Best Available Techniques in the Chlor-Alkali Manufacturing Industry. Institute for Prospective Technological Studies, Sevilla.
Sodium hydroxide is a white odorless pellet or solid that is very soluble. Sodium hydroxide is used for the synthesis of other chemicals, and is used in the metal industry, the pulp and paper sector, the textile industry and in other various sectors.

Euro Chlor (2013) An Eco-profile and Environmental Product Declaration of the European Chlor-Alkali Industry, Chlorine (The chlor-alkali process).

Chlorine is largely used in the synthesis of chlorinated organic compounds. PVC and isocyanates are the main drivers of chlor-alkali production in the EU-27 and EFTA countries (Euro Chlor 2013). These products are used in a wide range of applications, such as construction materials, plastics, clothing and pesticides.

This dataset represents the production of chlorine and sodium hydroxide (NaOH) by means of chlor-alkali electrolysis using a membrane cell. The chlor-alkali process is the main technology for the production of chlorine and sodium hydroxide. In this process, chlorine and sodium hydroxide are produced by electrolysis of a salt solution using either a mercury cell, diaphragm cell or membrane cell.

Geography: European average values.

Technology: In the membrane cell process, the anode and cathode compartments are separated by a perfluoropolymer cation-exchange membrane that selectively transmits sodium ions but suppresses the migration of hydroxyl ions (OH-) from the catholyte into the anolyte. Saturated brine flows through the anode compartment, where chlorine gas is produced at the anode. The electric field in the electrolysis cell causes hydrated sodium ions to migrate through the membrane into the cathode compartment. The cathode compartment is fed with diluted sodium hydroxide solution. Water is electrolysed at the cathode releasing gaseous hydrogen and hydroxyl ions, which combine with the sodium ions and thus increase the concentration of sodium hydroxide in the catholyte. Typically, the outlet concentration of sodium hydroxide is around 32 wt.-%. A part of the product stream is diluted with demineralised water to about 30 wt.-% and used as catholyte inlet. In some units, a more diluted 23 wt.-% NaOH solution is produced. In these cases, the inlet concentration is adjusted to 20-21 wt.-%. Usually the NaOH solution is evaporated to the marketable concentration of 50 wt.-% using steam. Depleted brine leaving the anode compartment is saturated with chlorine and is therefore sent to a dechlorination unit to recover the dissolved chlorine before it is resaturated with salt for recirculation. The advantages of the membrane cell technique are the very high purity of the sodium hydroxide solution produced and the comparably low energy demand. Disadvantages comprise the high requirements on brine purity, the need for sodium hydroxide evaporation to increase concentration, and the comparably high oxygen content in the produced chlorine. In general, multiple cell elements are combined into a single unit, called electrolyser, of whom the design can be either monopolar or bipolar. In a monopolar electrolyser, the anodes and cathodes of the cells are connected electrically in parallel, whereas in the bipolar design, they are connected in series. Therefore, monopolar electrolysers require high current and low voltage, whereas bipolar electrolysers require low current and high voltage. Since bipolar systems allow higher current densities inside the cells, investment and operating costs are usually lower than for monopolar systems.

References:

Euro Chlor (2013) An Eco-profile and Environmental Product Declaration of the European Chlor-Alkali Industry, Chlorine (The chlor-alkali process).

Liquefaction:

process-specific burdens, residual material landfill

Activity:

process-specific burdens, residual material landfill | cut-off

Geography:

Europe without Switzerland

Description:

inorganic landfill for polluted inorganic wastes like with carbon content below 5%

Technology: landfill with base seal, leachate collection system. Renaturation after closure.

zinc chloride

Activity:

Zinc chloride production

Geography:

RER

Description:

Additional data implemented as reaction happens:

$Zn + 2HCl \rightarrow ZnCl_2 + H_2$

sodium chloride, powder

Activity:

sodium chloride production, powder | cut-off

Geography:

RER

Description:

Gendorf (2016) Umwelterklärung 2015, Werk Gendorf Industriepark, www.gendorf.de.
Althaus H.-J., Chudacoff M., Hischier R., Jungbluth N., Osses M. and Primas A. (2007) Life Cycle Inventories of Chemicals. ecoinvent report No. 8, v2.0. EMPA Dübendorf, Swiss Centre for Life Cycle Inventories, Dübendorf, CH,.
This dataset represents the production of 1 kg of sodium chloride. Sodium chloride (NaCl) forms odorless cubic crystals. Depending on its degree of purity, the color varies between colorless when pure and white to gray when in the form of rock salt.
Sodium chloride has a huge variety of different uses. For example, salt is today the largest mineral feedstock consumed by the chemical industry. It is primarily used as a chemical feedstock for the production of chlorine and caustic soda in the chlor-alkali industry. Salt is also needed for the production of sodium chlorate and metallic sodium by electrolysis, and for the production of sodium sulfate and hydrochloric acid by reacting sodium chloride with sulfuric acid. Another very important area where sodium chloride is used is the human and animal nutrition, since all animals, humans included, need both sodium and chloride. Other relevant areas of use of salt are the maintenance and de-icing of roads as well as the conditioning of water.
References:
In Europe, the possibilities for producing salt by solar evaporation are rather poor and concentrated around the Mediterranean area. Therefore, this dataset represents the production of dry sodium chloride by underground mining (51%) and by solution mining (49%). This dataset is based on data from a European salt producer, as well as literature.

Geography: Data from one European solution mining site, used to represent the European mix of 41% solution mining and 59% rock salt. Some values are based on data from a large chemical factory located in Germany. These are assumed to be valid for this geography.

Technology: - Solution mining and mechanical evaporation: In this case, water is injected in a salt deposit, usually in about 150 to 500 m depth. The dissolution of the halite or salt deposits forms a cavern filled with brine. This brine is then pumped from the cavern back to the surface and transported to either an evaporation plant for the production of evaporated salt or transported directly to a chemical processing plant, e.g. a chlor-alkali plant.

As a fourth form on the market, the so-called 'salt in brine' may be found, which is especially used for the production of different chemicals. In this case, the solution mining technique without an evaporation step afterwards is used.

For the production of dry salt, three different types of sodium chloride production methods can be distinguished namely, underground mining of halite deposits, solution mining with mechanical evaporation and solar evaporation. Their respective products are rock salt, evaporated salt and solar salt:

- Underground mining: The main characteristic of this technique is the fact that salt is not dissolved during the whole process. Instead underground halite deposits are mined with traditional techniques like undercutting, drilling and blasting or with huge mining machines with cutting heads. In a second step, the salt is crushed and screened to the desired size and then hoisted to the surface.

References:

This dataset represents the production of dry sodium chloride by underground mining (51%) and by solution mining (49%) with modern solution mining technology (thermo compressing technology).

Althaus H.-J., Chudacoff M., Hischier R., Jungbluth N., Osses M. and Primas A. (2007) Life Cycle Inventories of Chemicals. ecoinvent report No. 8, v2.0. EMPA Dübendorf, Swiss Centre for Life Cycle Inventories, Dübendorf, CH.

- Solar evaporation: In this case salt is produced with the aid of the sun and wind out of seawater or natural brine in lakes. Within a chain of ponds, water is evaporated by sun until salt crystallizes on the floor of the ponds. Due to their natural process drivers, such plants must be located in areas with only small amounts of rain and high evaporation rates - e.g. in the Mediterranean area where the rate between evaporation and rainfall is 3:1, or in Australia, where even a ratio up to 15:1 can be found. There are some impurities due to the fact that seawater contains not only sodium chloride. That leads to impurities of calcium and magnesium sulfate as well as magnesium chloride. With the aid of clean brine from dissolved fine salt, these impurities are washed out.

Time period: The data in this dataset come from different years, but overall form the most realistic picture of the production. Some values are based on data published by the Gendorf factory that were collected between 2011 and 2015. The time period has been adjusted accordingly. For more details, see the comments of the exchanges.

potassium chloride, as K2O

Activity:

potassium chloride production | cut-off

Geography:

RER

Description:

Refers to 1 kg K2O, resp. 1.67 kg potassium chloride with a K2O-content of 60.0%
[This dataset was already contained in the ecoinvent database version 2. It was not individually updated during the transfer to ecoinvent version 3. Life Cycle Impact Assessment results may still have changed, as they are affected by changes in the supply chain, i.e. in other datasets. This dataset was generated following the ecoinvent quality guidelines for version 2. It may have been subject to central changes described in the ecoinvent version 3 change report (http://www.ecoinvent.org/database/ecoinvent-version-3/reports-of-changes/), and the results of the central updates were reviewed extensively. The changes added e.g. consistent water flows and other information throughout the database. The documentation of this dataset can be found in the ecoinvent reports of version 2, which are still available via the ecoinvent website. The change report linked above covers all central changes that were made during the conversion process.]
Geography: The data refer to Germany.
Technology: The potash salts stem from underground mines. Three different technologies are used to concentrate the salt: solution in hot water, flotation and electrostatic separation. The inventory describes a mixture of these processes.

Time period: Data come from an environmental report for the year 2000.

Hydropyrolysis:

hydrogen, gaseous

Activity:

hydrogen production, gaseous, petroleum refinery operation | cut-off

Geography:

Europe without Switzerland

Description:

Crude quality – API and sulfur content: Crude imports to Europe by country of origin were taken from BP Statistical Review of World Energy 2017 (Oil: Inter-area movements 2016) (BP, 2017) and matched with the crude quality reported for these regions in ENI World Oil Review 2018 (ENI, 2018). The resulting weighted average API grade of crude imports to Europe is 35, and the weighted average sulfur content 1.03%.

LCIs were generated for BREF type II, III and IV and for API 35. In the case of refinery gas and hydrogen, a sulfur content of 1% was used as proxy for the av. European sulfur content of curde intake of 1.03%. No intrapolation applied. This dataset was created as weighted average of types II-IV according to the above shares.

Fehrenbach, H., Liebich, A., Abdalla, N., Biemann, K., Fröhlich, T. Simon, B. (2017) Petroleum refinery industry and liquid fuels - Description of the ifeu refinery model and the calculation of LCI datasets for refinery products in Brazil, India, South Africa, Peru and Colombia. ecoinvent association, Zürich, Switzerland.

Oil and Gas Journal (OGJ) (2017) 2018 Worldwide Refining Survey: Global, Oil & Gas Journal, 5 December 2018, Pennwell Publishing, Tulsa, OK, USA, accessed December 2018.

Reference(s):

BP (2017) BP Statistical Review of World Energy June 2017, online at https://www.bp.com/content/dam/bp-country/de_ch/PDF/bp-statistical-review-of-world-energy-2017-full-report.pdf, last accessed March 2019.

The BREF (European Commission, 2015) contains not only aggregated numbers or weighted averages of emission and energy or water consumptions, but also encompasses primary data of the majority of refineries in Europe in anonymous form. This data source has been complemented by various specific confidential refinery datasets, by values from Eurostat (e.g. in the case of the energy source mix or process energy), and by literature data. In the case of the BREF, a range of values were mentioned as process parameters for which the arithmetic averages were applied. After adapting the model to the up-to-date mass and energy flows within the European refineries, it has been validated and calibrated by comparing the results to the dataset of the BREF, the Eurostat and the European Pollutant Release and Transfer Register (E-PRTR).

The ifeu petroleum refinery life cycle inventory (LCI) tool is based on the outputs of a complex refinery model that reproduces the complexity of petroleum refinery plants in which the combination and sequence of processes are usually very specific to the characteristics of the raw materials (i.e. the close relation between the composition of the crude oil and the products to be produced). Refineries differ not only in their configurations, process integration, feedstocks, product mixes, unit sizes, designs, and control systems but also the market situations, locations and ages of the refinery or environmental regulations can result in a wide variety of refinery concepts. It represents the current European state-of-the-art. The basic setting of the model reflects the technical characteristics of European refineries as described in the Best Available Techniques (BAT) Reference Document (BREF)for the Refining of Mineral Oil and Gas (European Commission, 2015). Further specific data was collected from companies and production plants and was incorporated in order to elaborate a comprehensive and robust model of a refinery.

Supporting documentation for the model underlying the ifeu tool can be found in the ecoinvent report on the petroleum refinery industry for the SRI project, by Fehrenbach et al. (2018).

European Commission (2015) Best Available Techniques (BAT) Reference Document (BREF) for the Refining of Mineral Oil and Gas, Industrial Emissions Directive 2010/75/EU Integrated Pollution Prevention and control, accessible online at http://eippcb.jrc.ec.europa.eu/reference/BREF/REF_BREF_2015.pdf, February 2019

Refinery complexity: The 2018 World Refining Survey (OGJ, 2018) reports the configuration of 107 refineries in Europe. According to their configuration each refinery was assigned a refinery type (I-IV) as defined in the BREF document. Weighted by the annual throughput volume, 62% of European refineries classify as type II, 29% as type II and 9% as type IV.

The simplified LCI tool can be adjusted to average conditions of a specific geography through the following parameters: refinery complexity (according to the complexity classes defined in the BREF document, type I-IV), crude oil sulfur content and American Petroleum Institute

(API) gravity classification. To create this dataset, the above parameters were set to represent the average situation in Europe without Switzerland:
This dataset describes the operation of a representative average petroleum oil refinery in the given geography. Since petroleum refineries are very complex the actual unit process modeling is done in a separate refinery tool, developed by ifeu (Institute for Energy and Environmental Research, Heidelberg, Germany) and this is a subdivided product-specific dataset.
ENI (2018) World Oil Review 2018, Volume 1, online at https://www.eni.com/docs/it_IT/eni-com/azienda/fuel-cafe/WORLD-OIL-REVIEW-2018-Volume-1.pdf, last accessed March 2019.
Geography: Global model calibrated with geography-specific information.

Technology: The technology level in Europe applied here represents a weighted average of BREF types II (62%), III (29%), IV (9%) refineries; API 35; sulfur content 1.03%.

Hydrodeoxygenation (HDO):

hydrogen, gaseous

Activity:

hydrogen production, gaseous, petroleum refinery operation | cut-off

Geography:

Europe without Switzerland

Description:

Crude quality – API and sulfur content: Crude imports to Europe by country of origin were taken from BP Statistical Review of World Energy 2017 (Oil: Inter-area movements 2016) (BP, 2017) and matched with the crude quality reported for these regions in ENI World Oil Review 2018 (ENI, 2018). The resulting weighted average API grade of crude imports to Europe is 35, and the weighted average sulfur content 1.03%.
LCIs were generated for BREF type II, III and IV and for API 35. In the case of refinery gas and hydrogen, a sulfur content of 1% was used as proxy for the av. European sulfur content of curde intake of 1.03%. No intrapolation applied. This dataset was created as weighted average of types II-IV according to the above shares.

Fehrenbach, H., Liebich, A., Abdalla, N., Biemann, K., Fröhlich, T. Simon, B. (2017) Petroleum refinery industry and liquid fuels - Description of the ifeu refinery model and the calculation of LCI datasets for refinery products in Brazil, India, South Africa, Peru and Colombia. ecoinvent association, Zürich, Switzerland.

Oil and Gas Journal (OGJ) (2017) 2018 Worldwide Refining Survey: Global, Oil & Gas Journal, 5 December 2018, Pennwell Publishing, Tulsa, OK, USA, accessed December 2018.

Reference(s):

BP (2017) BP Statistical Review of World Energy June 2017, online at https://www.bp.com/content/dam/bp-country/de_ch/PDF/bp-statistical-review-of-world-energy-2017-full-report.pdf, last accessed March 2019.

The BREF (European Commission, 2015) contains not only aggregated numbers or weighted averages of emission and energy or water consumptions, but also encompasses primary data of the majority of refineries in Europe in anonymous form. This data source has been complemented by various specific confidential refinery datasets, by values from Eurostat (e.g. in the case of the energy source mix or process energy), and by literature data. In the case of the BREF, a range of values were mentioned as process parameters for which the arithmetic averages were applied. After adapting the model to the up-to-date mass and energy flows within the European refineries, it has been validated and calibrated by comparing the results to the dataset of the BREF, the Eurostat and the European Pollutant Release and Transfer Register (E-PRTR).

The ifeu petroleum refinery life cycle inventory (LCI) tool is based on the outputs of a complex refinery model that reproduces the complexity of petroleum refinery plants in which the combination and sequence of processes are usually very specific to the characteristics of the raw materials (i.e. the close relation between the composition of the crude oil and the products to be produced). Refineries differ not only in their configurations, process integration, feedstocks, product mixes, unit sizes, designs, and control systems but also the market situations, locations and ages of the refinery or environmental regulations can result in a wide variety of refinery concepts. It represents the current European state-of-the-art. The basic setting of the model reflects the technical characteristics of European refineries as described in the Best Available Techniques (BAT) Reference Document (BREF)for the Refining of Mineral Oil and Gas (European Commission, 2015). Further specific data was collected from companies and production plants and was incorporated in order to elaborate a comprehensive and robust model of a refinery.

Supporting documentation for the model underlying the ifeu tool can be found in the ecoinvent report on the petroleum refinery industry for the SRI project, by Fehrenbach et al. (2018).

European Commission (2015) Best Available Techniques (BAT) Reference Document (BREF) for the Refining of Mineral Oil and Gas, Industrial Emissions Directive 2010/75/EU Integrated Pollution Prevention and control, accessible online at http://eippcb.jrc.ec.europa.eu/reference/BREF/REF_BREF_2015.pdf, February 2019

Refinery complexity: The 2018 World Refining Survey (OGJ, 2018) reports the configuration of 107 refineries in Europe. According to their configuration each refinery was assigned a refinery type (I-IV) as defined in the BREF document. Weighted by the annual throughput volume, 62% of European refineries classify as type II, 29% as type II and 9% as type IV.

The simplified LCI tool can be adjusted to average conditions of a specific geography through the following parameters: refinery complexity (according to the complexity classes defined in the BREF document, type I-IV), crude oil sulfur content and American Petroleum Institute (API) gravity classification. To create this dataset, the above parameters were set to represent the average situation in Europe without Switzerland:

This dataset describes the operation of a representative average petroleum oil refinery in the given geography. Since petroleum refineries are very complex the actual unit process modeling is done in a separate refinery tool, developed by ifeu (Institute for Energy and Environmental Research, Heidelberg, Germany) and this is a subdivided product-specific dataset.

ENI (2018) World Oil Review 2018, Volume 1, online at https://www.eni.com/docs/it_IT/eni-com/azienda/fuel-cafe/WORLD-OIL-REVIEW-2018-Volume-1.pdf, last accessed March 2019.

Geography: Global model calibrated with geography-specific information.

Technology: The technology level in Europe applied here represents a weighted average of BREF types II (62%), III (29%), IV (9%) refineries; API 35; sulfur content 1.03%.

wastewater, average

Activity:

treatment of wastewater, average, capacity 1E9l/year | cut-off

Geography:

Europe without Switzerland

Description:

Wastewater purified in a smaller municipal wastewater treatment plant (capacity class 4), with an average capacity size of 5320 per-captia-equivalents PCE.

Wastewater contains (in kg/m3): COD: 0.1556 (GSD=122.5%); BOD: 0.1036 (GSD=122.5%); DOC: 0.04575 (GSD=122.5%); TOC: 0.0673 (GSD=122.5%); SO4-S: 0.044 (GSD=122.5%); S part.: 0.002 (GSD=122.5%); NH4-N: 0.01495 (GSD=122.5%); NO3-N: 0.00105 (GSD=122.5%); NO2-N: 0.0004 (GSD=122.5%); N part.: 0.003279 (GSD=122.5%); N org. solv.: 0.008392 (GSD=122.5%); PO4-P: 0.002459 (GSD=122.5%); P part.: 0.0006147 (GSD=122.5%); Cl: 0.03003 (GSD=224.1%); F: 0.00003277 (GSD=224.1%); As: 0.0000009 (GSD=224.1%); Cd: 0.0000002806 (GSD=223.8%); Co: 0.000001618 (GSD=223.8%); Cr: 0.00001223 (GSD=223.8%); Cu: 0.00003744 (GSD=223.8%); Hg: 0.0000002 (GSD=223.8%); Mn: 0.000053 (GSD=224.1%); Mo: 0.0000009574 (GSD=223.8%); Ni: 0.000006589 (GSD=223.8%); Pb: 0.000008631 (GSD=223.8%); Sn: 0.0000034 (GSD=224.1%); Zn: 0.0001094 (GSD=223.8%); Si: 0.003126 (GSD=224.1%); Fe: 0.007093 (GSD=224.1%); Ca: 0.05083 (GSD=224.1%); Al: 0.001038 (GSD=224.1%); K: 0.0003989 (GSD=224.1%); Mg: 0.005707 (GSD=224.1%); Na: 0.002186 (GSD=224.1%);

Geography: Specific to the technology mix encountered in Switzerland in 2000. Well applicable to modern treatment practices in Europe, North America or Japan.

Technology: Three stage wastewater treatment (mechanical, biological, chemical) including sludge digestion (fermentation) according to the average technology in Switzerland