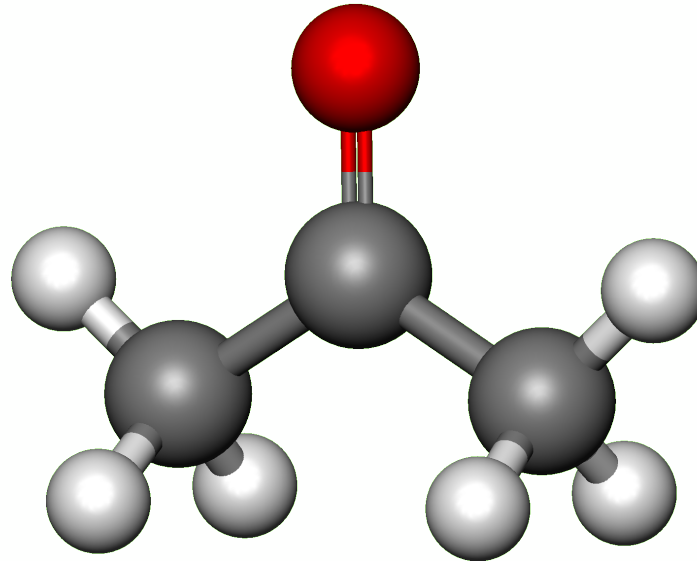




CHALMERS
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Life Cycle Assessment of acetone production from captured carbon dioxide

Using bio-fermentation at the PYROCO₂-pilot plant

Master's thesis in Industrial Ecology

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CHALMERS UNIVERSITY OF TECHNOLOGY
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Erik Jiresten
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Cover: Schematic illustration of an acetone molecule.

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Abstract

Due to its need of carbon feedstocks, the chemical industry is expected to become the major driver of oil consumption in the future, with its greenhouse gas emissions increasing annually. The PYROCO₂-project aims to reduce the industry's dependency on fossil resources, moving it in a direction of increased sustainability.

At the time of writing, the PYROCO₂-project is still in early development where the design process for a pilot plant, eventually to be constructed south of Oslo, Norway, is underway. The project aims to produce acetone via two fermentation processes, using captured carbon dioxide and hydrogen gas, produced through electrolysis, powered by renewable electricity. The aim of this thesis is to investigate how the future pilot-plant will perform regarding environmental impacts by applying life cycle assessment. This was further analysed using sensitivity scenarios, to verify the hotspots for environmental impacts within the production system. This provides providing important knowledge for the planned future construction of similar plants at other locations.

The environmental impact hotspots, identified for the pilot plant were the capture, purification and liquefaction of carbon dioxide, and the electrolysis, which performance is highly dependent on the electricity mix used. This was confirmed by the sensitivity analysis, using German electricity, as opposed to Norwegian. In terms of climate change, the PYROCO₂-pilot plant outperforms conventional acetone production considerably, potentially acting as a negative emissions technology. The impacts on toxicity was shown to be higher for the PYROCO₂-pilot plant. However, these are connected to metal use for the expansion of the electricity grid, where previous life cycle assessments have shown that embodied emissions for electricity transmission and distribution are negligible.

Keywords: Life Cycle Assessment, PYROCO₂, Acetone, Chemical Production, Fermentation, Carbon Capture and Utilisation, Negative Emission Technology, openLCA.

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Erik Jiresten & Oskar Larsson, Gothenburg, June 2022

List of Acronyms

1,4-DCB	1,4-Dichlorobenzene.
AC	Acidification.
AD-ER	Abiotic Energy Resources Depletion.
AD-MR	Abiotic Material Resources Depletion.
AD-R	Abiotic Resource Depletion.
AP	Acidification Potential.
ATP	Adenosine Triphosphate.
CC	Climate Change.
CC-CCA	Climate Change with Attributed Carbon Capture.
CCS	Carbon Capture and Storage.
CCU	Carbon Capture and Utilisation.
CCUS	Carbon Capture Utilisation and Storage.
CFC	Chlorofluorocarbon.
EOL	End-of-Life.
ET	Ecotoxicity.
ET-FW	Freshwater Ecotoxicity.
ET-MA	Marine Aquatic Ecotoxicity.
ET-T	Terrestrial Ecotoxicity.
EU	European Union.
F.U.	Functional Unit.
F1	Fermentation 1.
F2	Fermentation 2.
GHG	Greenhouse Gas.
GWP	Global Warming Potential.
HIP	Herøya Industrial Park.
HT	Human Toxicity.
IEA	International Energy Agency.

IPCC	International Panel on Climate Change.
ISO	International Organization for Standardization.
LCA	Life Cycle Assessment.
LCI	Life Cycle Inventory Analysis.
LCIA	Life Cycle Impact Assessment.
MEA	Monoethanolamine.
MMA	Methyl Methacrylate.
NET	Negative Emission Technology.
NMVOC	Non-Methane Volatile Organic Compound.
NO _x	Nitrogen Oxides.
PEM	Polymer Electrolyte Membrane.
PMMA	Polymethyl Methacrylate.
POF	Photochemical Oxidant Formation.
POFP	Photochemical Oxidant Formation Potential.
R.F.	Reference Flow.
RER	Region Europe.
SMR	Steam Methane Reforming.
SO _x	Sulphur Oxides.
STY	Space-Time- Yield.
TMP _{max}	Trans-membrane Maximum Pressure.
WLP	Wood-Ljungdahl pathway.

Nomenclature

Chemicals

Br Bromine

C₂H₄ Ethylene

CH₃COCH₃ Acetone

CH₃COO⁻ Acetate

CH₃COOH Acetic Acid

CH₄ Methane

Cl₂ Chlorine Gas

Cl Chlorine

CO₂ Carbon Dioxide

CO Carbon Monoxide

C Carbon

H⁺ Proton

H₂O Water

H₂ Hydrogen Gas

HCl Hydrogen Chloride

H Hydrogen

NaOH Sodium Hydroxide

Na Sodium

NH₃ Ammonia

NH₄⁺ Ammonium

Ni Nickel

NO Nitrogen Oxide

N Nitrogen

O₂ Oxygen Gas

O Oxygen

Sb Antimony

SO₂ Sulphur Dioxide

S Sulphur

Physical Quantities

ΔH_f Heat of Formation

ΔH_{vap} Heat of Vaporisation

A Area

C_P Specific Heat Capacity

k Heat Transfer Coefficient

M Molar Mass

m Mass

n Mole

q Mass Flow

T Temperature

V Volume

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1

Introduction

The global temperature has been on the rise for the last century, due to increasing concentration of Greenhouse Gases (GHGs) in the atmosphere. The world has decided to reach net zero emissions of GHGs by 2050, through the Paris Agreement and by that keeping the global temperature rise to 1.5 °C [1]. Regardless of the goals to reach net zero emissions and the ever-growing number of countries joining the agreement, the emissions of GHGs are still rising. There is a need for action, in order to go from political rhetoric to practice, to reach the net zero emission target.

The direct carbon dioxide gas (CO₂) emissions from primary chemical production have also increased annually by an average of 2.1% since 2015 and the petrochemical industry is expected to become the largest driver of global oil consumption in the future, due to its need of carbon feedstocks [2][3]. As part of the PYROCO₂-project, this thesis will explore one potential solution for reducing the CO₂-emissions from fertiliser and chemical industries. The aim of PYROCO₂ is not only to reduce the emissions from fertiliser production, but also to create industrial symbiosis with the chemical industry and by that reducing the emissions further [4].

In order to achieve the zero emissions goal by 2050, new technologies that are climate-positive and climate-neutral need to be implemented, reducing GHG-emissions to the atmosphere. PYROCO₂ is a project where carbon capture technologies are combined with chemical production and aims to become a representative for Carbon Capture and Utilisation (CCU) hubs around the world, where CO₂ is captured from one process and used as input to other industrial processes [4].

According to the International Panel on Climate Change (IPCC) scenarios to reach a maximum of 1.5°C global warming, almost all scenarios utilise carbon capture technologies; not using Carbon Capture Utilisation and Storage (CCUS) and CCU significantly raises the cost of reaching the goals of the Paris Agreement [5]. Generally, CCUS is considered more feasible for carbon capture from industrial processes, compared to energy generation. This is especially true for industries that have inherent process emissions, such as certain chemical production [6]. CCU currently has limited potential for keeping the global warming below 1.5°C, due to the lack of ability use of CO₂ with current technologies. However, IPCC has identified the use of CO₂ for production of carbon materials with a long life-time, such as plastics, as a development to make the techniques more feasible. International Energy Agency (IEA) predicts 7.6 Gt CO₂ to be captured annually by 2050 and emphasise the importance of CCU for the chemical industry, especially with regards to the need for carbon feedstock, aligning well with the ambitions with the PYROCO₂-project [1].

1.1 PYROCO₂-project

Acetone is an important chemical intermediate and solvent, with a global production of 6.85 Mt in 2021 [7][8]. Its largest application is in the synthesis of Methyl Methacrylate (MMA), used to produce Polymethyl Methacrylate (PMMA) (acrylic glass) [7][9]. It is also used as an intermediate in production of bisphenol A, diacetone alcohol, and other products [7].

Today, the vast majority of acetone is produced via 2-propanol dehydrogenation, the oxidation of cumene to phenol and acetone (Hock-process), and propene oxidation [7]. As acetone production is almost exclusively based on fossil feedstock, the chemical is of interest for investigation of potential new production processes, to decarbonise chemical production [10].

The PYROCO₂-project is an European Union (EU) based project, financed by the EU's Horizon 2020 research and innovation programme, via "The European Green Deal" [11]. The core in the project is to develop of a thermophilic microbial bioprocess, to produce acetone. In a two-step fermentation, bacteria will be fed with gaseous feedstock: 1) CO₂, captured from fertiliser production and originating from the use of Steam Methane Reforming (SMR), 2) hydrogen gas (H₂), and 3) oxygen gas (O₂); H₂ and O₂ being derived from renewable electricity through electrolysis.

The aim is to demonstrate the feasibility of CCU for bulk chemical production, by reaching a yearly production of at least 4000 tonnes of climate-positive acetone, at a pilot-plant in Herøya Industrial Park (HIP) in southern Norway. Part of the project is also to develop and implement efficient catalytic chemical industrial processes, for the production of valuable chemical products, using the produced acetone as feedstock. Full-scale financial, regulatory and environmental assessments will be executed, to demonstrate the process as a viable future low-emission production method.

1.2 Aim

The aim of this thesis is to perform a preliminary cradle-to-gate Life Cycle Assessment (LCA) of the PYROCO₂ fermentation and chemical pilot-plant, demonstrating production of acetone from captured CO₂ and green H₂ at HIP in southern Norway. The assessment will be used to identify environmental impact hotspots within the production, to compare environmental impacts of the production plant to those of conventional acetone production, and to evaluate the plants sensitivity to changes in foreground- and background systems. This initial assessment will be further built on and evaluated during the continuation of the PYROCO₂-project.

This report aims to answer the following questions:

1. How well does the PYROCO₂-pilot plant perform, compared to conventional acetone production, in terms of environmental impacts?
2. Where do the environmental impact hotspots for acetone production, through the PYROCO₂-production system, occur?
3. How do foreground- and background systems affect the environmental performance of the PYROCO₂-pilot plant?

2

Background

In this chapter, a short description of the technologies, used in this project, will be presented; also, the guidelines and definition used to conduct an Life Cycle Assessment (LCA)-study.

2.1 Carbon Capture Utilisation and Storage

CCUS are technologies to capture CO₂ from stationary sources, such as industrial processes or the atmosphere, and subsequently distribute it for intermediate utilisation or final storage [12]. While Carbon Capture and Storage (CCS) offers potential reduction of GHG-emissions, as captured CO₂ is stored long-term, CCU instead has the potential of displacing the need for CO₂, extracted from natural resources; to create low-carbon products or intermediates, e.g. through chemical- or biological processes, such as in the PYROCO₂-project [13]. CCUS applications have been identified to play a crucial role in limiting the global warming to 1.5°C, as stated in the Paris Agreement, especially for industries with inherent process emissions, as these processes cannot otherwise reach net zero carbon emissions with current technologies [5][6].

Liquified CO₂ for commercial applications is almost exclusively captured as a by-product from industrial processes [14]. The concentration of CO₂ in flue gases and whether a diluted feedstock can be used, as opposed to pure CO₂-streams, have been identified as important aspects [15]. This is due to the energy intensity of CO₂-recovery processes. For this reason, access to low-cost and low-emission electrical energy sources are of high importance for the potential to reduce overall GHG-emissions, when using CCUS [6]. For CCS-applications, the CO₂ typically needs to be concentrated to >85% [16].

Today, chemical absorption by Monoethanolamine (MEA) is the most common technique, for capture and recovery of CO₂ from industrial flue gas [15]. However, there are also other techniques available, such as the cryogenic process and membrane separation. There is no "one-size-fits-all-technology", as each technique has different compatibility depending on the industrial application: 1) cryogenic CO₂-separation requires no chemical absorbents but is highly energy intensive, 2) membrane separation of CO₂, from biogas, produces a purified stream of methane but has a lower CO₂-removal rate, 3) chemical absorption with MEA is less energy-intensive, but generally only economically viable for industries with readily available recoverable heat [15][17].

2.2 Electrolysis

Electrolysis of water (H_2O) can be used to produce H_2 , and O_2 as a by-product. H_2 is valued for its future potential uses; an energy carrier, fuel for vehicles, as storage for power generation and use in chemical and industrial processes [18]. Electrolysis is conducted in an electrolyser, using an anode (positively charged) in one cell, and a cathode (negatively charged) in the other. The two nodes are separated by a membrane, see Figure 2.1. There are several types of electrolysis systems and in the PYROCO₂-project, Polymer Electrolyte Membrane (PEM) electrolysis will be used.

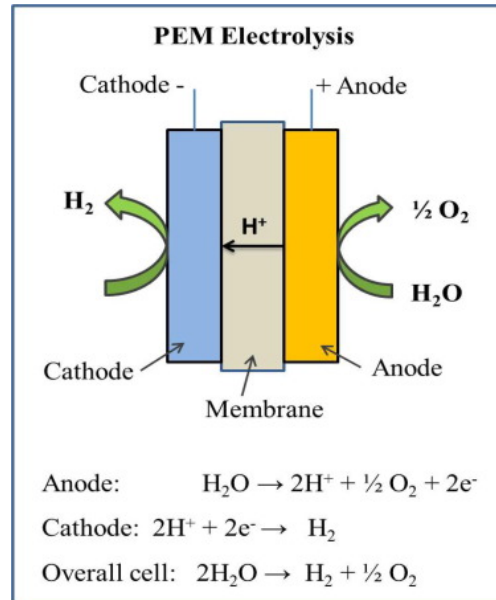
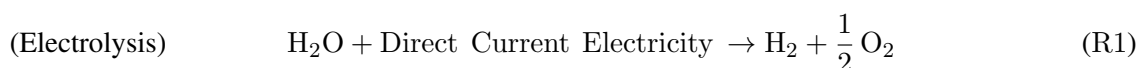


Figure 2.1: Conceptual process of Polymer Electrolyte Membrane (PEM) electrolysis, where H_2 and O_2 is produced from water and electricity, from [19].

The major benefit of producing H_2 from electrolysis, as opposed to from fossil feedstocks, is the potentially low GHG-emissions in the production phase; the only needed inputs being water and electricity, see Reaction R1. This makes O_2 the only direct emission from the production phase, which can potentially also be collected and used; hence, there are no direct emissions of GHGs. The GHG-emissions attributed to the use of electrolysis would instead be from the manufacturing of electrolysers, and generation of electricity, used in the the production process. When produced via electrolysis using renewable energy, the term *green H₂* is often used [18]. In order to access the full potential of green H_2 , the use of clean and renewable energy is critical. Currently, electrolysis for H_2 -production is not widely applicable, due to the lack of renewable electricity; hence, most of the current H_2 -production is based on fossil sources [18]. If green H_2 would replace all fossil-based H_2 , GHG-emissions could be reduced with the equivalent of the United Kingdom and Indonesia combined emissions, showing the potential environmental benefits of the technology [18].



The production system for electrolysis can be split into the following three steps: 1) *plant manufacturing and installation*, 2) *plant operation*, and 3) *storage and delivery of the hydrogen* [20]. When looking at the life cycle perspective of these steps, the operating phase is where the majority of environmental impacts occur; hence, the manufacturing and installation has negligible impact [20]. For operation, the energy-intensive production process causes the main environmental impacts, largely dependent on the energy-mix. Therefore, if the energy-mix is fully powered by renewable energy sources, the overall environmental impacts can be reduced significantly.

2.3 Thermophilic fermentation

The PYROCO₂-process will use a two-step thermophilic fermentation process. In Fermentation 1 (F1), acetic acid (CH₃COOH) is produced, which is then consumed in Fermentation 2 (F2), to produce acetone (CH₃COCH₃). Both fermentations use bacteria developed by project partners. F1 is sustained by inputs of feed media, see C.1 in Appendix C, CO₂, H₂ and NH₃. F2 is sustained by NH₃, O₂, and input of broth from F1.

The production of acetic acid is performed by thermophilic acetogen bacteria, via the catabolic (energy generation and product formation) Wood-Ljungdahl pathway (WLP), see Reaction R2 [21].



Reaction R3 shows the anabolic (biomass growth) pathway, for thermophilic acetogen [22].



Reaction R4 shows the Adenosine Triphosphate (ATP)-balanced (energy-balanced) reaction for thermophilic acetogen, including biomass growth [22].



In F2, the production of acetone is performed by aerobic thermophilic bacteria, via Reaction R5 [22]. F2 will operate at 60 °C, easing the separating of the acetone gas from the broth, as acetone boils at 56 °C, making the thermophilic bacteria a good match for acetone production.



Reaction R6 shows the anabolic (biomass growth) reaction for the aerobic thermophile [22].



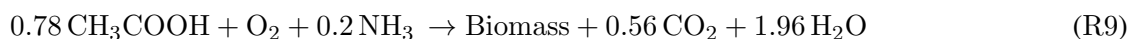
Reaction R7 shows the catabolic (energy generating) reaction for the aerobic thermophile [22].



As the product formation for the aerobic thermophile is ATP-negative, see Reaction R5, the reactions for biomass growth and product formation need to be decoupled and balanced using the catabolic pathway, see Reaction R7. Reaction R8 shows the ATP-balanced (energy-balanced) reaction for acetone production, using the aerobic thermophile [22].



Reaction R9 shows the ATP-balanced (energy-balanced) reaction for the biomass growth of the aerobic thermophile [22].



2.4 Life Cycle Assessment Framework

LCA is used to evaluate a product's environmental impact, the potential impacts related to the product and to interpret these impacts [23]. An LCA-study can be divided into the following four phases: *Goal and scope definition*, *Inventory analysis*, *Impact assessment* and *Interpretation*, visualised in Figure 2.2 [23]. This framework is based on the International Organization for Standardization (ISO) standard for LCA, ISO 14040. An LCA does not only include the resources put into the system, but also production processes and the End-of-Life (EOL) journey of the product. The interpretations of this assessment could then be used by the target audience, e.g. the manufacturer or policy makers, to identify and implement improvements for production processes and policies for the targeted system [23].

2.4.1 Goal and Scope Definition

In the goal and scope phase of the assessment, the purpose of the study is defined, in accordance to the ISO 14040 standard [23]. Further, the intended audience, application of the study, and background to why the study is conducted, are identified. LCA-studies are iterative processes. The F.U. is also defined, in accordance with the function of the product.

The system boundaries of the production system are set, including time horizon, geographical- and technical system boundaries [23]. Under the goal and scope definition, the environmental impacts

intended to be used to evaluate the product should be defined and described. The data quality requirements, whether site-specific or average data will be used, are also considered during this phase.

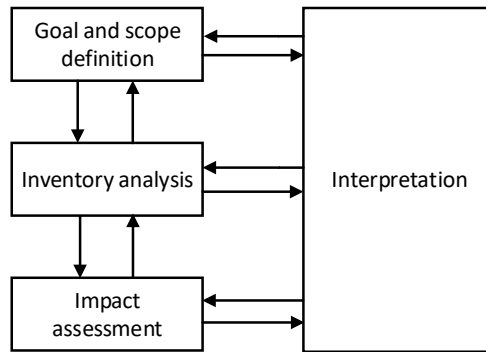


Figure 2.2: Life Cycle Assessment (LCA) framework from [23].

2.4.2 Inventory Analysis

The Life Cycle Inventory Analysis (LCI) phase of the assessment is based on the goal and scope definition and its purpose is to construct a system following the requirements stated in the goal and scope [23]. This is used to build up a system, with system boundaries and a more detailed description of the technical system and its processes.

The intended production system should be visualised with a flowchart, showing the processes included in the assessment (e.g. transportation, processes, use and waste management) [23]. In this section, data collection is performed and presented, including input- and output data for the activities within the system, showing the emissions from each process. These values should be normalised and scaled to the Reference Flow (R.F.) or F.U. used in the assessment.

2.4.3 Impact Assessment

The purpose of the Life Cycle Impact Assessment (LCIA) is to quantify the environmental impacts from the process data, presented in the inventory analysis [23]. This translation is done through *classification*, describing the environmental impact a certain emission will have, by aggregating emissions to e.g. impacts on climate change or acidification. After classification, a *characterisation* is performed, calculating the resource use and emissions via characterisation factors, connecting it to the environmental impacts chosen for assessment within the project [23]. The classification and characterisation can be performed using different life cycle impact methods.

2.4.4 Interpretation

Depending on the size and complexity of the system examined, the inventory results may contain hundreds of result parameters. In order to interpret and present conclusions, these results need to be refined. This process may differ depending on the intended use and audience of the study; for

example, it could consist of presenting the most relevant inventory flows, aggregated characterisation results, or the impacts could be weighted and aggregated further into a single number, that could be used to compare alternatives [23].

As LCAs often give unexpected results, the interpretation of results is an important part of the iterative process. For example, reformulation of the goal and scope may be needed, depending on preliminary results [23]. Depending on the goal and scope of the study, different results may be presented. These could include impact hotspots, comparative impacts, absolute impacts, different scenarios, sensitivity analysis and more.

2.5 Previous LCA Studies

The PYROCO₂ production process is new of its kind; hence, no previous LCA-studies have been conducted on the process. However, studies have been performed on systems that are part of the production processes, as well as novel technologies used, such as CCU.

LCAs of CCU have shown that impacts on Global Warming Potential (GWP) has a high variability, depending on application [17]. For production of chemicals, specifically dimethylcarbonate, application of CCU has been shown to reduce the GWP by 4.3 times and ozone layer depletion by 13 times, compared to conventional production. An LCA on application of carbon capture technologies on power-production has shown that the use of MEA carbon capture technology has the highest environmental impacts, compared to other capturing technologies [24]. However, the application of carbon capture significantly reduced the production's GWP, and the MEA-process has a lower electric energy use than membrane separation [17] [24]. Also, the MEA is a proven and commercially available technology; one of the main complications being the need for a large amount of heat, it is suitable for applications where excess industrial heat is readily available [17] [25].

One study performed a comparative LCA on H₂-production; comparing H₂-production from natural gas via SMR, and H₂-production with renewable energy, using electrolysis [26]. The results from the study indicate that the environmental performance of H₂ produced via electrolysis with energy from solar-, wind- or hydro power outperforms H₂ produced from natural gas via SMR. This is further supported by [27].

An LCA has shown the potential reduction of Climate Change (CC)-impacts for acetone and chemical production from using carbon waste streams together with fermentation processes; here, a process similar to the PYROCO₂-process was examined, where acetone is produced from fermentation processes with gene modified organisms [28]. According to this study, the production of acetone using these fermentation processes significantly reduces GHGs-emissions, compared to conventional acetone production; similar to the results of the PYROCO₂-pilot plant. Further, the study supports the attribution of the captured off-gases as a negative impact, hence making the acetone production act as a Negative Emission Technology (NET) [28].

An LCA on ethanol production, via fermentation of spruce wood chips, was used to argue for the negligible impacts of the electricity needed for stirring of the fermentation tanks [29]. Whether capital emissions should be included or not is dependent on their contributions to environmental

impact; if emissions are negligible they do not need to be included [30].

LCAs on environmental impacts from transmission and distribution of electricity conclude that the majority of emissions can be attributed to operational electrical losses, and that embodied impacts (impacts from construction and maintenance of the network) are insignificant, in comparison [31][32].

3

Method

Literature was studied throughout the thesis process, to get the needed understanding of the technical system processes and the corresponding application of data. As the thesis is centred around the LCA-process, the first step was to define the project, its goals and scope. Afterwards, data gathering, through literature studies and exploration of the ecoinvent data set was performed [33]. The gathered data was merged with data received from partners of the PYROCO₂-project, and flow- and heat calculations were performed. This data was entered into an LCA-software (openLCA); a virtual system was built, including processes and flows. Calculations of environmental impacts were then performed, using the system constructed in openLCA. The output of the environmental impact assessment was interpreted and discussed, to reach conclusions regarding the environmental performance of the system and its implications for the PYROCO₂-project and future applications.

As performing an LCA is an iterative process, goal and scope definitions, data gathering, system construction, impact assessment, analysis and interpretation of results were reevaluated and changed throughout this thesis project, depending on preliminary results and changes to the system. The system, its flows and processes, were also continually updated with the latest information from other project partners, as the planning of the pilot plant progressed within the PYROCO₂-project.

3.1 Goal and Scope

The goal of this study is to investigate and evaluate the environmental performance of the PYROCO₂-pilot plant, located at HIP. The study will look into acetone production via thermophilic fermentation, with captured CO₂ as part of the input resources. The assessment will provide and aggregate data for the PYROCO₂-project group and Chalmers University of Technology, in order to identify the hotspots and estimate the environmental impacts pilot plant. Hence, the intended audience of the assessment is the PYROCO₂-project group, academia, and companies related to the project.

3.2 System Description

In Figure 3.1, an aggregated flowchart, of the cradle-to-gate acetone production system, can be seen; the system boundary for this LCA is indicated by the black dashed box; the red dashed box represents the system boundary related to the PYROCO₂-project.

The first step is the inflow of deionised water, produced on site at HIP. The water is then split

into H_2 and O_2 via PEM-electrolysis, using Norwegian low-emission electricity, see Section F.1 in Appendix F. Subsequently, the H_2 is used in Fermentation 1 (F1), and the O_2 is used as input for Fermentation 2 (F2) and emitted to the atmosphere, due to overproduction. At HIP, the CO_2 is captured from industrial off-gas, from fertiliser production, and purified, liquefied, and transported by truck to the PYROCO₂-pilot plant, to be used as input to F1.

The first fermentation step, F1, will be using thermophilic acetogen bacteria to convert H_2 and CO_2 to acetic acid. This is subsequently used as input to F2, where it is converted to the final product, acetone, by aerobic thermophile bacteria. Both fermentation steps are operating at 60 °C, and heated by excess industrial waste heat, available from industrial processes at HIP.

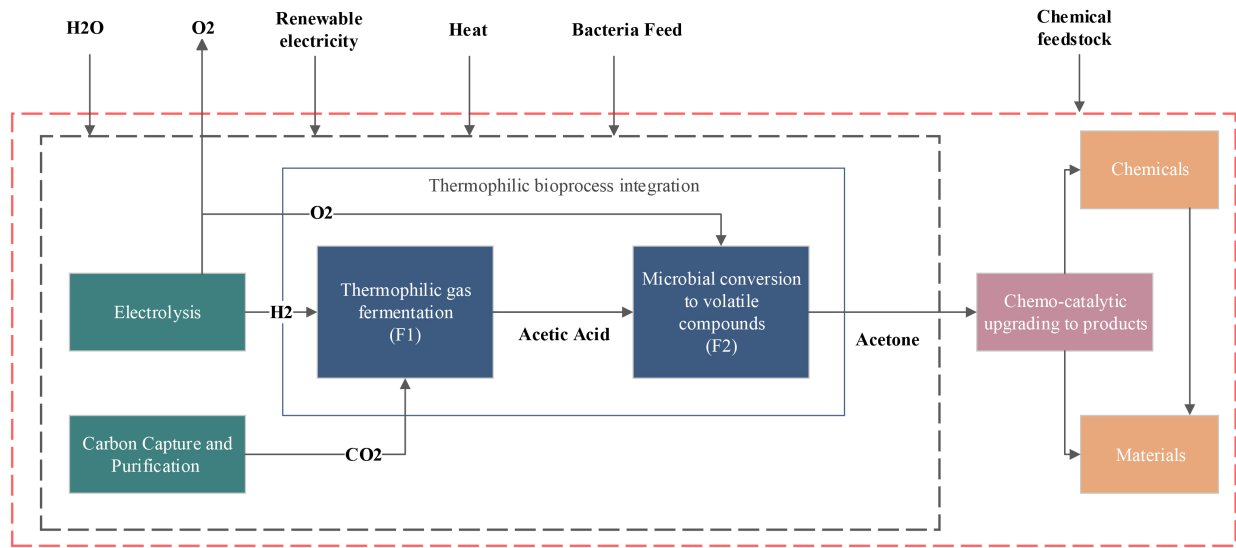


Figure 3.1: Initial flowchart, with the modelled system in this report highlighted in the black dashed box and entire PYROCO₂-process indicated by the red dashed box.

3.3 Functional Unit

The function of the studied system is to produce acetone via a two-step thermophilic fermentation, using captured CO_2 , and H_2 produced from electrolysis. Hence, the F.U. of this production system will be 4000 tonnes of acetone produced, with a R.F. of 500 kg of acetone; as the plant is set to produce 500kg of acetone per hour, and has an operating time of 8000 hours per year.

3.4 System Boundaries

In this section, the assessment's system boundaries will be presented. The system boundaries will be divided into geographical, technical and temporal boundaries.

3.4.1 Geographical System Boundaries

The geographical system boundaries for the acetone production will be limited to Norway and Germany, for background system data. Transportation will be using global, regional or local averages for emissions and type of transportation, depending on where the transportation takes place and how it is modelled in the ecoinvent processes used. For the comparative production of conventional acetone, European average was used. For other inputs to the production system: where available and appropriate, national averages were used; otherwise, European averages were used.

3.4.2 Technical System Boundaries

For the physical implementation of the PYROCO₂-process, a new production plant needs to be built. Hence, the environmental assessment will include impacts from capital emissions.

Personnel activities, such as commuting to and from the production plant, and emissions from employees building the plant, will not be included in the assessment. However transportation of process inputs for both construction and operations will be considered.

The capture and purification of CO₂ will be included in the production system; hence, capital emissions for the CO₂-production plant will be included. The production of membranes, used in the membrane purification processes, will be included; however, capital emissions are excluded for this process; the emissions from transportation of membranes is assumed to be negligible. Further refinement, use, and EOL of the produced acetone are not included.

3.4.3 Temporal System Boundaries

The temporal system boundary will be 20 year, a common assumption for the lifetime of a chemical production plant. The predicted yearly production capacity of the PYROCO₂-pilot is 4000 tonnes of acetone, with 18 800 tonnes of CO₂ captured annually.

3.5 Type of Life Cycle Assessment

In order to investigate the environmental impacts when applying CCU in the PYROCO₂-production system, an attributional cradle-to-gate LCA will be conducted. An attributional LCA was selected due to the large differences between the PYROCO₂-production process and the current conventional acetone production. The result from the attributional LCA will then be used comparatively against the conventional processes for acetone production, in order to evaluate its environmental performance. Further, a scenario analysis will be conducted, to evaluate the PYROCO₂-production's sensitivity to changes in foreground- and background systems, in terms of environmental performances; this being of special importance, as there are plans to implement the PYROCO₂-process at other production sites across Europe.

3.6 Impact Assessment Choices

The results of the study needs to provide enough information to shed light on the environmental performance of the PYROCO₂-project and to support effective decision making from the intended audience, regarding the project. The intended audience was assumed to have the required expertise to interpret environmental impacts and uncharacterised inventory data is often cumbersome to interpret. Consequently, the data, collected for the industrial system, was aggregated into mid-point categories. Further aggregation, weighting and evaluation will be the responsibility of the intended audience, such as other actors within the PYROCO₂-project, depending on the indented application.

The impact assessment method chosen, in openLCA, was *ei - CML v4.8 2016*. CML is a database with characterisation factors for LCIA, developed by Leiden University, Netherlands, and contains the most commonly used impact categories [34]. The chosen impact categories are presented in Table 3.1.

Table 3.1: Environmental and health impact categories chosen for evaluation.

Impact category	Abbreviation	Comment	Unit
Acidification	AC	Expressed relative to SO ₂ (European average, including fate).	kg SO ₂ -eq
Climate Change	CC	Expressed relative to CO ₂ , with a time horizon of 100 years (GWP100).	kg CO ₂ -eq
Freshwater Aquatic Ecotoxicity	ET-FW	Freshwater ecotoxicity on a global scale, for an infinite time horizon (FAETP inf.), relative to 1,4-dichlorobenzene.	kg 1,4-DCB
Abiotic Material Resources Depletion	AD-MR	Expressed relative to antimony (Sb) depletion (element, ultimate reserves).	kg Sb-eq
Human Toxicity	HT	Expressed in terms of human toxicity potential on a global scale, for an infinite time horizon (HTP inf.), relative to 1,4-dichlorobenzene.	kg 1,4-DCB
Photochemical Oxidant Formation	POF	Photochemical oxidation (high NO _x), relative to ethylene.	kg ethylene-eq

The most important for Acidification (AC) pollutants are Sulphur Oxides (SO_x), Nitrogen Oxides (NO_x), hydrogen chloride (HCl) and NH₃ [23]. Common for all acidifying pollutants are their ability to form H⁺-ions. Acidification can occur in many ways, one of which is the deposition of atmospheric pollutants through rain (acid rain). There are also many potential impacts, e.g. damaging forests and increasing freshwater fish mortality [23]. The Acidification Potential (AP) is commonly expressed using the reference unit *kg sulphur dioxide (SO₂) equivalents*. This reflects the maximum acidification a substance can cause, not taking into account areas' susceptibility for acidification [23][35].

The most important compounds for Climate Change (CC) include CO₂, methane (CH₄), Chlorofluorocarbons (CFCs) and NO_x. They all enhance the atmospheric radiative forcing by absorbing infrared radiation [23]. Impacts from CC have global ramifications, with broad impacts on ecosystems and human society, including climatic disturbance, desertification and rising sea levels [23][35]. The GWP is commonly expressed using the reference unit *kg CO₂ equivalents*, the radiative forcing potential of the gas compared to CO₂. Gases have different characterisation factors depending on their momentary radiative forcing potential and the time horizon used for calculations [23].

Toxicity is a complex impact category, due to the many types of pollutants and impacts; the toxic impacts of e.g. organic solvents, heavy metal and pesticides, all differ. Toxicity causes include carcinogens, mutagens, neurologically damaging substances and more. Due to the wide variety of sources, impacts and fates of emissions, toxicity is divided into Human Toxicity (HT) and Ecotoxicity (ET); where ET is further split into Freshwater Ecotoxicity (ET-FW), Marine Aquatic Ecotoxicity (ET-MA) and Terrestrial Ecotoxicity (ET-T) [23]. The toxicity is commonly expressed using the reference unit *kg 1,4-Dichlorobenzene (1,4-DCB) equivalents* [35]. For CML 2016, the *USES-LCA* method is used to calculate characterisation factors, based on generic fate, exposure and effect analysis, using EUs toxicity model *EUSES*; a model including theories about dispersion between soil, air and water [23][35].

Abiotic Resource Depletion (AD-R) is used to show the impact on depletion of deposit [23]. There are a number of sub-categories, referring to the depletion of non-biological resources. These sub-categories include Abiotic Material Resources Depletion (AD-MR), depletion of metals, and Abiotic Energy Resources Depletion (AD-ER), depletion of fossil fuels [35]. The application of these categories is highly debated; some regard diminishing resource pools as an environmental problem and others as a societal problem, making it outside the scope of LCAs [23]. Depending on the sub-category examined, the reference unit will differ; for AD-MR, *kg antimony (Sb) equivalents* is commonly used, reflecting the scarcity of the substance.

Photochemical Oxidant Formation (POF) measures the impact from pollutants that are formed in the lower atmosphere [35]. When substances such as carbon monoxide (CO), SO_x, nitrogen oxide (NO), ammonium (NH₄⁺) and Non-Methane Volatile Organic Compounds (NMVOCs) are exposed to sunlight, they cause formation of photochemical ozone [35]. Although ozone works protectively in the stratosphere, it is toxic in high concentrations, forming photochemical smog that causes irritation of respiratory systems and damage to vegetation [23][35]. POF is commonly expressed using the reference unit *kg ethylene (C₂H₄) equivalents* [35]. The Photochemical Oxidant Formation Potential (POFP) is calculated using a 5-day dispersion model of pollutants within Europe [23].

3.7 Data

The open-source software *openLCA* was used for the modelling of flows and processes, in order to calculate the environmental impacts of the defined system, see Section 3.2. For details about flow calculations, see Appendix A.

For processes used in the system, the *ecoinvent 3.8* database was used, see Chapter 4. The processes for inputs that were known to be produced locally at HIP (water treatment and CO₂-capture and purification), were modified to use Norwegian electricity, see Section 4.2.3 and 4.3. Industrial heat is available in excess at HIP. Therefore, an elementary flow without attributed impacts was used to model the inputs and outputs of heat, for processes within the system.

The requirements on data quality depend on areas of application and the availability of data. Generally, average data is to be used for the foreground system, where rough data for the production processes will be supplied by PYROCO₂-partners and calculated using flow analysis, and average data will be used for background systems, such as electricity mix.

For the background system, more specific data is preferable. For example, national and regional averages are preferred over global averages. This is especially important for the electricity mix, as energy intensive processes such as electrolysis is assumed to have a large overall contribution to the environmental impacts of the system. Background data, and data for auxiliary processes and products, will largely be retrieved from the *ecoinvent* data set [33].

The data used will also depend on the defined temporal boundaries of the project. As the production plant planned in the PYROCO₂-project is on a pilot-scale, and the project is only in the early stages of development, the implementation of a full-scale production plant will likely take more time than the time-frame for completing this assessment. Hence, data gathering will be a mixture of primary data, from project-partners, and secondary data, from literature and *ecoinvent*.

3.8 Limitations and Assumptions

At the time of this assessment, the PYROCO₂-project is in its early stages. Therefore, a major limiting factor, when modelling the impacts for the PYROCO₂-plant, is the availability of plant-specific- and experimental data; although, process step specific data is available from literature.

Major limitations and assumptions regarding data collection include: 1) an electrolyser model matching the criteria for the PYROCO₂-pilot plant was selected by the authors and may not match the final design, as this is yet to be defined in the project, see Section 4.2.2, 2) all heat needed for the pilot-plant is assumed to be industrial waste heat, if not otherwise mentioned, as excess heat is available at HIP, see Section 4.2.4, 3) heat losses are only estimated for the fermentation tanks, as systems such as piping and pumps are yet to be decided, see Appendix B, 4) no mass losses within system, e.g. due to leakage or maintenance, except for a liquid purge from F2 and biomass loss in purification, see Appendix A for mass balance calculations, 5) media feed is not fully modelled, as the defined media to be used is yet to be decided, and 6) transportation of locally produced inputs are not modelled, and average data from *ecoinvent* is used for other inputs.

4

Life Cycle Inventory Analysis

In this chapter, the inventory analysis will be presented together with assumptions and limitations used for the collected data. The processes and flows for inputs, and their corresponding impacts, were obtained from the *ecoinvent 3.8* database, if other sources are not mentioned. A detailed inventory for all flows can be found in Appendix A and process providers used for the modelling can be found in Appendix I.

4.1 General Description of Overall Flowchart

In Table 4.1, the total in- and outputs from the modelled production system of the PYROCO₂-pilot plant can be seen. These values are based on the R.F., representing one hour of production in a steady-state system.

Table 4.1: Total in- and output from the PYROCO₂-pilot plant modelled system for R.F.

Resource	Value	Unit
Input		
Heat	13518	MJ
Electricity	14898	kWh
CO ₂	2348	kg
Feed Media	2799	kg
NH ₃	54	kg
Membranes	0.14	items
Water, ultra pure	6000	kg
Water, deionised	3184	kg
Output		
Heat	20158	MJ
Acetone	500	kg
Water, purged	4875	kg
Acetone, purged	125	kg
O ₂	1993	kg

Figure 4.1 shows a detailed flowchart for the PYROCO₂-pilot plant model and its processes. The modelled process starts with water entering the electrolysis, producing H₂ and O₂; subsequently, the H₂ is used as input to F1. CO₂ is captured, purified, and liquefied, see Section 4.3, and used as input to F1. The bacteria media feed, see recipe in Section C.1 in Appendix C, is mixed and added to F1. In F1, all input resources are mixed together to produce acetic acid, see Section 4.5.1. After the fermentation, in F1, the broth mixture goes through a purification step, see Section 4.6, to remove the bacteria used in F1, avoiding contamination of F2. For full inventory data, see Appendix A.

In F2, the O₂, co-produced with H₂ in the electrolysis, is added together with the broth from F1 to produce the final product, acetone, see Section 4.5.2. Excess O₂ is released to the atmosphere. From F2, an hourly purge of 2% of the reactor volume is assumed to be needed¹. From F2, a flow of broth is recirculated back to F1, with another purification step in between, to avoid contamination of F1. Stripping gas, consisting of steam, acetone, O₂ and CO₂, is harvested from F2 and goes through a condensation process; here, liquid condensate, consisting of liquid acetone and water, is separated from the gas, see Section 4.7. From the condensation process, a subcooled gas stream, consisting of water, acetone and CO₂ is split; one stream is recirculated to F2, the other is deoxygenated and recirculated to F1. From the condenser, a third flow, consisting of liquid condensate is harvested; it is transported to the distillation step, where acetone is distilled to pure acetone and harvested, see Section 4.8. The water residue from the distillation is recirculated to F1.

4.2 Background System

In this section, the background systems will be explained in more detailed; the HIP, electricity mix, and what kind of water and industrial waste heat are accessible at the industrial plant.

4.2.1 Herøya Industrial Park

Located in Norway, southwest of Oslo, is the Herøya Industrial Park (HIP). At the site, the PYROCO₂ pilot-plant will be integrated with the current industrial park, accessing the Norwegian electrical grid, Section 4.2.2. The industrial park does also allow access to systems on site, such as the supply of water of varying degrees of purification, Section 4.2.3, excess industrial waste heat, Section 4.2.4. The CO₂ used in F1 is also produced, captured and purified at the industrial park, Section 4.3.

4.2.2 Electricity Mix

For all calculations regarding on-site processes of the pilot-plant (within the system boundaries in Figure 4.1), the Norwegian market for medium voltage electricity was used, *market for electricity, medium voltage | electricity, medium voltage | Cutoff, U - NO*. The mix consists of mostly renewable and nuclear energy generation (95%) with hydro-power being the dominating source of electricity (87%), see Appendix F for detailed electricity mix.

¹Based on communication with project partners.

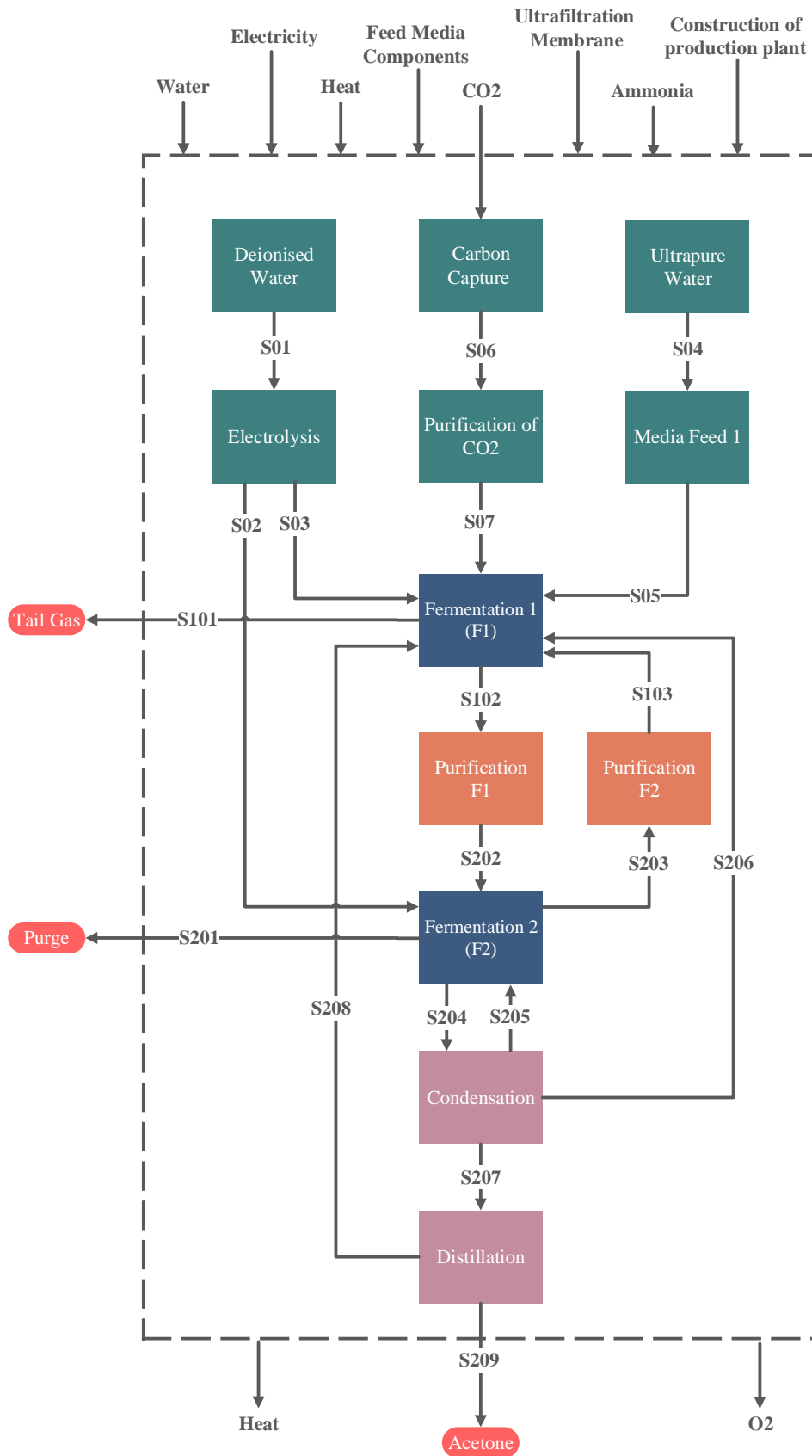


Figure 4.1: Detailed flowchart of the modelled PYROCO2-production process.

4.2.3 Water Purification

To estimate the on-site production of water, existing ecoinvent datasets were modified to better represent the production at HIP. For the production of deionised water, used for electrolysis, the process for deionised water production within Switzerland, *water production, deionised* | *water, deionised* | *Cutoff, U - CH*, was modified to use the Norwegian electricity mix, see Section 4.2.2. For the production of ultrapure (distilled) water, used within the fermentations, the process for ultrapure water production within Region Europe (RER), *water production, ultrapure* | *water, ultrapure* | *Cutoff, U - RER*, was modified to use the Norwegian electricity mix, see Section 4.2.2. The electricity mix for inputs to the water purification processes, such as *treatment of sewage sludge by anaerobic digestion* | *sewage sludge* | *Cutoff, U*, were also modified.

4.2.4 Excess Industrial Waste Heat

Industrial waste heat is available, in excess, from exothermic processes at HIP. An elementary flow without attributed impacts, *Energy, waste*, was used to model this in openLCA. See Appendix B for detailed calculations and heat data.

4.2.5 Capital Emissions for the PYROCO₂-pilot plant

To include the capital emissions for the PYROCO₂-pilot plant in the model, the process *ethanol fermentation plant* was used and modified to match the requirements for the PYROCO₂-pilot plant.

4.3 Carbon Capture

To estimate the CO₂ capture and purification of the industrial waste gas, containing CO₂, the process *carbon dioxide production, liquid* | *carbon dioxide, liquid* | *Cutoff, U* was used, henceforth known as CO₂-production. This process was deemed to be a good estimation for the process at HIP; the data set includes industrial waste gas produced through SMR for NH₃ production, captured and purified using MEA, the same processes used at HIP. Capital emissions from the construction of the purification plant are also included. However, the process includes methane emissions from the industrial gas, which should not be attributed to the PYROCO₂-process, see Section 5.1.1 for results and further discussion. The process was modified, to better fit the system at HIP; the electricity mix was changed to Norwegian, see Section 4.2.2, and industrial heat was changed to the elementary flow, without environmental impacts, described in Section 4.2.4.

4.4 Electrolysis

The electrolysis used by the PYROCO₂-project will be a PEM electrolysis, manufactured by NEL hydrogen. Due to the early process of the project, the dimensions for the electrolysis is not yet set and the model M2000 was chosen to simulate the electrolysis production and provide an overview of the water and electricity consumption needed [36]. The electricity need for producing H₂ via PEM electrolysis is 50 kWh per kg of H₂, and the water consumption is about 11 kg of water per kg of H₂. See Appendix A for full inventory data.

4.5 Thermophilic Fermentation

The thermophilic fermentation is divided into two continuous fermentations, F1 and F2, using thermophilic acetogen and aerobic thermophile bacteria strains, respectively. The F1 and F2 fermentations are connected to each other via a purification process. Due to uncertainties regarding what type of purification will be used in the PYROCO₂-pilot plant, this assessment models the purification using membrane filtration, see Section 4.6. Due to negligible impacts from electricity use for stirring, this is not included in the model [29].

4.5.1 Fermentation 1

In this model, the first fermentation, F1, will have a reactor volume of 943 m³. It will operate at a temperature of 60 °C and a pressure of 10 bar. The pH will be kept between 6.0 and 6.7, due to the early stage of the PYROCO₂-project, the pH stabilisation will not be included in this assessment. The cell density was assumed to be 20 g cDW per litre of reactor volume with a Space-Time-Yield (STY) of 2 g acetic acid/L.h and an acetic acid (product) concentration of 40 g/L. The fermentation process in F1 is exothermic and produces an excess of 5 000 MJ heat per R.F., which leaves the modelled system. For metabolic pathways used in this fermentation, see Section 2.3. The biomass need 36 kg of NH₃, per R.F., to sustain growth in the fermentation process, it is modelled using the process *ammonia, anhydrous, liquid* from ecoinvent. The full inventory data and calculations can be seen in Appendix A, and the heat data and calculations can be seen in Appendix B.

4.5.2 Fermentation 2

In this model, the second fermentation, F2, will have a reactor volume of 250 m³. It will operate at a temperature around 60 °C and a pressure of 10 bar. The pH will be kept between 6 and 7, due to the early stage of the PYROCO₂-project, the pH stabilisation will not be included in this assessment. The cell density was assumed to be 20 g cDW per litre of reactor volume with a STY of 2.5 g acetone/L.h and an acetone (product) concentration of 25 g/L. F2 was assumed to have a purge out of the system corresponding to 2 % of the reactor volume, resulting in 5000 L/h of purge. The fermentation process taking place in F2 need about 12 000 MJ of heat per R.F., provided by the excess heat at HIP, see Section 4.2.4. For metabolic pathways used in F2, see Section 2.3. The biomass need 18 kg of NH₃, per R.F. to sustain growth in the fermentation process, it is modelled using the process *ammonia, anhydrous, liquid* from ecoinvent. The full inventory data and calculations can be seen in Appendix A, and the heat data and calculations can be seen in Appendix B.

4.6 Broth Purification

In the PYROCO₂-production process, cell retention will be used to purify the stream between F1 and F2. As the PYROCO₂-pilot plant is still under development, the purification was modelled using membrane filtration. The data was collected from a previous LCA of membrane filtration [37] and modified to match the PYROCO₂-pilot plant; all electricity use was changed to Norwegian

electricity. The Trans-membrane Maximum Pressure (TMP_{max}) was chosen to be 20 kPa and the flux was assumed to be 10 L/m²h.

A model for the manufacturing of a membranes was built and the full inventory analysis for membrane production can be seen in Appendix D. In the membrane filtration LCA-report, different scenarios of how often cleaning is needed were examined. As the PYROCO₂-pilot plant is still in the early stages of development and the purification process has not yet been fully defined, the cleaning process was excluded. For the full inventory of the purification process, see Appendix A.1.

4.7 Condensation

Condensation was used to remove a mixture of acetone and water from the stripping gas, output from F2. The stripping gas inflow will contain 0.1055 g water and 0.0462 g acetone per g CO₂ and the condensate will consist of 76.9 g acetone/L of condensate. As only part of the acetone in the stripping gas will be condensed, the rest of the stripping gas will be recirculated to the fermentors, with the vast majority going back to F2. The recirculating flow contains 0.0059 g water and 0.0379 g acetone per g CO₂. The acetone and water loads were calculated by project partners, using the Aspen modelling software.

The condensation process will use cooling water at 5 °C, resulting in coolant outflow temperature of 12 °C. The excess heat will, partly, be used to heat up and evaporate liquid CO₂. The rest of the excess heat was removed through the use of water from a nearby lake (usually between 5-7 °C). Approximately 15 000 MJ of heat per R.F. is output from the process. For heat calculations see Appendix B and for full inventory data, see Appendix A.

4.8 Distillation of Acetone

The distillation process separates water from the acetone product and is assumed to work at the boiling point of acetone (56°C). The product outflow is assumed to contain 100% pure acetone and the separated water is recycled to F1. The process needs approximately 1 300 MJ of heat per R.F. For full heat calculations and data, see Appendix B.

4.9 Conventional Acetone Production

To evaluate how the PYROCO₂-production process performs, in terms of environmental impacts, compared to conventional acetone production, theecoinvent process *market for acetone, liquid | acetone, liquid | Cutoff, U - RER* was used in openLCA. The process includes different acetone production processes and ratios between them, based on total production. In turn, these acetone production processes include resources, and their production processes, e.g. fossil carbon feedstock, electricity, heat, chemicals, metals etc., as well as process emissions. Impact assessment results from production via this process was compared to the PYROCO₂-process.

4.10 Sensitivity Analysis

In order to investigate the system's sensitivity to changes, a sensitivity analysis was performed which is presented in this section. Several different scenarios were constructed to analyse the sensitivity of the resulting environmental impacts of the system. The scenarios include changing the electricity mix, whether industrial waste heat is available in excess or needs to be produced, and the effect of using fossil H₂, as opposed to electrolysis.

4.10.1 German Electricity Mix

The Norwegian electricity mix, see Section 4.2.2, is to a large extent based on renewable energy sources and hence has low emissions of GHGs. The low emissions from the Norwegian electricity mix combined with the use of electrolysis for H₂ production makes it interesting to look at how this system would perform in a more carbon intensive electricity mix.

According to the grant agreement and project partners, Germany is one potential future candidate for implementation of another PYROCO₂-production plant, similar to the one in Norway. An evaluation on the environmental performance of the product system using a German electricity mix is therefore of interest. As the German electricity mix is largely fossil-based, see Appendix F, this would further show how dependent the production process is on the choice of electricity source. For this scenario *market for electricity, medium voltage | electricity, medium voltage | Cutoff, U - DE* was used as the provider of electricity, in openLCA.

4.10.2 No Excess Heat

There is a needed heat input into the production system, mainly due to the use of thermophilic bacteria in F1 and F2. In HIP, industrial waste heat is readily available. However, this may not be the case for other production sites and it would therefore be interesting to see how the system responds to the need of industrial heat production. In this scenario, the total heat input needed for processes were divided between *market for heat, district or industrial, natural gas | heat, district or industrial, natural gas | Cutoff, U - Europe without Switzerland* and *market for heat, district or industrial, other than natural gas | heat, district or industrial, other than natural gas | Cutoff, U - Europe without Switzerland*, using 35.42% from natural gas and the rest from other sources [38].

4.10.3 No PEM Electrolysis

The PYROCO₂-pilot plant in Norway uses low-carbon H₂, from electrolysis. However, as the majority of H₂ produced in the world is fossil-based, it would be interesting to evaluate the environmental performance when using the European H₂-market. In openLCA, *market for hydrogen, liquid | hydrogen, liquid | Cutoff, U* was used to simulate the environmental impact for the H₂-production. The electrolysis also produces O₂; hence, O₂-production needs to be added as input to the production system. For this, *market for oxygen, liquid | oxygen, liquid | Cutoff, U - RER* was used as input to F2.

4.10.4 Reduced Purge in Fermentation 2

The current model of the PYROCO₂-pilot plant includes a liquid purge from F2, leaving the system. The hourly purge is assumed to be 2 % of the reactor volume, in this case 5000 kg/h, and this flow is assumed to contain 125 kg of acetone, constituting 20% of the total acetone production. Therefore, another model was evaluated regarding environmental impacts; here, the same purge only contains 12.5 kg of acetone, hence increasing the yield of acetone in F2, reducing the need of inputs to the system,.

4.10.5 Modelling of Scenarios

To construct the different sensitivity analysis scenarios, see Section 4.10, global parameters were used; they were set to either one or zero, to control the flow from certain processes. For example, if the value of the parameter *electricity_mix* was set to one, 100% of electricity was provided by the Norwegian electricity mix; if set to zero, all processes were provided with 100% German electricity mix. This was done for all scenarios, except for the *reduced purge* scenario; here, the parameter represented the purge percentage compared to the base case, i.e. a parameter value of one represented 125 kg acetone purged and 0.1 represented 12.5 kg acetone purged, see Section 4.10.4. For the *no industrial heat* scenario, a parameter was also used to control the ratio of industrial heat from natural gas versus other sources, see Section 4.10.2. See Appendix I for all process modelling in openLCA.

5

Result and Discussion

In this chapter, the results of the environmental impact assessment, together with discussions about the environmental impacts' causes, and what they entail for the PYROCO₂-project.

5.1 Environmental Impacts of the Pilot Plant

Figure 5.1 shows the environmental impacts of the Norwegian PYROCO₂-pilot plant, compared to conventional acetone production. As can be seen, the PYROCO₂-pilot plant has significantly lower impacts for Acidification (AC)(61%¹) and Photochemical Oxidant Formation (POF)(27%¹). In conventional acetone production, the Acidification (AC) is mainly due to NO_x- and SO_x emissions to air, in the acetone production process; emissions that are avoided in the PYROCO₂-model. In conventional acetone production, the POF is mainly due to gas emissions of 2-propanol, the use of which is avoided in the PYROCO₂-process. However, it is important to note that the model used for the PYROCO₂-pilot plant, in this study, does not include leaking and venting of acetone gas, which would result in increased POF.

For the PYROCO₂-pilot plant, higher impacts have been calculated for Freshwater Ecotoxicity (ET-FW) (1057%¹), Abiotic Material Resources Depletion (AD-MR) (1250%¹) and Human Toxicity (HT) (778%¹), compared to conventional acetone production, see Figure 5.1. For the PYROCO₂-pilot plant, the impacts on ET-FW and AD-MR are dominated by the construction of a CO₂-production plant (45% of total) and the increased use of electricity in the electrolysis (46% of total), and thereby the use and dissipation of metals (mainly copper) in construction of the plant and transmission networks. The increase for HT is mainly attributed to ethylene oxide emissions from MEA-production, used for the capture and purification of CO₂, and the construction of a CO₂-production plant.

Although the impact on Climate Change (CC) is higher for the PYROCO₂-pilot plant (121%¹), it is important to note that this does not include attribution for reduction of GHG-emissions due to the capture of CO₂ from off-gases in fertiliser production. For Climate Change with Attributed Carbon Capture (CC-CCA)-results, see Section 5.3.2.

For other impact categories, the trends and their causes closely follow those for the categories presented in Figure 5.1. The results for absolute impacts in all categories can be found in Section H.1 in Appendix H.

¹Relative impact, compared to conventional acetone production.

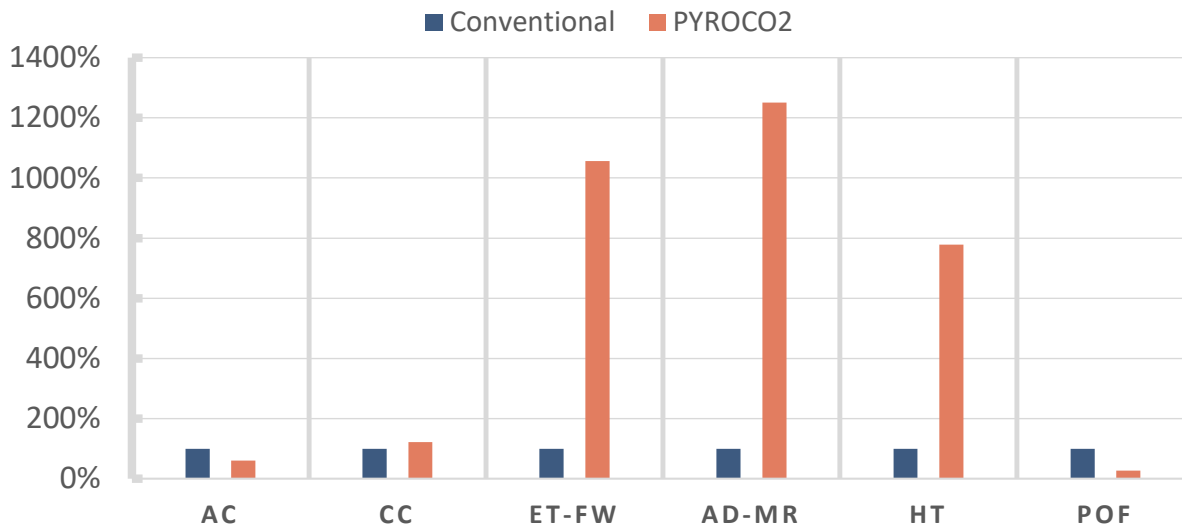


Figure 5.1: Environmental impacts for *Conventional* and *PYROCO2* acetone production, relative to conventional acetone production, for impact categories: Acidification (AC), Climate Change (CC), Freshwater Ecotoxicity (ET-FW), Abiotic Depletion of Material Resources (AD-MR), Human Toxicity (HT) and Photochemical Oxidant Formation (POF).

5.1.1 Performance Without CO₂-production

Figure 5.2 shows the environmental impacts of the Norwegian PYROCO₂-pilot plant with (*PYROCO2*) and without (*No CO₂-production*) CO₂-production, compared to conventional acetone production. As can be seen, removing the capture and purification of CO₂ considerably reduces the impacts of the pilot plant, for all categories.

For CC, this may be a reasonable assumption; the emissions of methane gas in the CO₂-production is the main contributor (47% of total CC-impact and 98% of impact from the CO₂-production, see Section G.7 in Appendix G). The methane emissions, being part of the industrial off-gas from the industrial process from which the CO₂ is captured, could instead be attributed to this upstream industrial process; without the PYROCO₂-plant, this methane gas would be emitted to the air anyways.

Omitting the other impacts from CO₂-production may be more questionable, as these are inherent impacts from the use of MEA and the construction of the CO₂-production plant. However, in a future large-scale application of the PYROCO₂-process, the purification grade of the CO₂ would probably be lower than the food-grade CO₂ that is planned to be used at the pilot plant; the purification process used at the planned pilot plant would likely not be economically or environmentally feasible, as can be seen in these results. Therefore, the impacts for these other categories may be lower for a large-scale plant, compared to *PYROCO2*.

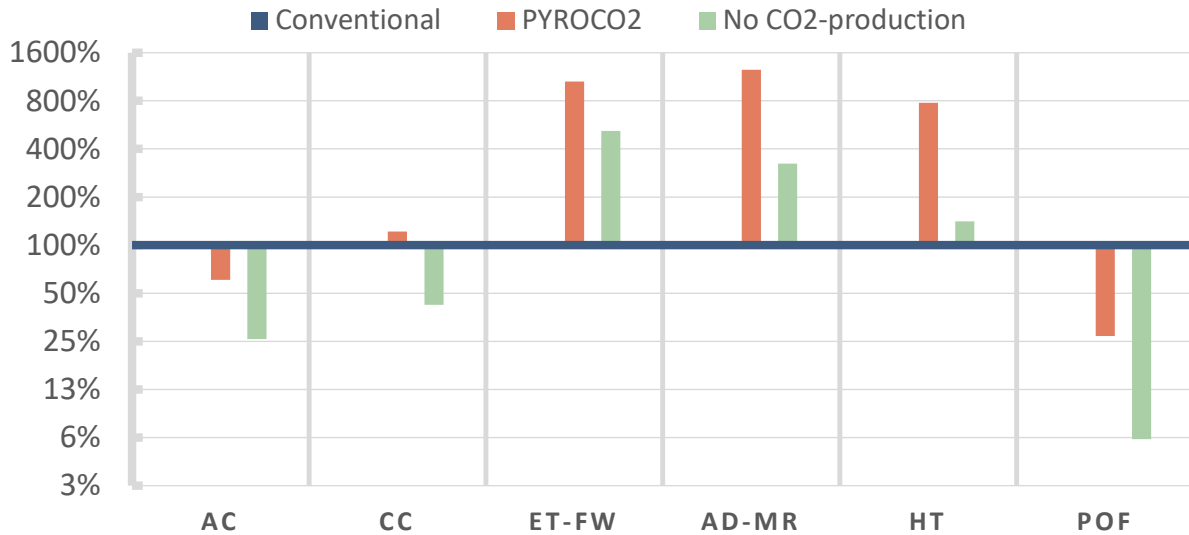


Figure 5.2: Environmental impacts for *PYROCO2* and *PYROCO2* without CO₂-production (No CO₂-production), relative to conventional acetone production, for impact categories: Acidification (AC), Climate Change (CC), Freshwater Ecotoxicity (ET-FW), Human Toxicity (HT), Abiotic Material Resources Depletion (AD-MR) and Photochemical Oxidant Formation (POF), on a logarithmic scale.

5.1.2 Hotspots Identification

For *PYROCO2*, the contributions of processes for environmental impacts, are presented in Figure 5.3. The major contributors are the CO₂-production and electrolysis. The CO₂-production contributing between 50-82%, depending on impact category, with the lowest contribution in ET-FW and highest in HT. The high contribution of this process is due to MEA-production, see Section 5.1. The electrolysis has a contribution between 16-47%, depending on impact category, with its lowest contribution in HT and its highest in ET-FW. The impacts on toxicity from electrolysis are mainly due to the use of metals in transmission networks, see Section 5.1, and for other categories the electricity generation is the major contributor. The third largest contributor is NH₃-production, contributing 1-11%, depending on impact category, with the lowest contribution in HT and the highest in CC. The impacts are mainly due to use of fossil resources in industrial processes used for production on the European market. The *CO2-production* includes both the capturing, purification and liquefaction of CO₂, and *NH3* indicates the production of NH₃, needed to sustain biomass growth.

Further, neither of the fermentation processes contribute to any environmental impacts. This is also expected, as the use of electricity for stirring is excluded, and excess waste heat is used, excluding industrial waste heat production; hence, no contribution is allocated for heat use in the distillation process. For the category *Other*, the following processes are included: *acetone production plant*, *media feed*, *condensation* and *purification*; its contribution is around 1% for all impact categories. For full contribution data, see Section G.1 in Appendix G.

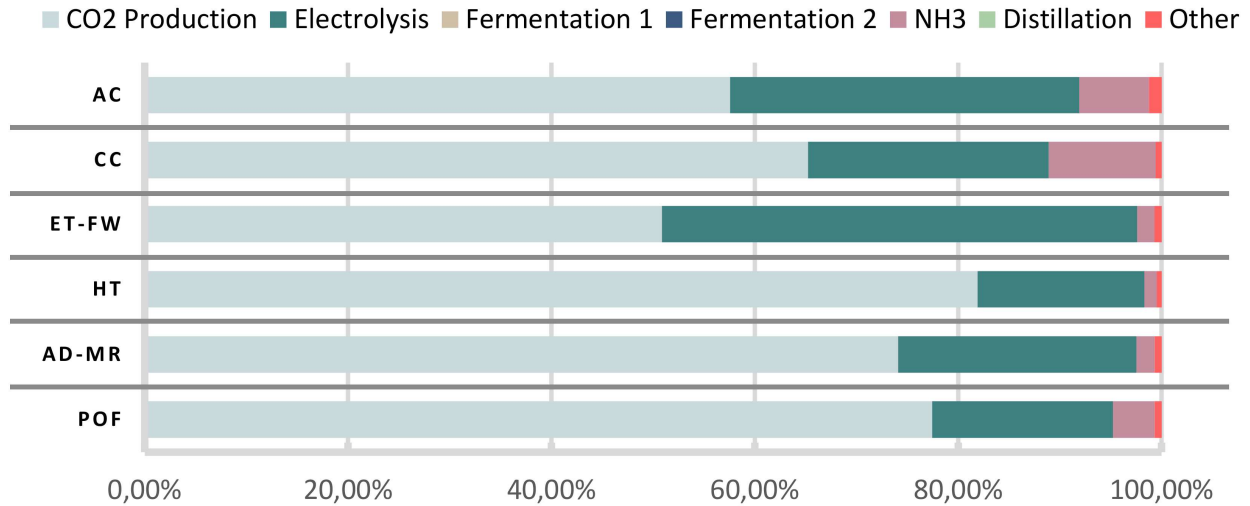


Figure 5.3: Contributions for the *PYROCO2*-pilot plant for the following impact categories: Acidification (AC), Climate Change (CC), Freshwater Ecotoxicity (ET-FW), Human Toxicity (HT), Abiotic Material Resources Depletion (AD-MR) and Photochemical Oxidant Formation (POF).

5.2 Hotspots Identification - Scenarios

In this section, process contributions for each scenario will be presented and compared with the base case of *PYROCO2*, see Section 5.1; thereby, also identifying hotspots for each scenario. In the category *Other*, the following processes are included: *acetone production plant, media feed, condensation and purification*. The *CO2-production* includes both the capturing, purification and liquefaction of CO_2 , and *NH3* indicates the production of NH_3 , needed to sustain biomass growth.

5.2.1 German Electricity Mix

Looking at the *German Electricity Mix* scenario and its contributions, presented in Figure 5.4; the top three contributors are: electrolysis, CO_2 -production and NH_3 -production; this is the case for all impact categories. To a large extent, this is due to the carbon-intensive electricity mix used in Germany, see Section 4.10.1. Hence, the energy-intensive electrolysis now has a larger contribution than the CO_2 -production, in all categories, as opposed to for *PYROCO2*. The energy-intensive electrolysis process, combined with the fossil-based electricity mix, explains the increased absolute impacts for all impact categories, which are several times higher for most impact categories, see Section 5.3.1. Looking at Figure 5.4, the contribution from NH_3 -production has been reduced significantly, compared to *PYROCO2*; this is the case for all categories, except for AD-MR. Even though the absolute impacts for NH_3 -production have not changed, the absolute impacts for the entire system have increased, see Section 5.3.1, thereby reducing its relative contribution. The NH_3 -production has its largest contribution in CC and AD-MR, with 1.5% in both categories.

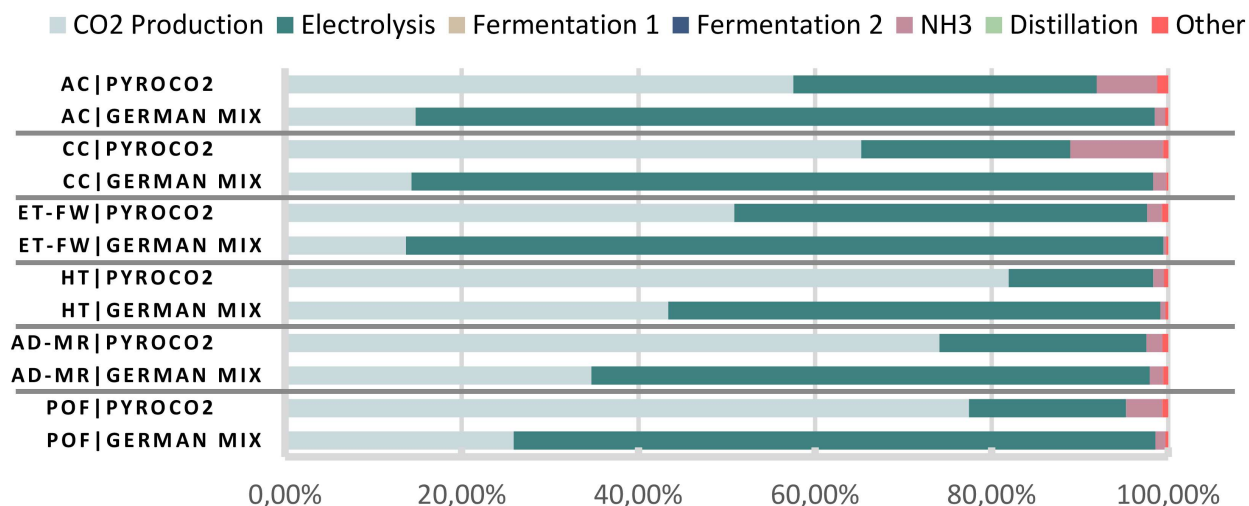


Figure 5.4: Contributions for scenario *German Electricity Mix* (German Mix) and *PYROCO2* for the following impact categories: Acidification (AC), Climate Change (CC), Freshwater Ecotoxicity (ET-FW), Human Toxicity (HT), Abiotic Material Resources Depletion (AD-MR) and Photochemical Oxidant Formation (POF).

Looking into the other processes for the *German Electricity Mix* scenario, neither of the fermentations have any impacts. This is explained by: 1) the lack of input materials, not covered by other processes, 2) the fact that excess waste heat is used, and 3) that the electricity for stirring is assumed to be negligible. Further, the distillation does not contribute with any impacts, due to the use of excess industrial waste heat. The category *Other* has an impact below 1 %, for all impact categories. The hotspots identified for this scenario are mainly the electrolysis and CO₂-production. For full contribution data, see Section G.2 in Appendix G.

5.2.2 No PEM Electrolysis

Assessing the contribution from processes in the *No PEM Electrolysis* scenario, compared to the base case of *PYROCO2*; the electrolysis does not have any impact in this scenario, due to H₂ and O₂ being bought on the European market, rather than being produced on site, see Section 4.10.3. The combined contribution from H₂ and O₂, bought from the European market in the *No PEM Electrolysis* scenario, exceeds the impacts from electrolysis in *PYROCO2*, amounting to 55 % and 43 % for AC and CC. The combined contribution for H₂ and O₂ are smaller for ET-FW, HT, AD-MR, compared to *PYROCO2*. This is due to the reduced need of electricity, and thereby the use of copper.

For the *No PEM Electrolysis* scenario, the CO₂-production still contributes between 40 - 90% of the overall impact, depending on the impact category, with its highest contribution in the HT-category and its lowest contribution in AC. In this scenario, the CO₂-production is the same process, with the same input as in *PYROCO2*; hence, the absolute impact is higher in the categories where the CO₂-production has a lower contribution, compared to *PYROCO2*. Looking into the third largest contributor, the NH₃-production, it generally has a lower contribution for the *No PEM*

Electrolysis scenario, with the exception for ET-FW, HT and AD-MR, where they are relatively the same, between 1-4%.

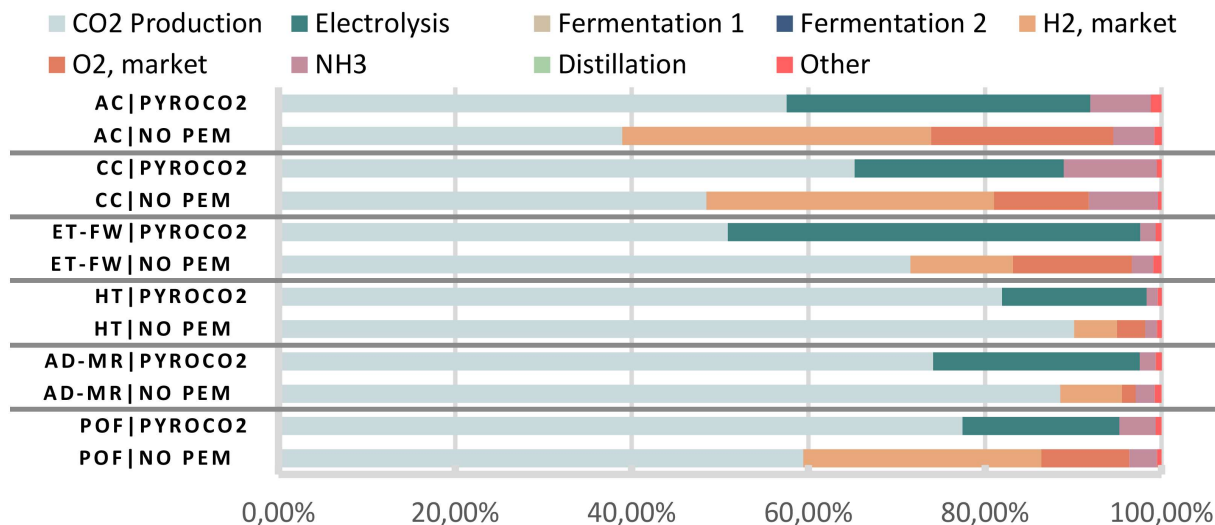


Figure 5.5: Contributions for scenario *No PEM Electrolysis* (No PEM) and *PYROCO2* for the following impact categories: Acidification (AC), Climate Change (CC), Freshwater Ecotoxicity (ET-FW), Human Toxicity (HT), Abiotic Material Resources Depletion (AD-MR) and Photochemical Oxidant Formation (POF).

For this scenario, neither fermentation contributes with any impacts, similar to the *PYROCO2*, due to no changes in the heat input source, and the electricity use for stirring is still assumed to be negligible. The contribution from the distillation is also kept at zero, as excess industrial waste heat is used. The *Other* category contributes with less than 1% in all impact categories. For full contribution data, see Section G.3 in Appendix G.

5.2.3 No Excess Industrial Waste Heat

Looking at the contribution for the *No Excess Industrial Waste Heat* scenario, and comparing it to the *PYROCO2*-base case, the CO₂-production still acts as the main contributor, with a contribution between 43-78%, with the lowest contribution in AC and its highest in HT. This is lower than for the *PYROCO2* scenario, for all impact categories. NH₃-production has a contribution between 1-5%, with the lowest contribution in HT, and the highest in CC, similar to *PYROCO2*. The electrolysis is still identified as one of the hotspots in this scenario; however, compared to *PYROCO2*, the contribution from the electrolysis is lower, despite the fact that the electrolysis process is the same for both scenarios. This is due to the new impacts from production of needed industrial heat.

Looking into the processes needing heat to operate, F2 and the distillation, both of these processes now contribute with an impact for all categories. The contribution of F2 varies from 1% to 40%, depending on impact category, with its lowest in AD-MR and highest in CC. For the distillation, the contribution is between 3% and 5%, for AC, CC and POF; the contribution for ET-FW, HT and AD-MR are all less than 1%. It is important to note that some processes (F1 and condensation)

have a high heat output, while others (F2 and distillation) require heat input; therefore, heat exchangers should be used between these processes, to reduce the overall need for heat input and the corresponding environmental impacts. See Appendix A for heat inputs and outputs of processes.

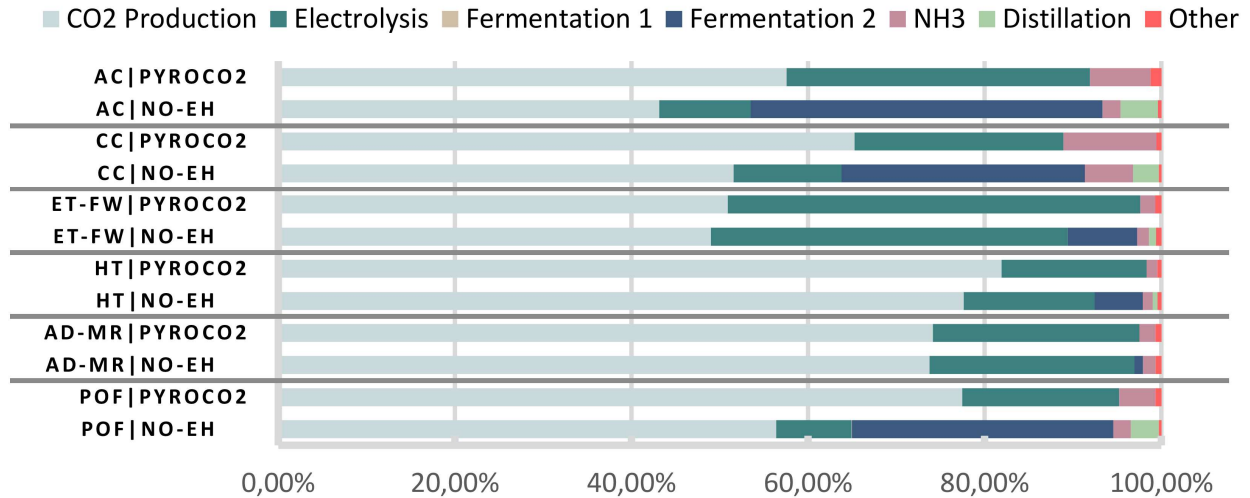


Figure 5.6: Contributions for scenario *No Excess Industrial Waste Heat* (NO-EH) and *PYROCO2* for the following impact categories: Acidification (AC), Climate Change (CC), Freshwater Ecotoxicity (ET-FW), Human Toxicity (HT), Abiotic Material Resources Depletion (AD-MR) and Photochemical Oxidant Formation (POF).

The *Other* category contributed with less than 1 % in all impact categories. For full contribution data, see Section G.4 in Appendix G.

5.2.4 Reduced Purge in F2

Looking at the scenario with *Reduced Purge* in F2 (increased product yield), see Section 4.10.4, the contributions of this scenario are the same as for *PYROCO2*, see Figure 5.7. This is an expected result, as all impact contributing processes are located before the purge process, resulting in a reduction of all input resources. However, the absolute emissions are reduced for this scenario, see Section 5.3. For full contribution data, see Section G.5 in Appendix G.

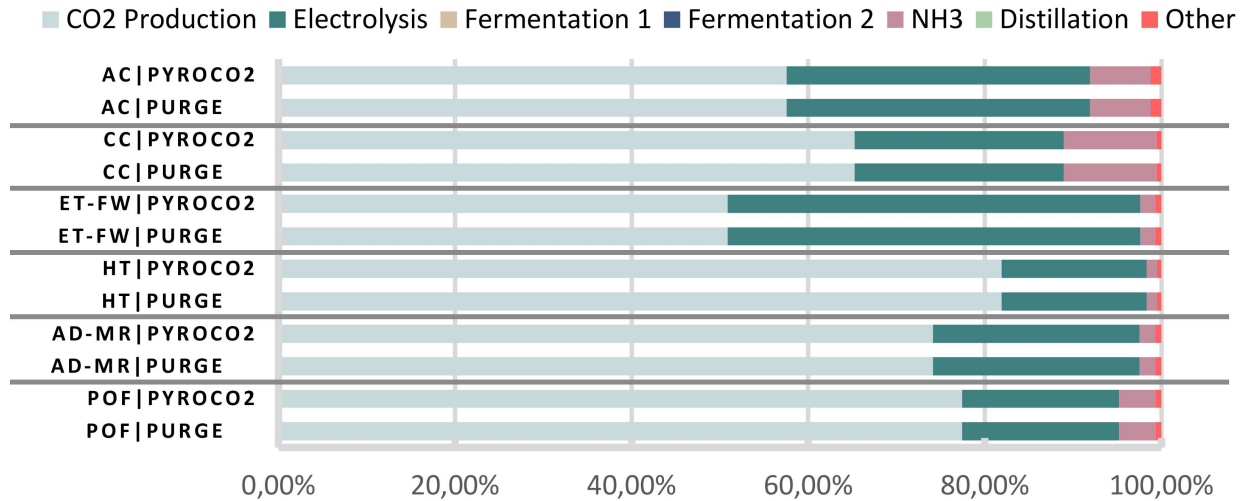


Figure 5.7: Contributions for scenario *Reduced Purge* (Purge) and *PYROCO2* for the following impact categories: Acidification (AC), Climate Change (CC), Freshwater Ecotoxicity (ET-FW), Human Toxicity (HT), Abiotic Material Resources Depletion (AD-MR) and Photochemical Oxidant Formation (POF).

5.2.5 German Electricity Mix and No PEM Electrolysis

The *German Electricity Mix* scenario has high impacts in all categories, see Section H.2 in Appendix H, where the electrolysis is the major contributor. Due to the increased contribution from the electrolysis, a scenario where the electrolysis was removed and replaced with H₂ and O₂ bought from the European market was modelled. In Figure 5.8, the combined contribution from H₂ and O₂ from the market is reduced, for all impact categories, compared to the electrolysis in *German Electricity Mix*. Hence, one can conclude that a system, where the electrolysis is removed, could make the system less sensitive to the electricity mix used.

Whether this scenario is suitable for application, or not, and if it performs better from an environmental point-of-view can be seen in Section 5.3.1. For full contribution data, see Section G.6 in Appendix G.

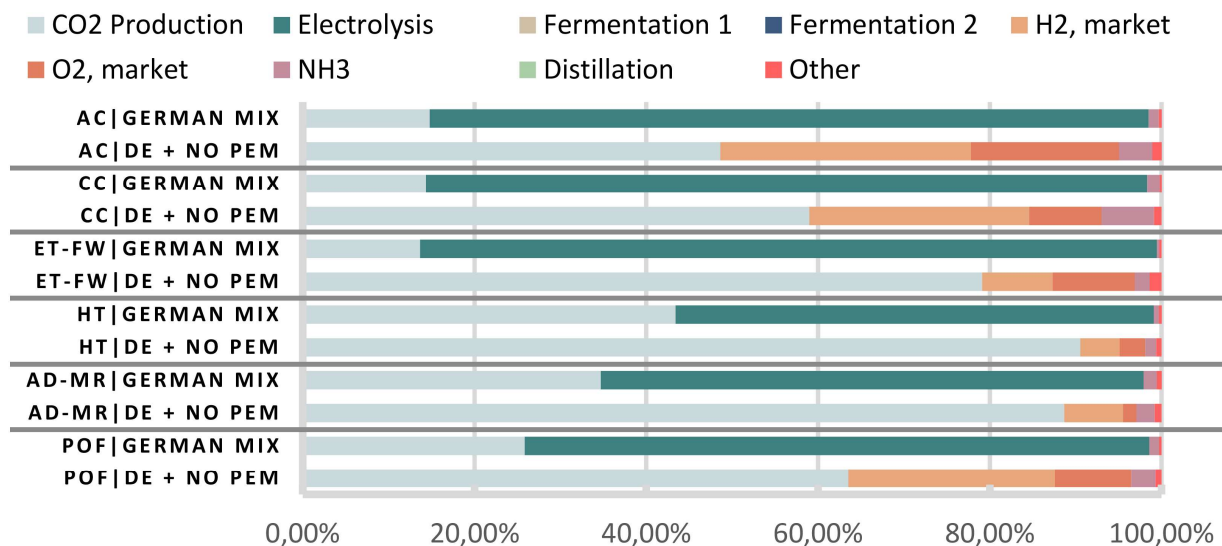


Figure 5.8: Contributions for scenarios *German Electricity Mix* (German Mix) and *German Electricity and No PEM Electrolysis* (DE + NO PEM), for the following impact categories: Acidification (AC), Climate Change (CC), Freshwater Ecotoxicity (ET-FW), Human Toxicity (HT), Abiotic Material Resources Depletion (AD-MR) and Photochemical Oxidant Formation (POF).

5.3 PYROCO2-pilot plant Scenarios' Performance

5.3.1 Scenarios' Overall Performance

Figure 5.9 shows the impacts on CC, AC and POF for the sensitivity analysis scenarios, described in Chapter 4. Due to extreme values, the *German Electricity Mix* scenario has been excluded, but can be found in Section H.2 in Appendix H. For this scenario, the CC is many times higher, compared to conventional acetone production and the other scenarios. This is due to the high use of electricity in the production of H₂ via electrolysis, combined with the high use of fossil fuels in the German electricity mix, see Section F.2 in Appendix F. This is also the reason for the high impacts on AC, ET-FW and HT, compared to the other scenarios. For the *Reduced Purge* scenario, the lower impacts in all categories can be directly attributed to the increased yield of acetone from F2, reducing the need of all inputs to the system.

As can be seen in Figure 5.9, for the *No PEM Electrolysis* scenario, the CC and AC is high, compared to *PYROCO2*, due to the use of fossil resources in the production of H₂. The higher impact on POF is mainly attributed to the use of fossil fuels in the production of electricity used for O₂-production, see contribution in Section 5.2.2.

Comparing *No Excess Industrial Waste Heat* to *PYROCO2*, the higher impacts for CC, AC and POF, see Figure 5.9, are attributed to the use of fossil fuels (natural gas, coal and petroleum) for the production of industrial heat, see Section F.3 in Appendix F.

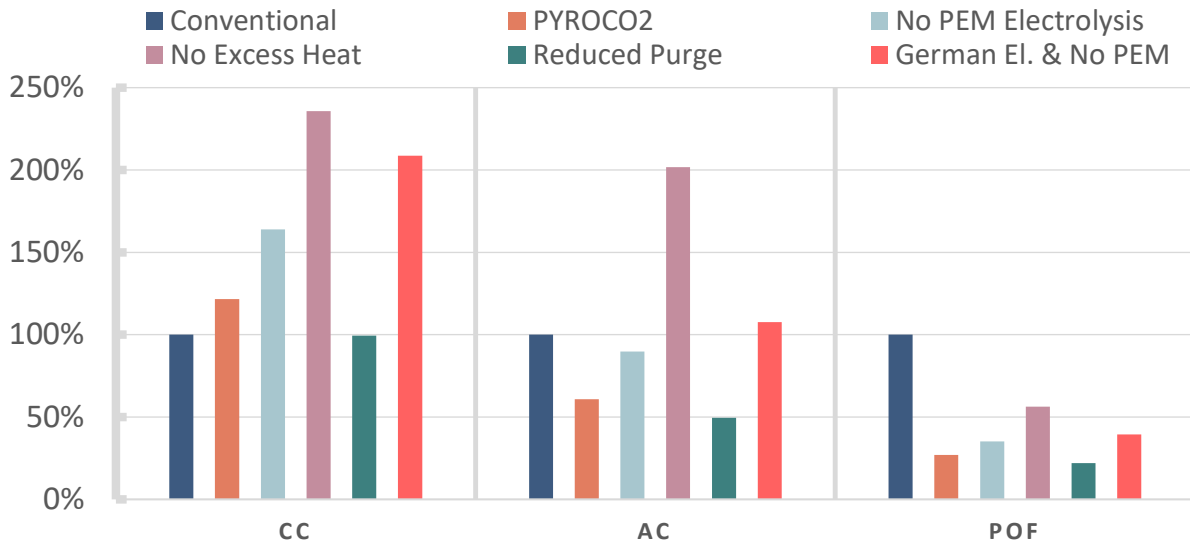


Figure 5.9: Environmental impacts for sensitivity scenarios, relative to conventional acetone production, for impact categories: Climate Change (CC), Acidification (AC) and Photochemical Oxidant Formation (POF).

For the last scenario, *German Electricity Mix and No PEM Electrolysis*, the results in Figure 5.9 are a combination of the scenarios *German Electricity Mix* and *No PEM Electrolysis*. The increased impacts on CC, AC and POF, compared to the *PYROCO2*-scenario, are mainly due to the burning of fossil fuels in the German electricity mix, see Section F.2 in Appendix F. The reduction of impacts, compared to the *German Electricity Mix*-scenario, see Section H.2 in Appendix H, is due to the removal of electricity needed for the production of H₂ gas via electrolysis; making it a suitable candidate for implementation in a location where the electricity mix is relying on fossil energy sources.

Figure 5.10 shows the impacts on HT, ET-FW and AD-MR. As can be seen, the impacts for all these categories are several times higher for the *PYROCO2*-pilot plant and the sensitivity scenarios, compared to conventional acetone production. For ET-FW and AD-MR this is due to the construction of a CO₂-production plant and the increased use of electricity, and for HT the main contributor is the production of MEA, see Section 5.1 for more details.

As the *No PEM Electrolysis* scenario does not use electricity for hydrogen production, its impacts on HT, ET-FW and AD-MR are lower. However, they are still high due to metal use for the construction of the CO₂-production plant and the use of MEA in the CO₂-production process, and some additional impact from the production of H₂, bought from the market.

For the *No Excess Industrial Waste Heat* scenario, the increase in HT, ET-FW and POF is dominated by emissions from the burning of coal for industrial heat production.

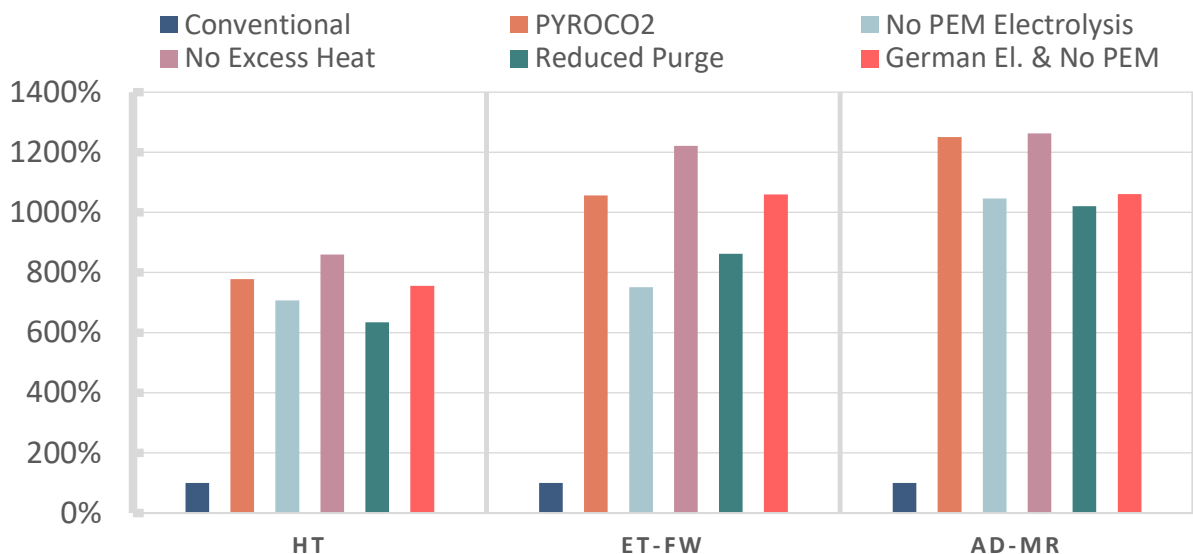


Figure 5.10: Environmental impacts for sensitivity scenarios, relative to conventional acetone production, for impact categories: Human Toxicity (HT), Freshwater Ecotoxicity (ET-FW) and Abiotic Material Resources Depletion (AD-MR).

For the scenario *German Electricity Mix and No PEM Electrolysis*, the impacts on HT and ET-FW are very similar to those of the *PYROCO2* scenario. However, it is important to note that impacts are lower for this scenario, compared to the scenario *German Electricity Mix*, see Section H.2 in Appendix H. This does highlight the importance of what type of electricity mix is used in the *PYROCO2*-process, due to the electricity demand for the electrolysis. Hence it is of interest for the *PYROCO2*-project group to take into consideration how the electricity mix is in locations for future production plants.

5.3.2 Climate Change Impacts Including Attribution of Captured CO₂

Figure 5.11 shows the absolute CC-impacts for the F.U. (4000 tonnes acetone produced), for *conventional acetone production*, *PYROCO2*, and the different *scenarios*. The chart shows both the CC- and CC-CCA impacts, where the CO₂ used as input for F1 has been attributed as a negative impact. The *German Electricity Mix* is an extreme outlier and is hence excluded, but is presented in Section H.3 in Appendix H.

Attributing captured carbon as a negative impact significantly changes the results of the scenarios' performance, with several scenarios now acting as NETs, with the exception of *No Excess Industrial Waste Heat* and *German Electricity Mix and No PEM Electrolysis*. However, for all these scenarios, the overall CC-impact is reduced significantly, and all scenarios, except *German Electricity Mix*, perform better than conventional acetone production.

For *PYROCO2*, this would result in a CO₂-sink, with 1.9 kg of CO₂ removed from the atmosphere per kg of acetone produced, see Section H.1 in Appendix H. It is important to note that this system, and its performance, is based on a cradle-to-gate system, excluding the use of the acetone.

Including the whole, cradle-to-grave, life cycle may result in the PYROCO₂-process not performing as a carbon sink, as the captured carbon may eventually be released to the atmosphere. This is dependant on the use for the acetone in later stages.

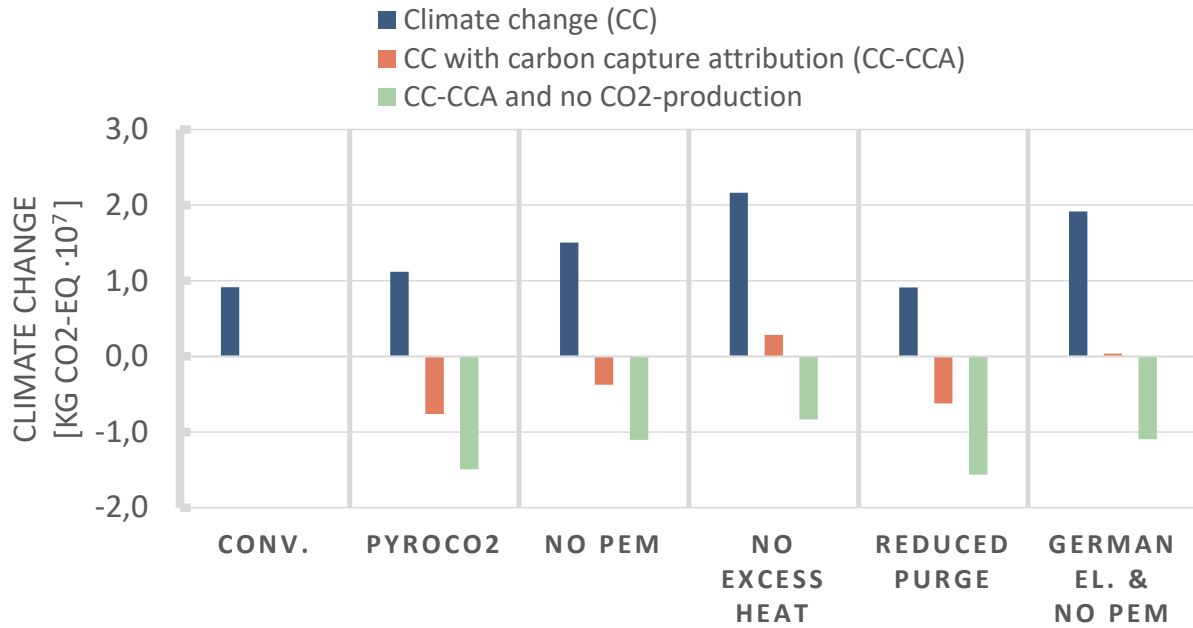


Figure 5.11: Climate change impacts per Functional Unit (F.U.) (4000 tonnes acetone produced) for the different sensitivity scenarios, including attribution of captured CO₂ (CC with carbon capture attribution (CC-CCA)), and attribution of captured CO₂ without CO₂-production (CC-CCA and no CO₂-production).

6

Conclusions

For the PYROCO₂-pilot plant, the environmental impacts for AC and POF are lower than for the conventional acetone production used in this assessment. The PYROCO₂-process outperforms conventional acetone production in CC, to the extent where the PYROCO₂-process starts acting as a NET if the captured CO₂ is attributed as a negative emission. Without attribution of captured CO₂, the emissions of CH₄ and CO₂ from the CO₂-production should not be accounted for; thereby improving the environmental performance of the PYROCO₂-process, compared to conventional acetone production. However, it's important to note that the result may change if the whole cradle-to-grave is evaluated, especially regarding CC. For example, at the EOL of a product the captured CO₂ may be released to the atmosphere.

Further, the impacts for ET-FW, AD-MR and HT are higher for the PYROCO₂-process, compared to conventional acetone production. This is due to: 1) emissions in production of MEA, used in the CO₂-production, and 2) increased need for and dissipation of metals, for the construction of the CO₂-production plant and expansion of the electrical grid, needed due to the large amount of electricity used for the electrolysis. However, previous LCAs have concluded that the embodied impacts of transmission networks are generally insignificant. Therefore, the high relative impacts for these categories are due to very low impacts in conventional acetone production; hence, the reduced impacts for CC, AC and POF are more important when looking at the PYROCO₂-pilot plant.

Generally, the CO₂-production and electrolysis are identified as the major hotspots, acting as the two largest contributors for all impact categories, with NH₃-production being the third largest. However, it's important to note that at a full-scale plant, it would likely not be economically or environmentally feasible to purify the CO₂ to the grade used at the pilot plant. For a full-scale implementation, the impacts may fall between the results shown for the scenarios *PYROCO₂* and *No CO₂-production*. For the *No Excess Industrial Waste Heat* scenario, F2 is also a major hotspot, due to its need of industrial heat.

The scenario analyses show that evaluation of the local electricity mix will be of critical importance when implementing the PYROCO₂-process at different locations, as the overall environmental impacts are largely dependent on it. This should be taken into consideration by the PYROCO₂-project group. For example, the impacts for AC, CC, ET-FW and HT are much higher when using a German electricity mix, which is largely fossil-based, due to the high use of electricity for H₂-production, using electrolysis; these emissions are high enough to warrant the use of fossil H₂, lowering the impacts for all categories. For all scenarios not using a German electricity mix, the

PYROCO₂-process reduces CC-impacts considerably, compared to conventional acetone production; it can be considered a NET, if the captured carbon is attributed as a negative impact.

The scenarios also show that access to excess industrial waste heat is of importance; conventional heat generation, using fossil fuels, has a significant impact for all impact categories. However, these impacts could be reduced considerably by integrating heat exchangers between F1, F2, and acetone condensation and distillation, reducing the overall heat input needed for F2 and distillation. Reducing the purge from F2 would also reduce emissions, by increasing the yield of the plant. This would also make the process more economically viable, by reducing the needed plant size, and inputs per kg of produced acetone.

6.1 Further Research Suggestions

As this study is an assessment of a preliminary PYROCO₂-process, further research and assessment is needed. The model used in this thesis should be further developed; adding processes for the finalised system, such as pumps, heat exchangers between F1, F2 and acetone condensation, further acetone purification steps, purge treatment, and other system processes. Also, updated experimental data for the continuous fermentation processes is needed; inputs of and emissions from the use of defined media, and acid and base used to sustain pH. Losses and emissions from the system should also be modelled, e.g. heat losses from processes and piping, purge rate and its components, and the need of a tail gas purge in F1. The system modelled in this assessment should also be expanded, to include the different products from chemo-catalytic upgrading of acetone; their production and use may greatly affect the CC-impacts of the system, as the captured CO₂ may be released again when the products are degraded, or incinerated at their EOL.

Further investigation into the CO₂-production process will be critical. The results from this model show that it has a potentially large contribution to environmental impacts. However, if the PYROCO₂-process is to be applied at an industrial scale, a lower purification grade may be used and CO₂ would not be liquefied, but piped directly to the fermentations as a gas. CO₂-accounting should also be evaluated; attribution of captured CO₂, as a negative impact for the PYROCO₂-process, and allocation of CH₄ and CO₂ emissions, between the PYROCO₂-process and the industrial process where they originate, will be of critical importance.

Also, the absolute impacts on HT, ET-FW and AD-MR should be further investigated, especially the impacts from use of copper in the construction of the PYROCO₂-plant and electrical transmission networks.

For production plants at alternative locations, background systems need thorough assessment, including electricity mix and access to excess industrial heat. Here, other uses for the heat, such as district heating, should be investigated and appropriate attribution and allocation be performed. Alternatives that could reduce impacts from the PYROCO₂-process should also be assessed, e.g. the use of "green" ammonia and heat from renewable sources.

6.2 Final Thoughts

It is important to note that impacts such as toxicity are highly dependent on context, such as nearby ecosystems and human exposure to toxins. Also, valuation of impact categories is not strictly a scientific question, but also need to regard ethics and people's personal values. However, as highlighted by the Paris Agreement and the efforts to reduce GHG-emissions, CC is of paramount importance. In this category, the PYROCO₂-pilot plant outperforms the conventional acetone production and should hence be a preferred method for production of acetone in the future.

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A

Appendix

In this Appendix, all flows and input data for the PYROCO₂-pilot plant model are presented. All flows are calculated for the R.F. of 500 kg of acetone produced.

A.1 Flows for the PYROCO₂-pilot plant

The flows, used in the PYROCO₂-pilot plant, were calculated via mass balancing, starting with the end-product of 500 kg of acetone per hour, hence why this was set as the R.F. Starting with 500 kg of acetone, the mass balances are calculated backwards to the previous process, where assumptions helped to complete the balance; this approach was used for all processes, see Figure 4.1 in Section 3.2. The base of this model was made by Henri Steinweg, at Karlsruhe Institute of Technology, and was further refined by the authors, to match the PYROCO₂-pilot plant used in this report. Further, all flows mentioned are provided as the unit *per hour*.

A.1.1 Distillation of Acetone

The distillation was assumed to produce 500 kg of acetone, from a total mixed flow of 6500 kg, where 6000 kg of the stream is consisting of water. See Table A.1 for full inventory data for the distillation process.

Table A.1: Inventory data for all flows in distillation for the PYROCO₂-pilot plant

Flow	Resource	Value	Unit
Input			
S207	Condensate outlet	6500	kg
S207a	<i>Mass flow of acetone</i>	500	kg
S207b	<i>Mass flow of water</i>	6000	kg
-	Heat	1278	MJ
Output			
S209	Acetone, 100 % pure,	500	kg
S208	Aqueous distillation residue	6000	kg

A.1.2 Condensation of Acetone

The output of 6500 kg is based on a AspenPlus-model¹, where the liquid concentration of acetone in F2 is 25 g per litre of water, and the water is assumed to have a density of 1 kg/L; hence making the liquid condensate outlet have an acetone concentration of 76,9 g/L. This concentration is calculated based on the AspenPlus-model of the water load in the stripping gas outlet from F2 being 0.1055 g/g CO₂ and an acetone load of 0.0462 g/g CO₂. The water load for the condenser gas outlet is 0.0059 g/gCO₂ and the acetone load of 0.0379 g/gCO₂. The CO₂ mass flow is calculated based on the assumption of 0.108 g condensate per g dry CO₂. In the condensation, the heat losses were assumed to be negligible, see Section B.1.6 in Appendix B. For full inventory data, see Table A.2.

Table A.2: Inventory data for all flows in condensation for the PYROCO₂-pilot plant

Flow	Resource	Value	Unit
Input			
S204	Stripping gas circular, total	69380	kg
S204a	<i>Mass flow of CO2 dry.</i>	60241	kg
S204b	<i>Mass flow of acetone</i>	2783	kg
S204c	<i>Mass flow of water</i>	6355	kg
Output			
-	Heat	15271	MJ
S205	Stripping gas circular flow, in, F2 total	61965	kg
S205a	<i>Mass flow of CO2 dry.</i>	59365	kg
S205b	<i>Mass flow of acetone</i>	2250	kg
S205c	<i>Mass flow of water</i>	350	kg
S206	CO ₂ from F2, raw, deoxygenated, to F1	915	kg
S206a	<i>Mass flow of CO2 dry.</i>	876	kg
S206b	<i>Mass flow of water</i>	5	kg
S206c	<i>Mass flow of acetone</i>	33	kg
S207	Condensate outlet	6500	kg
S207a	<i>Mass flow of acetone</i>	500	kg
S207b	<i>Mass flow of water</i>	6000	kg

A.1.3 Fermentation 2

The F2 operating settings are described in Section 4.5.2 in Chapter 4. For the production of acetone, see reactions in Section 2.3 in Chapter 2. The consumption of substances were normalised to acetic acid. The consumption of acetic acid was divided into two phases, one for product formation and one for biomass-growth. For acetone production the acetic acid consumption per acetone was assumed to be 2.27 mol/mol, the O₂-consumption per acetone was assumed to be 0.25 mol/mol; per acetic acid, the production of CO₂ was assumed to be 0.69 mol/mol, and the production of H₂O

¹Simulated with previously given assumptions: Vapour-Liquid-Equilibrium calculated by AspenPlus (R), UNIFAC - Dortmund modified database.

to be 0.69 mol/mol. For biomass-growth, the acetic acid consumption per biomass was assumed to be 0.78 mol/mol, the O₂-consumption per acetic acid was assumed to be 0.78 mol/mol, the NH₃-consumption per acetic acid was assumed to be 0.156 mol/mol. The production of CO₂ per acetic acid was assumed to be 0.4368 mol/mol and the production of H₂O per acetic acid was assumed to be 1.5288 mol/mol.

The concentration of biomass in the fermentation tank was assumed to be 20g cDW/L². The growth reaction was based on 10% of the biomass lost in the purification process, the rest being recirculated to the fermentor.

The hourly purge was assumed to be 2% of the reactor volume², and consists of the same concentration as the fermentation tank: 25g/L of acetone, with the rest assumed to be water. The full input and output inventory data is presented in Table A.3.

Table A.3: Inventory data for all flows in Fermentation 2 for the PYROCO₂-pilot plant

Flow	Resource	Value	Unit
Input			
S02	Oxygen	369	kg
-	Ammonia	18,46	kg
S202	Broth transfer from F1, purified, F2	47151	kg
S202a	<i>Mass flow of rest</i>	45265	kg
S202b	<i>Mass flow of acetic acid</i>	1886	kg
S202c	<i>Mass flow of acetone</i>	898	kg
S205	Stripping gas circular flow, in, F2 total	61965	kg
S205a	<i>Mass flow of CO₂ dry.</i>	59365	kg
S205b	<i>Mass flow of acetone</i>	2250	kg
S205c	<i>Mass flow of water</i>	350	kg
-	Heat	12239	MJ
-	Electricity	0	kWh
Output			
S204	Broth out, recycle stream F2.	34591	kg
S204a	<i>Mass flow of rest.</i>	33726	kg
S204b	<i>Mass flow of acetone</i>	865	kg
S201	Broth out, bleed stream	5000	kg
S201a	<i>Mass flow of rest</i>	4875	kg
S201b	<i>Mass flow of acetone</i>	125	kg
S203	Stripping gas circular, total	69380	kg
S203a	<i>Mass flow of CO₂ dry.</i>	60241	kg
S203b	<i>Mass flow of acetone</i>	2783	kg
S203c	<i>Mass flow of water</i>	6355	kg

²Based on communication with project partners.

A.1.4 Broth Purification F2

The purification process taking place between F2 and F1 was assumed to have no losses, in terms of the mass flow of broth; hence, the same mass of input and output was assumed. For the cell retention, it was assumed that 10 %³ of the biomass is lost through the purification process, although this is not modelled in the purification process, except for the production of new biomass. For electricity consumption and number of needed membranes, see Section D.1 in Appendix D. The full input and output inventory data is presented in Table A.4.

Table A.4: Inventory data for all flows in broth purification F2 for the PYROCO2-pilot plant

Flow	Resource	Value	Unit
Input			
S203	Broth out, recycle stream F2.	34591	kg
<i>S203a</i>	<i>Mass flow of rest.</i>	<i>33726</i>	<i>kg</i>
<i>S203b</i>	<i>Mass flow of Acetone</i>	<i>865</i>	<i>kg</i>
-	Membrane filters	0.06	items
-	Electricity	4	kWh
Output			
S103	Broth recycle in, purified F1	34591	kg
<i>S103a</i>	<i>Mass flow of rest</i>	<i>33726</i>	<i>kg</i>
<i>S103b</i>	<i>Mass flow of Acetone</i>	<i>865</i>	<i>kg</i>

A.1.5 Broth Purification F1

The purification process taking place between F1 and F2 was assumed to have no losses in terms of the mass flow of broth, hence the same mass of input and output was assumed. For the cell retention, it was assumed that 10 %³ of the biomass is lost through the purification process, although this is not modelled in the purification process, except for the production of new biomass. For electricity consumption and the number of needed membranes, see Section D.1 in Appendix D. The full input and output inventory data is presented in Table A.5.

³Based on communication with project partners.

Table A.5: Inventory data for all flows in broth purification F1 for the PYROCO₂-pilot plant

Flow	Resource	Value	Unit
Input			
S102	Broth out, F1	47151	kg
<i>S102a</i>	<i>Mass flow of water</i>	<i>44367</i>	<i>kg</i>
<i>S102b</i>	<i>Mass flow of acetic acid, total</i>	<i>1886</i>	<i>kg</i>
<i>S102c</i>	<i>Mass flow of acetone</i>	<i>898</i>	<i>kg</i>
-	Membrane filters	0.08	items
-	Electricity	5	kWh
Output			
S202	Broth transfer from F1, purified, F2	47151	kg
<i>S202a</i>	<i>Mass flow of rest</i>	<i>45265</i>	<i>kg</i>
<i>S202b</i>	<i>Mass flow of acetic acid</i>	<i>1886</i>	<i>kg</i>
<i>S202c</i>	<i>Mass flow of acetone</i>	<i>898</i>	<i>kg</i>

A.1.6 Fermentation 1

The F1 operating settings are described in Section 4.5.1 in Chapter 4. For the production of acetic acid, see reactions in Section 2.3 in Chapter 2. The consumption of substances were normalised to acetic acid. For this fermentation, there is no separate pathway for biomass growth and product formation; hence, the acetic acid production was assumed to be the limiting factor.

The consumption of CO₂ per acetic acid was assumed to be 2.33 mol/mol. The H₂-consumption per acetic acid produced was assumed to be 4.7 mol/mol, while the production of H₂O was assumed to be 2.5 mol/mol per acetic acid produced. The consumption of NH₃ was assumed to be 0.06 mol/mol per acetic acid produced. The concentration of biomass in the fermentation tank was assumed to be 20g cDW/L⁴. The loss of biomass via purification was not modelled for this fermentation process. The full input and output inventory data is presented in Table A.6.

⁴Based on communication with project partners.

Table A.6: Inventory data for all flows in Fermentation 1 for the PYROCO₂-pilot plant

Flow	Resource	Value	Unit
Input			
S07	CO ₂ in from carbon capture	2349	kg
S03	Hydrogen	298	kg
S208	Water residue from distillation	6000	kg
S05	Growth media	2799	kg
-	Ammonia	36	kg
S103	Broth recycle in, purified F1	34591	kg
<i>S103a</i>	<i>Mass flow of rest</i>	<i>33726</i>	<i>kg</i>
<i>S103b</i>	<i>Mass flow of acetone</i>	<i>865</i>	<i>kg</i>
S206	CO ₂ from F2, raw, deoxygenated, to F1	915	kg
<i>S206a</i>	<i>Mass flow of CO₂ dry.</i>	<i>876</i>	<i>kg</i>
<i>S206b</i>	<i>Mass flow of water</i>	<i>5</i>	<i>kg</i>
<i>S206c</i>	<i>Mass flow of acetone</i>	<i>33</i>	<i>kg</i>
-	Formation of water	164	kg
-	Electricity	0	kWh
Output			
-	Heat	4887	MJ
S102	Broth out, F1	47151	kg
<i>S102a</i>	<i>Mass flow of water</i>	<i>44367</i>	<i>kg</i>
<i>S102b</i>	<i>Mass flow of acetic acid, total</i>	<i>1886</i>	<i>kg</i>
<i>S102b1</i>	<i>Mass flow of acetic acid, product</i>	<i>1469</i>	<i>kg</i>
<i>S102b2</i>	<i>Mass flow of acetic acid, growth</i>	<i>417</i>	<i>kg</i>
<i>S102c</i>	<i>Mass flow of acetone</i>	<i>898</i>	<i>kg</i>
S101	Tail gas, out	0	kg

A.1.7 Electrolysis

The electrolysis produces both H₂ and O₂, with the excess O₂ being released to the atmosphere. The electricity and H₂O consumption was based on model M2000 [36]. The full input and output inventory data is presented in Table A.7.

Table A.7: Inventory data for all flows in the electrolysis for the PYROCO₂-pilot plant

Flow	Resource	Value	Unit
Input			
S01	Deionized water	3184	kg
-	Electricity	14898	kWh
Output			
S02	Oxygen	2362	kg
S03	Hydrogen	298	kg

B

Appendix

In this appendix, all heat data and calculations are presented.

B.1 Heat Calculations

The heat needed- or produced by different processes within the PYROCO₂-pilot plant was estimated using the temperatures, masses and specific heat capacities of process inputs and outputs, enthalpies of vaporisation, and the enthalpy of formation for the two fermentation reactions in F1 and F2. Heat losses from the fermentation reactors were also calculated, using heat transfer rates and the reactor volumes of F1 and F2.

B.1.1 Specific Heat Capacity

Equation B.1 shows the Shomate equation, used for calculation of the specific heat capacity at different temperatures for substances (hydrogen gas, liquid and gaseous water, carbon dioxide gas and oxygen gas), using parameters (**A** to **E**), see Table B.1, and temperature (**T**), see Section E.3 in Appendix E.

$$C_{H_2O(l),T} = A + B \cdot \frac{T}{1000} + C \cdot \left(\frac{T}{1000}\right)^2 + D \cdot \left(\frac{T}{1000}\right)^3 + \frac{E}{(T/1000)^2} \quad (\text{B.1})$$

Equation B.3 shows a calculation example for liquid water at room temperature (20°C):

$$\begin{array}{lll} A = -203.606 & B = 1523.29 & C = -3196.413 \\ D = 2474.455 & E = 3.855326 & T = 293.15K \end{array}$$

$$\begin{aligned} C_{H_2O(l),293.15K} &= -203.606 + 1523.29 \cdot \frac{293.15}{1000} - 3196.413 \cdot \left(\frac{293.15}{1000}\right)^2 + \\ &+ 2474.455 \cdot \left(\frac{293.15}{1000}\right)^3 + \frac{3.855326}{(293.15/1000)^2} = 75.456 J/(mol \cdot K) \end{aligned} \quad (\text{B.2})$$

Table B.1 shows the parameter values used to calculate the heat capacity of substances at different temperatures, see Table B.2 , via the Shomate equation, Equation B.1.

Table B.1: Parameter values used for the Shomate equation.

Shomate equation parameters						
Substance	A	B	C	D	E	Source
H2(g); 298-1000K	33,0662	-11,3634	11,4328	-2,7729	-0,1586	Literature [39]
H2O(l); 298-500K	-203,606	1523,29	-3196,41	2474,455	3,855326	Literature [40]
H2O(g); 298-500K	30,092	6,832514	6,793435	-2,53448	0,082139	Literature [41]
CO2(g); 298-1200K	24,99735	55,18696	-33,6914	7,948387	-0,13664	Literature [42]
O2(g); 100-700K	31,32234	-20,2353	57,86644	-36,5062	-0,00737	Literature [43]

Table B.2 shows the values used for specific heat capacities. For heat capacities that were not calculated using Equation B.1, linear interpolation was performed between the literature values for the closest temperatures, lower and higher than the specified temperature.

Table B.2: Specific heat capacity of substances at different temperatures: room, Fermentation 1 (F1), Fermentation 2 (F2) and condensation outlet.

Substance	Heat capacity [J/mol*K]				Source
	Temperature [K]				
	Room temp 293,15K	F1 temp 333,15K	F2 temp 333,15K	Cond. temp 285,15K	
H2(g); 298K-1000K	28,80259	29,01825	-	-	Equation B.1
H2O(l); 298K-500K	75,45633	75,34311	75,34311	75,64494	Equation B.1
H2O(g); 298K-500K	33,57071	33,7686	33,7686	33,54409	Equation B.1
CO2(g); 298K-1200K	36,89033	38,70632	38,70632	36,49829	Equation B.1
O2(g); 100K-700K	29,35774	29,58719	29,58719	29,32028	Equation B.1
CH3COCH3(g); 1 bar	74,234	80,86931	80,86931	72,9764	Literature [44]
CH3COCH3(l)	124,5	124,5	124,5	124,5	Literature [45]
CH3COOH(g)	62,628	69,01748	69,01748	61,3288	Literature [46]
CH3COOH(l)	123,1	123,1	123,1	123,1	Literature [47]
NH3(l)	80,8	80,8	80,8	80,8	Literature [48]

B.1.2 Heat Content

Equation B.3 shows the calculation of the total heat content ($H_{cp,i}$) of a substance flow (i), using: the mass flow (q_i), see Appendix A; molar mass (M_i), see Section E.1.1 in Appendix E; specific heat capacity ($C_{p,i}$), see Table B.2; temperature (T_i), see Section E.3 in Appendix E. The heat contents of mixed flows were calculated by summarising the heat content of each substance in the mix, assuming no interactions between the substances that change the substances' specific heat capacity. For the full summary of the calculated heat content of flows, see Section B.1.6.

$$H_{cp,i} = \frac{q_i \cdot C_{p,i} \cdot T_i}{M_i} \quad (\text{B.3})$$

Equation B.3 shows a calculation example for the heat content of CO₂ outflow from F2:

$$\begin{aligned} q_{CO_2} &= 60241 \text{ kg/h} & C_{p,CO_2} &= 38.4909 \text{ J/(K} \cdot \text{mol)} \\ M_{CO_2} &= 44.01 \text{ g/mol} & T_{CO_2} &= 328.15 \text{ K} \end{aligned}$$

$$H_{cp,CO_2} = \frac{60241 \text{ kg/h} \cdot 38.4909 \text{ J/(K} \cdot \text{mol)} \cdot 328.15 \text{ K}}{44.01 \text{ g/mol}} = 17289 \text{ MJ/h} \quad (\text{B.4})$$

B.1.3 State of Matter Transitions

Equation B.5 shows the heat calculation for state of matter transitions in a process ($H_{som,j}$) for a substance (j), using the mass flows of outputs ($q_{j,out}$) and inputs ($q_{j,in}$) in a state of matter, see Appendix A, and heat of vaporisation ($\Delta H_{vap,j}$), see Table B.3. Where substances condensate, a negative value was used for $\Delta H_{vap,j}$, corresponding to a heat output. For the full summary of the calculated heat of vaporisation and condensation, see Section B.1.6.

$$H_{som,j} = \left(\sum q_{j,out} - \sum q_{j,in} \right) \cdot \Delta H_{vap,j} \quad (\text{B.5})$$

Equation B.6 shows a calculation example for the heat of vaporisation of water in F2:

$$\begin{aligned} q_{H_2O(g),out} &= 6355 \text{ kg/h} & C_{H_2O(g),in} &= 350 \text{ kg/h} & \Delta H_{vap,H_2O} &= 2369.8 \text{ kJ/kg} \end{aligned}$$

$$H_{som,H_2O(g)F2} = (6355 \text{ kg/h} - 350 \text{ kg/h}) \cdot 2369.8 \text{ kJ/kg} = 14231 \text{ MJ/h} \quad (\text{B.6})$$

Table B.3 shows the heat of vaporisation for substances at different temperatures. The heats of vaporisation were calculated using linear interpolation between the literature values for the closest temperatures, lower and higher than the specified temperature.

Table B.3: Heat of vaporisation of substances at different temperatures: room, Fermentation 1 (F1), Fermentation 2 (F2) and condensation outlet.

Heat of vaporisation [kJ/kg]					
Substance	Temperature [K]				Source
	Room temp	F1 temp	F2 temp	Cond. temp	
	293.15K	333.15K	333.15K	285.15K	
H2O	2453.6	2357.6	2369.8	2472.5	Literature [HvapH2O]
CH3COCH3	534	534	534	534	Literature [45]
CO2	179.5	179.5	179.5	179.5	Literature [49]

B.1.4 Heat of Reactions

Equation B.7 shows the calculation for heat of reactions ($H_{r,k}$) for product (k), using: the mass of outflow ($q_{out,k}$) and inflow ($q_{in,k}$), see Appendix A; molar mass (M_k), see Section E.1.1 in Appendix E; heat of formation (ΔH_f), see Table B.4; molar ratio per reaction (N_k), see Reaction R2 and R5 in Section 2.3. Due to lack of data, the calculations for heat of reaction only takes into account the product formation, excluding formation of biomass.

$$H_{r,k} = \frac{(q_{out,k} - q_{in,k})}{M_k \cdot N_k} \cdot \Delta H_f \quad (\text{B.7})$$

Equation B.8 shows a calculation example for the heat of reaction for acetone production, in F2:

$$\begin{aligned} q_{acetone,out} &= 3773 \text{ kg/h} & q_{acetone,in} &= 3148 \text{ kg/h} & M_{acetone} &= 58.08 \text{ g/mol} \\ \Delta H_f &= 41.3 \text{ kJ/mol} & N_k &= 1 \end{aligned}$$

$$H_{r,acetoneF2} = \frac{(3773 \text{ kg/h} - 3148 \text{ kg/h})}{58.08 \text{ g/mol} \cdot 1} \cdot 41.3 \text{ kJ/mol} = 444.6 \text{ MJ/h} \quad (\text{B.8})$$

Table B.1.4 shows the heat of formation for Reaction R2 and R5 in Section 2.3, balanced for one mole of product (acetic acid and acetone, respectively). The values were calculated using the heat of formation for substrates and products, see Section E.1.2 in Appendix E.

Table B.4: Heat of reaction for product formation.

Heat of reaction [kJ/mol]	
Fermentation	ΔH_r°
Fermentation 1	-268.78
Fermentation 2	41.317

B.1.5 Heat Losses

Equation B.9a shows the heat loss equation for fermentors. The heat loss is based on conductive heat transfer, calculated using the heat transfer coefficient (k), see Section E.2.3 in Appendix E, the fermentor surface area (A), the temperature of the fermentor (T_f) and the surrounding (T_o), see Section E.2.1 in Appendix E, and the number of seconds in one hour ($t_{s,h}$). The area of the fermentor is calculated with Equation B.9b, using the diameter (d) and height (h) of the fermentor, respectively calculated using Equation B.9d and B.9c, using the fermentor volume (V), see Section E.2.2 in Appendix E, and its height-diameter ratio (α), see Section E.2.2 in Appendix E.

$$H_{loss} = k \cdot A \cdot (T_f - T_o) \cdot t_{s,h} \quad (\text{B.9a})$$

$$A = \pi \cdot \left(d \cdot h + 2 \left(\frac{d}{2} \right)^2 \right) \quad (\text{B.9b})$$

$$h = d \cdot \alpha \quad (\text{B.9c})$$

$$d = \sqrt[3]{\left(\frac{4V}{\pi \cdot \alpha} \right)} \quad (\text{B.9d})$$

Equation B.10 shows a calculation example for the heat loss in F2:

$$\begin{array}{lll} k = 0.136 \text{W}/(\text{m}^2 \cdot \text{K}) & \alpha = 1 \text{m}/\text{m} & t_{s,h} = 3600 \text{s}/\text{h} \\ T_f = 333.15 \text{K} & T_o = 293.15 \text{K} & V = 250 \text{m}^3 \end{array}$$

$$d = \sqrt[3]{\left(\frac{4 \cdot 250 \text{m}^3}{\pi \cdot 1 \text{m}/\text{m}} \right)} = 6.83 \text{m} \quad (\text{B.10a})$$

$$h = 6.83 \cdot 1 \text{m}/\text{m} = 6.83 \text{m} \quad (\text{B.10b})$$

$$A = \pi \cdot \left(6.83 \text{m} \cdot 6.83 \text{m} + 2 \left(\frac{6.83 \text{m}}{2} \right)^2 \right) = 219.7 \text{m}^2 \quad (\text{B.10c})$$

$$H_{loss} = 0.136 \frac{\text{W}}{(\text{m}^2 \cdot \text{K})} \cdot 219.7 \text{m}^2 \cdot (333.15 \text{K} - 293.15 \text{K}) \cdot 3600 \frac{\text{s}}{\text{h}} = 4.30 \text{MJ}/\text{h} \quad (\text{B.10d})$$

B.1.6 Total Heat Input

Equation B.5 shows the heat calculation for the total heat input needed for a process ($\Delta \mathbf{H}_{tot}$), using the total heat content of outputs ($\mathbf{H}_{cp,out,i}$) and inputs ($\mathbf{H}_{cp,in,i}$), see Section B.1.2, the heat for state of matter transitions ($\mathbf{H}_{som,j}$), see Section B.1.3, the heat from chemical reactions ($\mathbf{H}_{r,k}$), see Section B.1.4, and heat losses (\mathbf{H}_{loss}), see Section B.1.5.

$$\Delta H_{tot} = \sum H_{cp,out,i} - \sum H_{cp,in,i} + \sum H_{som,j} + \sum H_{r,k} + H_{loss} \quad (\text{B.11})$$

Equation B.12 shows a calculation example for the total heat input to F2.

$$\begin{array}{lll} \sum H_{cp,out,i} = 77399 \text{MJ} & \sum H_{cp,in,i} = 80124 \text{MJ} & \sum H_{som,j} = 14516 \text{MJ} \\ \sum H_{r,k} = 445 \text{MJ} & H_{loss} = 4 \text{MJ} & \end{array}$$

$$\Delta H_{tot,F2} = 77399 \text{MJ} - 80124 \text{MJ} + 14516 \text{MJ} + 445 \text{MJ} + 4 \text{MJ} = 12239 \text{MJ} \quad (\text{B.12})$$

B.2 Calculated Heat Data

The following sections show the heat data, calculated for F1, F2, and condensation and subsequent distillation of acetone. The data was calculated using the methods demonstrated in Section B.1. For total heat input needed for different processes, see Appendix A.

B.2.1 Fermentation 1 (F1)

Table B.5: Calculated heat data for Fermentation 1 (F1).

Flow	Resource	Heat input [MJ]	Assumptions
Heat capacity			
Input			
S07	CO2 in from carbon capture	577	
S03	Hydrogen	1246	
S208	Water residue from destillation	7367	
S05	Growth media	3437	Assumed water
-	<i>Ammonia in</i>	76	
S103	Broth recycle in, purified F1	47607	
<i>S103a</i>	<i>Massflow of rest</i>	46989	<i>Assumed water</i>
<i>S103b</i>	<i>Massflow of Acetone</i>	618	
S206	CO2 from F2, raw, deoxygenated, to F1	227	
<i>S206a</i>	<i>Massflow of CO2 dry.</i>	207	
<i>S206b</i>	<i>Massflow of Water</i>	2	
<i>S206c</i>	<i>Massflow of Acetone</i>	18	
Output			
<i>S102</i>	<i>Broth out, F1</i>	63743	
<i>S102a</i>	<i>Massflow of Water</i>	61814	Assumed water
<i>S102b</i>	<i>Massflow of acetic acid, total</i>	1288	
<i>S102c</i>	<i>Massflow of Acetone</i>	641	
<i>S101</i>	<i>Tail gas, out</i>	0	
State of matter and chemical reactions			
S01	Carbon dioxide vaporisation	422	
S206b	Acetone condensation	-3	
S206c	Water condensation	-82	
-	Energy of formation	-8441	
	Heat lossess	10	

B.2.2 Fermentation 2

Table B.6: Calculated heat data for Fermentation 2 (F2).

Flow	Resource	Heat input [MJ]	Assumptions
Heat capacity			
Input			
S02	Oxygen in	99	
S202	Broth transfer from F1, purified, F2	64994	
<i>S202a</i>	<i>Massflow of rest</i>	63065	Assumed water
<i>S202b</i>	<i>Massflow of acetic acid</i>	1288	
<i>S202c</i>	<i>Massflow of acetone</i>	641	
S205	Stripping gas circular flow, in, F2 Total	15031	
<i>S205a</i>	<i>Massflow of CO2 dry.</i>	14039	
<i>S205b</i>	<i>Massflow of Acetone</i>	806	
<i>S205c</i>	<i>Massflow of Water</i>	186	
Output			
S204	Broth out, recycle stream F2.	47607	
<i>S204a</i>	<i>Massflow of rest.</i>	46989	Assumed water
<i>S204b</i>	<i>Mass of Acetone</i>	618	
S201	Broth out, bleed stream	6881	
<i>S201a</i>	<i>Mass of rest</i>	6792	Assumed water
<i>S201b</i>	<i>Mass of Acetone</i>	89	
S203	Stripping gas circular, total	22910	
<i>S203a</i>	<i>Massflow of CO2 dry.</i>	17651	
<i>S203b</i>	<i>Massflow of Acetone</i>	1291	
<i>S203c</i>	<i>Massflow of Water</i>	3969	
State of matter and chemical reactions			
S203b-S205b	Acetone vaporisation	285	
S203c-S205c	Water vaporisation	14231	
-	Energy of formation	445	
-	Heat lossess	4	

B.2.3 Condensation

Table B.7: Calculated heat data for the condensation process.

Flow	What	Heat input [MJ]	Assumptions
Heat capacity			
Input			
S204	Stripping gas circular, total	22910	
S204a	<i>Massflow of CO2 dry.</i>	17651	
S204b	<i>Massflow of Acetone</i>	1291	
S204c	<i>Massflow of Water</i>	3969	
Output			
S205	Stripping gas circular flow, in, F2 Total	15031	
S205a	<i>Massflow of CO2 dry.</i>	14039	
S205b	<i>Massflow of Acetone</i>	806	
S205c	<i>Massflow of Water</i>	186	
S206	CO2 from F2, raw, deoxygenated, to F1	222	
S206a	<i>Massflow of CO2 dry.</i>	207	
S206b	<i>Massflow of Water</i>	3	
S206c	<i>Massflow of Acetone</i>	12	
S207	Condensate outlet	7489	
S207a	<i>Massflow of Acetone</i>	306	
S207b	<i>Massflow of Water</i>	7184	
State of matter and chemical reactions			
S207a	Acetone condensation	-267	
S207b	Water condensation	-14835	

B.2.4 Distillation

Table B.8: Calculated heat data for the distillation process.

Flow	What	Heat input [MJ]	Assumptions
Heat capacity			
Input			
S207	Condensate outlet	7489	
S207a	<i>Massflow of Acetone</i>	306	
S207b	<i>Massflow of Water</i>	7184	
Output			
S209	Acetone, 100 % pure,	229	<i>Specific heat capacity assumed as for 55C</i>
S208	Aqueous distillation residue	8272	
State of matter and chemical reactions			
S209	Acetone vaporisation	267	

C

Appendix

In this appendix, the recipe for feed media will be presented.

C.1 Feed Media Recipe

The recipe can not be disclosed due to confidentiality.

D

Appendix

In this appendix the inventory and calculations used to simulate the membrane filtration and the membrane manufacturing is presented.

D.1 Inventory Data for Membrane Filtration

To model the purification processes used in the PYROCO₂-pilot plant, a membrane filtration model was built using data from [37]. The first step was to estimate the environmental impact of the manufacturing of the membranes, instead of using the environmental impacts presented in [37], a new model was built using the inventory data from the LCA-study and combining them with new data from *ecoinvent 3.8* database. The inventory data for manufacturing of one membrane, for flux 10 and TMP_{max} of 20 kPa, is given in Table D.1.

Table D.1: Inventory data from and flows used in openLCA for manufacturing of one membrane

Inventory data from	Flow used in openLCA	Amount	Unit
Hard casing made of Acrylonitrile-butadiene-styren	Acrylonitrile-butadiene-styren copolymer	12,948	kg
Mesh made of polyethylene	packaging film, low density polyethylene	0,404	kg
Polyurethane glue	polyurethane adhesive	1,33	kg
Fibre made of polypropylene	textile, nonwoven polypropylene	1,2	kg

In order to calculate the number of membranes required to filter one litre of liquid in the PYROCO₂-pilot plant a model was built up using data from [37] and combining the settings for the PYROCO₂-pilot plant; this is represented by Equation D.1 from the regression made in Figure D.1, with $R^2 = 0.9968$.

$$Y = 0.0003e^{0.0276*flux} \quad (D.1)$$

Equation D.1 was modeled by dividing all electricity produced input for *membrane operations* (*MJ/ML*), in [37], for TMP_{max} 20 kPa, by 1 000 0000 for all fluxes, and the plotting the data set in excel. Then performing a regression dependent on the flux in order to be able to change the flux. See Table D.2 for all electricity use per litre of filtrated liquid.

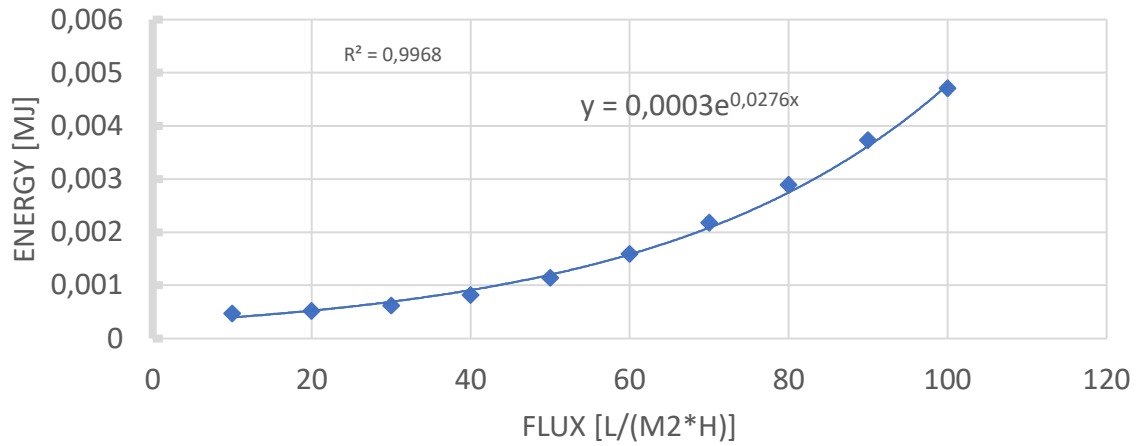


Figure D.1: Regression of data for energy required to filter one litre of liquid for various flux.

Table D.2: Inventory data for energy needed to filtrate one litre of liquid in PYROCO2-pilot plant model.

Flux	MJ
10	0,000471
20	0,000517
30	0,000619
40	0,000815
50	0,00114
60	0,001593
70	0,002176
80	0,002889
90	0,003732
100	0,004705

E

Appendix

In this appendix, physical and chemical constants together with parameters used in the modelling will be presented.

E.1 Physical and Chemical Constants

This section contains data for physical and chemical constants, used for calculations within the model.

E.1.1 Molar Masses

Table E.1 shows molar masses, used for calculations within the model. The molar masses for substances were calculated using their element composition together with the molar mass of each respective element.

Table E.1: Molar masses.

Molar masses		
Substance	Molar mass [g/mol]	Source
Elements		
Hydrogen (H)	1.0079	Literature [50]
Carbon (C)	12.01	Literature [50]
Nitrogen (N)	14.007	Literature [50]
Oxygen (O)	16	Literature [50]
Sodium (Na)	22.99	Literature [50]
Sulphur (S)	32.065	Literature [50]
Chlorine (Cl)	35.45	Literature [50]
Nickel (Ni)	58.6934	Literature [50]
Bromine (Br)	79.904	Literature [50]
Common substances		
Water (H ₂ O)	18.0158	Calculated
Hydrogen gas (H ₂)	2.0158	Calculated
Oxygen gas (O ₂)	32	Calculated
Carbon dioxide gas (CO ₂)	44.01	Calculated
Acetic acid (CH ₃ COOH)	60.052	Calculated
Acetone (CH ₃ COCH ₃)	58.08	Calculated
Chlorine gas (Cl ₂)	70.9	Calculated
Sodium hydroxide (NaOH)	39.9971	Calculated
Hydrogen chloride (HCl)	36.4579	Calculated
Bacteria		
Biomass, thermophilic acetogen (C-mole: CH _{1.8} O _{9.5} N _{0.2})	24.6	Literature [51]

E.1.2 Heat of Formation

Table E.2 shows heat of formation for different substances at standard state (25°C, 1 atm), used for calculations within the model.

Table E.2: Heat of formation, standard state (25°C, 1 atm).

Heat of formation		
Substance	ΔH_f° [kJ/mol]	Source
CH ₃ COCH ₃ (l)	-247.609	Literature [50]
CH ₃ COCH ₃ (g)	-216.648	Literature [50]
CH ₃ COOH (l)	-484.131	Literature [50]
CH ₃ COOH (g)	-434.843	Literature [50]
H ₂ O (l)	-285.83	Literature [50]
H ₂ O (g)	-241.818	Literature [50]
CO ₂ (g)	-393.505	Literature [50]
H ₂ (g)	0	Literature [50]
H ⁺	0	Literature [50]

E.2 System Parameters

This section contains data for system parameters, used for calculations within the model.

E.2.1 System Temperatures

Table E.3 shows the temperatures of different systems and processes within the modelled system.

Table E.3: Temperatures for different processes and flows within the modelled system, in degrees Celsius and Kelvin.

Temperatures		
Process/Flow	[°C]	[K]
Room	20	293,15
Fermentor 1	60	333,15
Fermentor 2	60	333,15
Condensation output	12	285,15
Distillation output, water	56	329,15
Distillation output, acetone	56	329,15

E.2.2 Fermentation Reactor Dimensions

Table E.4 shows the reactor volumes for F1 and F2.

Table E.4: Fermentation reactor volumes.

Fermentation reactor volumes		
Reactor	Value	Unit
Fermentation 1	943	m ³
Fermentation 2	250	m ³

The height-diameter ratio, of the fermentation reactors, was assumed to be 1, to have a high ratio between the gas-liquid interface area and the reactor volume [52].

E.2.3 Heat Transfer Coefficient

The heat transfer coefficient (**k**) was assumed to be $0.136\text{W}/(\text{m}^2 \cdot \text{K})$, corresponding to a reactor using a 30cm insulating layer [53].

F

Appendix

In this appendix the electricity mix, and industrial heat mix used in the report is presented.

F.1 Norwegian Electricity Mix

Figure F.1 shows the Norwegian electricity mix in 2018, calculated from *ecoinvent process market for electricity, medium voltage | electricity, medium voltage | Cutoff, U - NO*, using impact assessment *ei - cumulative energy demand*. The electricity mix in Norway is dominated by renewable energy (hydro, nuclear and wind), with only a small share of fossil-based energy generation.

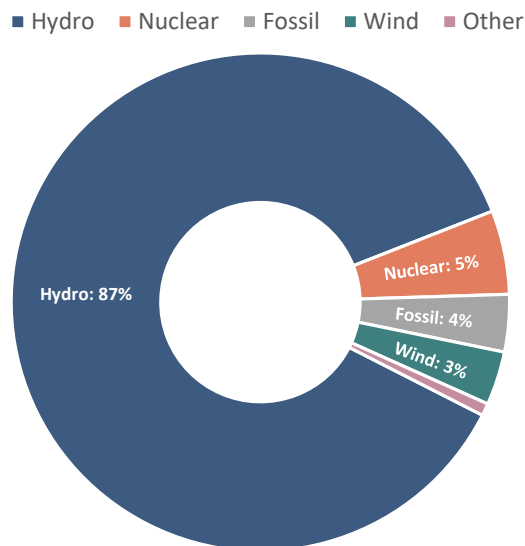


Figure F.1: Norwegian electricity mix, calculated from *ecoinvent process market for electricity, medium voltage | electricity, medium voltage | Cutoff, U - NO*, using impact assessment *ei - cumulative energy demand*.

F.2 German Electricity Mix

Figure F.2 shows the German electricity mix in 2018, calculated from *ecoinvent process market for electricity, medium voltage | electricity, medium voltage | Cutoff, U - DE*, using impact assessment

ei - cumulative energy demand. The electricity mix in Germane is dominated by fossil-based energy (lignite, hard coal, natural gas and petroleum), with a smaller share of low-carbon energy generation, mainly nuclear power.

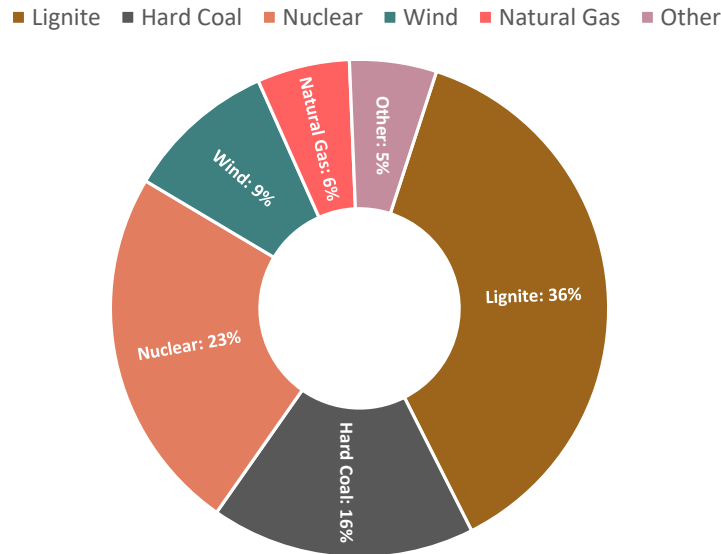


Figure F.2: German electricity mix, calculated from *ecoinvent process market for electricity, medium voltage | electricity, medium voltage | Cutoff, U - DE*, using impact assessment *ei - cumulative energy demand*.

F.3 Industrial Heat Energy Mix

Figure F.3 shows the European energy mix for industrial heat generation in 2009, calculated with using impact assessment *ei - cumulative energy demand* for *ecoinvent processes market for heat, district or industrial, natural gas | heat, district or industrial, natural gas | Cutoff, U - Europe without Switzerland* and *market for heat, district or industrial, other than natural gas | heat, district or industrial, other than natural gas | Cutoff, U - Europe without Switzerland*, using 35.42% natural gas and the rest from other [54]. The European industrial heat generation is dominated by fossil-based energy (natural gas, hard coal and petroleum), with a smaller share from biomass.

■ Natural gas ■ Hard coal ■ Petroleum ■ Biomass ■ Other

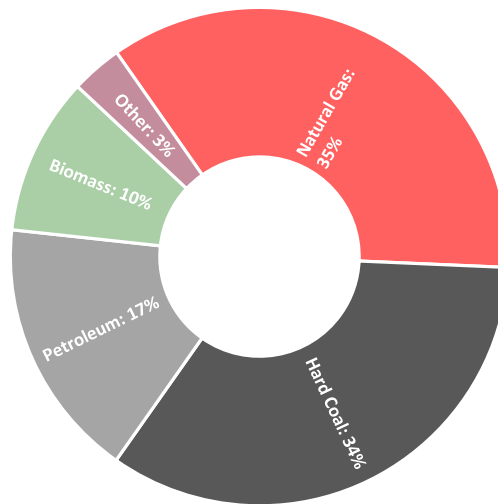


Figure F.3: Industrial heat energy mix, calculated from *ecoinvent* processes *market for heat, district or industrial, natural gas* | *heat, district or industrial, natural gas* | *Cutoff, U - Europe without Switzerland* and *market for heat, district or industrial, other than natural gas* | *heat, district or industrial, other than natural gas* | *Cutoff, U - Europe without Switzerland*, using impact assessment *ei - cumulative energy demand*.

G

Appendix

In this appendix, full inventory results for contribution for all scenarios will be presented.

G.1 Contribution for PYROCO₂-Pilot Plant

Table G.1: Contribution for PYROCO₂, calculated with openLCA

PYROCO ₂						
Process	AC	CC	ET-FW	HT	AD-MR	POF
acetone distillation	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
aqueous residue sink	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
broth purification, F1,out	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
broth purification, F2, out	0,05%	0,04%	0,02%	0,01%	0,01%	0,04%
carbon dioxide production, liquid carbon dioxide, liquid Cutoff, U - NO	57,55%	65,24%	50,88%	81,92%	74,11%	77,44%
electrolysis, PEM - NO	34,36%	23,68%	46,72%	16,39%	23,42%	17,78%
ethanol fermentation plant construction ethanol fermentation plant Cutoff, U - CH	0,36%	0,12%	0,32%	0,18%	0,19%	0,20%
feed media blend, F1	0,75%	0,37%	0,34%	0,27%	0,45%	0,38%
fermentation, F1	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
fermentation, F2	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	2,34%	3,59%	0,58%	0,42%	0,62%	1,40%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	4,52%	6,93%	1,12%	0,81%	1,20%	2,71%
market for hydrogen, liquid hydrogen, liquid Cutoff, U - RER	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
market for oxygen, liquid oxygen, liquid Cutoff, U - RER	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
membrane filtration	0,07%	0,05%	0,02%	0,01%	0,01%	0,05%
stripping gas condensation, C1, moderate temp	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
stripping gas sink, C1	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%

G.2 Contribution for German Electricity Mix Scenario

Table G.2: Contribution for German Electricity, calculated with openLCA

German Electricity						
Process	AC	CC	ET-FW	HT	AD-MR	POF
acetone distillation	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
aqueous residue sink	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
broth purification, F1,out	0,00%	0,01%	0,00%	0,00%	0,00%	0,00%
broth purification, F2, out	0,03%	0,03%	0,02%	0,02%	0,01%	0,03%
carbon dioxide production, liquid carbon dioxide, liquid Cutoff, U - NO	14,78%	14,33%	13,67%	43,40%	34,69%	25,87%
electrolysis, PEM - NO	83,71%	83,97%	85,79%	55,69%	63,21%	72,68%
ethanol fermentation plant construction ethanol fermentation plant Cutoff, U - CH	0,06%	0,02%	0,05%	0,13%	0,18%	0,05%
feed media blend, F1	0,21%	0,13%	0,14%	0,14%	0,37%	0,18%
fermentation, F1	0,00%	0,00%	0,01%	0,00%	0,00%	0,00%
fermentation, F2	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	0,40%	0,51%	0,10%	0,21%	0,52%	0,39%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	0,78%	0,98%	0,19%	0,40%	1,01%	0,76%
market for hydrogen, liquid hydrogen, liquid Cutoff, U - RER	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
market for oxygen, liquid oxygen, liquid Cutoff, U - RER	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
membrane filtration	0,04%	0,03%	0,03%	0,02%	0,02%	0,04%
stripping gas condensation, C1, moderate temp	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
stripping gas sink, C1	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%

G.3 Contribution for No PEM Electrolysis Scenario

Table G.3: Contribution for No PEM Electrolysis, calculated with openLCA

No PEM Electrolysis						
Process	AC	CC	ET-FW	HT	AD-MR	POF
acetone distillation	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
aqueous residue sink	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
broth purification, F1,out	0,00%	0,00%	0,00%	0,01%	0,00%	0,00%
broth purification, F2, out	0,04%	0,03%	0,02%	0,01%	0,01%	0,03%
carbon dioxide production, liquid carbon dioxide, liquid Cutoff, U - NO	38,93%	48,45%	71,55%	90,08%	88,54%	59,42%
electrolysis, PEM - NO	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
ethanol fermentation plant construction ethanol fermentation plant Cutoff, U - CH	0,25%	0,09%	0,45%	0,19%	0,23%	0,15%
feed media blend, F1	0,51%	0,27%	0,47%	0,30%	0,53%	0,29%
fermentation, F1	0,00%	0,01%	0,00%	0,00%	0,00%	0,01%
fermentation, F2	0,00%	0,00%	0,00%	0,00%	0,01%	0,00%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	3,06%	5,14%	1,58%	0,89%	1,43%	2,08%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	1,58%	2,66%	0,82%	0,46%	0,74%	1,08%
market for hydrogen, liquid hydrogen, liquid Cutoff, U - RER	34,96%	32,57%	11,59%	4,87%	6,97%	26,96%
market for oxygen, liquid oxygen, liquid Cutoff, U - RER	20,64%	10,75%	13,49%	3,19%	1,53%	9,95%
membrane filtration	0,05%	0,04%	0,03%	0,01%	0,01%	0,04%
stripping gas condensation, C1, moderate temp	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
stripping gas sink, C1	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%

G.4 Contribution for No Excess Industrial Heat Scenario

Table G.4: Contribution for No Excess Industrial Heat, calculated with openLCA

No Excess Industrial Heat						
Process	AC	CC	ET-FW	HT	AD-MR	POF
acetone distillation	4,24%	2,94%	0,82%	0,58%	0,06%	3,16%
aqueous residue sink	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
broth purification, F1,out	0,00%	0,01%	0,00%	0,00%	0,00%	0,00%
broth purification, F2, out	0,02%	0,02%	0,01%	0,01%	0,01%	0,02%
carbon dioxide production, liquid carbon dioxide, liquid Cutoff, U - NO	43,14%	51,55%	49,00%	77,64%	73,75%	56,39%
electrolysis, PEM - NO	10,34%	12,22%	40,40%	14,83%	23,19%	8,54%
ethanol fermentation plant construction ethanol fermentation plant Cutoff, U - CH	0,11%	0,06%	0,28%	0,16%	0,19%	0,09%
feed media blend, F1	0,23%	0,19%	0,29%	0,25%	0,44%	0,18%
fermentation, F1	0,00%	0,00%	0,00%	0,00%	0,00%	0,02%
fermentation, F2	39,84%	27,57%	7,86%	5,42%	0,98%	29,61%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	1,36%	3,58%	0,97%	0,73%	1,19%	1,30%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	0,70%	1,85%	0,36%	0,38%	0,18%	0,67%
market for hydrogen, liquid hydrogen, liquid Cutoff, U - RER	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
market for oxygen, liquid oxygen, liquid Cutoff, U - RER	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
membrane filtration	0,02%	0,02%	0,02%	0,01%	0,01%	0,02%
stripping gas condensation, C1, moderate temp	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
stripping gas sink, C1	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%

G.5 Contribution for Reduced Purge in F2 Scenario

Table G.5: Contribution for Reduced Purge in F2, calculated with openLCA

Reduced Purge in F2						
Process	AC	CC	ET-FW	HT	AD-MR	POF
acetone distillation	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
aqueous residue sink	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
broth purification, F1,out	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
broth purification, F2, out	0,05%	0,04%	0,02%	0,01%	0,01%	0,04%
carbon dioxide production, liquid carbon dioxide, liquid Cutoff, U - NO	57,55%	65,24%	50,88%	81,92%	74,11%	77,44%
electrolysis, PEM - NO	34,36%	23,68%	46,72%	16,39%	23,42%	17,78%
ethanol fermentation plant construction ethanol fermentation plant Cutoff, U - CH	0,36%	0,12%	0,32%	0,18%	0,19%	0,20%
feed media blend, F1	0,75%	0,37%	0,34%	0,27%	0,45%	0,38%
fermentation, F1	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
fermentation, F2	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	4,52%	6,93%	1,12%	0,81%	1,20%	2,71%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	2,34%	3,59%	0,58%	0,42%	0,62%	1,40%
market for hydrogen, liquid hydrogen, liquid Cutoff, U - RER	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
market for oxygen, liquid oxygen, liquid Cutoff, U - RER	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
membrane filtration	0,07%	0,05%	0,02%	0,01%	0,01%	0,05%
stripping gas condensation, C1, moderate temp	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
stripping gas sink, C1	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%

G.6 Contribution for German Electricity Mix and No PEM Electrolysis Scenario

Table G.6: Contribution for German Electricity and No PEM Electrolysis, calculated with openLCA

German Electricity and No PEM Electrolysis						
Process	AC	CC	ET-FW	HT	AD-MR	POF
acetone distillation	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
aqueous residue sink	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
broth purification, F1,out	0,00%	0,00%	0,00%	0,01%	0,00%	0,00%
broth purification, F2, out	0,09%	0,11%	0,13%	0,03%	0,02%	0,07%
carbon dioxide production, liquid carbon dioxide, liquid Cutoff, U - NO	48,63%	58,97%	79,09%	90,56%	88,66%	63,52%
electrolysis, PEM - NO	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
ethanol fermentation plant construction ethanol fermentation plant Cutoff, U - CH	0,21%	0,07%	0,32%	0,28%	0,25%	0,13%
feed media blend, F1	0,68%	0,55%	0,79%	0,28%	0,53%	0,43%
fermentation, F1	0,0%	0,00%	0,00%	0,00%	0,00%	0,01%
fermentation, F2	0,01%	0,00%	0,00%	0,00%	0,00%	0,00%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	2,55%	4,04%	1,12%	0,83%	1,41%	1,85%
market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER	1,32%	2,09%	0,58%	0,43%	0,73%	0,96%
market for hydrogen, liquid hydrogen, liquid Cutoff, U - RER	29,17%	25,59%	8,22%	4,56%	6,87%	24,06%
market for oxygen, liquid oxygen, liquid Cutoff, U - RER	17,22%	8,44%	9,57%	2,98%	1,51%	8,88%
membrane filtration	0,13%	0,14%	0,18%	0,04%	0,02%	0,09%
stripping gas condensation, C1, moderate temp	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%
stripping gas sink, C1	0,00%	0,00%	0,00%	0,00%	0,00%	0,00%

G.7 Contribution for CO₂-Production

Table G.7: Contribution of methane- (CH₄) and carbon dioxide (CO₂) emissions in *carbon dioxide production, liquid | carbon dioxide, liquid | Cutoff, U - NO*, as a share of total emissions and emissions from *carbon dioxide production, liquid | carbon dioxide, liquid | Cutoff, U - NO*.

Methane and carbon dioxide contributions		
	Methane	Carbon dioxide
Total emissions	47,11%	0,84%
Carbon dioxide capture and purification	98,25%	1,75%

H

Appendix

In this appendix the absolute impacts will be presented.

H.1 Total Environmental Impact for the PYROCO₂-Pilot Plant with the CML Impact Methode

In this section the absolute impacts for 1 F.U. is presented in Table H.1

Table H.1: Total environmental impact for Functional Unit (F.U.) and the PYROCO₂-pilot plant for the CML impact methode

Impact Category	Conventional	PYROCO ₂	De-Elec	No PEM	No-EH	Reduced Purge	De-Elec and No PEM	Without CO ₂ -production
Acidification [kg SO ₂ -Eq]	4,02E+04	2,44E+04	1,43E+05	3,61E+04	8,12E+04	2,00E+04	4,33E+04	1,04E+04
Climate change [kg CO ₂ -Eq]	9,18E+06	1,12E+07	7,88E+07	1,50E+07	2,16E+07	9,12E+06	1,91E+07	3,88E+06
Ecotoxicity - Freshwater [kg 1,4-DCB-Eq]	1,10E+06	1,17E+07	6,77E+07	8,30E+06	1,35E+07	9,52E+06	1,17E+07	5,73E+06
Ecotoxicity - Marine [kg 1,4-DCB-Eq]	2,96E+09	1,32E+10	1,52E+11	1,37E+10	2,04E+10	1,08E+10	2,21E+10	5,18E+09
Ecotoxicity - Terrestrial [kg 1,4-DCB-Eq]	6,95E+03	1,23E+05	2,18E+05	4,77E+04	1,56E+05	1,01E+05	5,35E+04	9,45E+04
Energy resources: non-renewable, abiotic depletion potential [MJ]	2,37E+08	6,31E+07	7,85E+08	2,23E+08	1,85E+08	5,15E+07	2,67E+08	3,65E+07
Eutrophication [kg PO ₄ -Eq]	1,89E+04	1,63E+04	3,57E+05	2,10E+04	2,73E+04	1,33E+04	4,17E+04	8,06E+03
Human toxicity [kg 1,4-DCB-Eq]	4,63E+06	3,60E+07	7,30E+07	3,28E+07	3,98E+07	2,94E+07	3,50E+07	6,51E+06
Material resources [kg Sb-Eq]	2,63E+01	3,28E+02	3,91E+02	2,75E+02	3,32E+02	2,68E+02	2,79E+02	8,51E+01
Ozone depletion [kg CFC-11-Eq]	1,24E-01	3,80E-01	1,81E+00	1,20E+00	1,14E+00	3,10E-01	1,29E+00	2,96E-01
Photochemical oxidant formation [kg ethylene-Eq]	8,71E+03	2,35E+03	8,44E+03	3,07E+03	4,90E+03	1,92E+03	3,44E+03	5,31E+02
Climate change with attributed captured carbon [kg CO ₂ -Eq]	9,18E+06	-7,62E+06	6,00E+07	-3,75E+06	2,84E+06	-6,22E+06	3,55E+05	-1,49E+07

H.2 Relative Impacts - All Scenarios Included

In this section, the total relative impacts for all scenarios is presented in Figure H.1

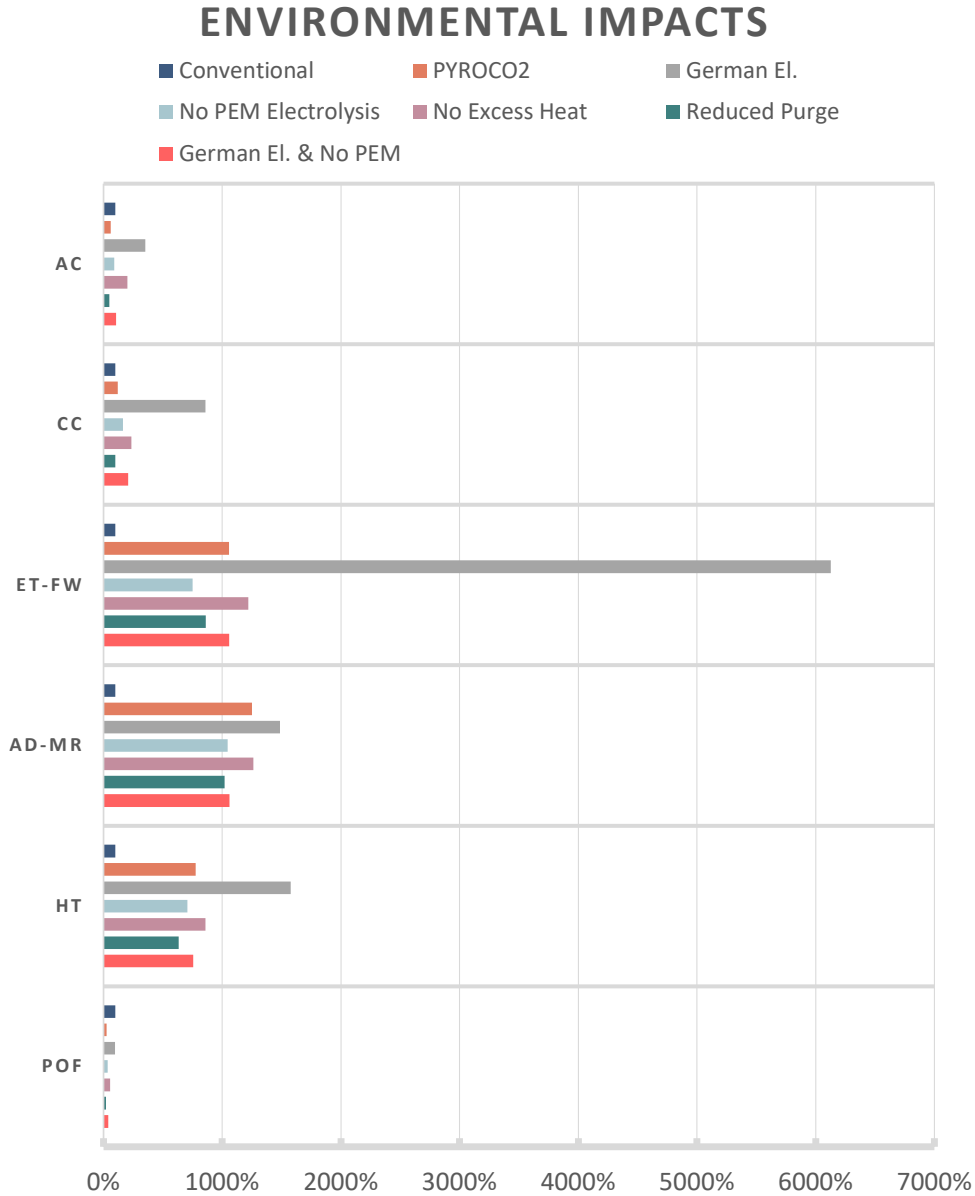


Figure H.1: Environmental impacts for acetone production in all scenarios, relative to conventional acetone production, for impact categories: Acidification (AC), Climate Change (CC), Freshwater Ecotoxicity (ET-FW), Abiotic Depletion of Material Resources (AD-MR), Human Toxicity (HT) and Photochemical Oxidant Formation (POF).

H.3 Climate Change Impacts Including Attribution of Captured CO₂ - With German Electricity Mix

In this section, the absolute impact per F.U. is presented for CC in Figure H.2.

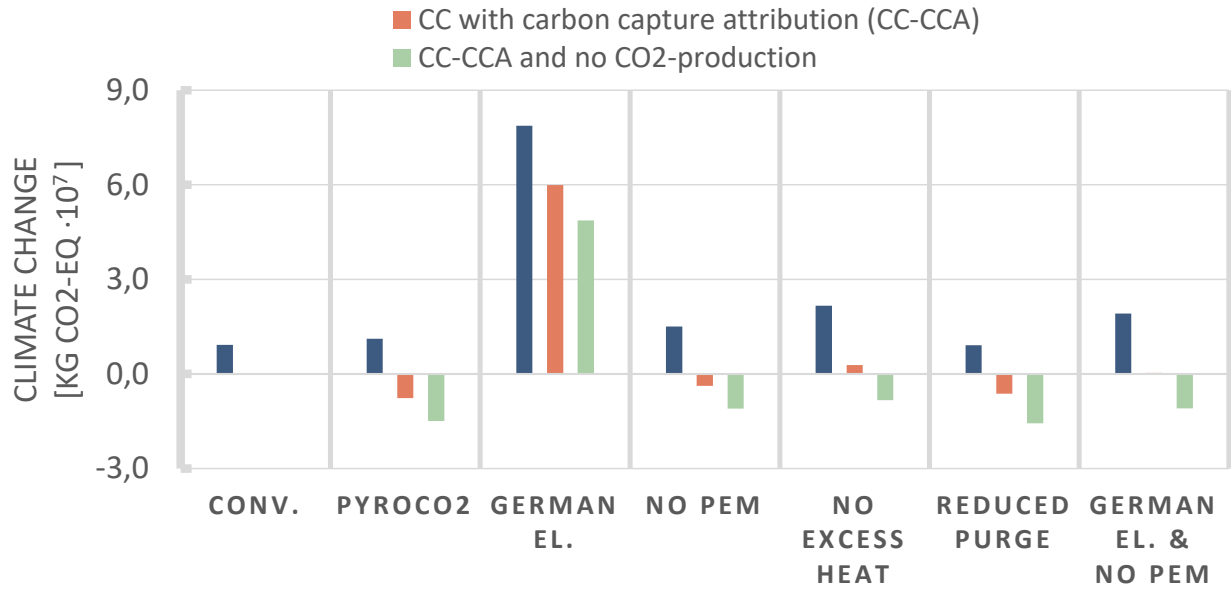


Figure H.2: Climate Change (CC) impacts per F.U. (4000t of acetone produced) for all sensitivity scenarios, including attribution of captured CO₂ and without CO₂ capture and purification.

I

Appendix

In this appendix all processes modelled or edited in openLCA, using the *ecoinvent 3.8* data base is presented.

I.1 openLCA Flows

Here, tables for all openLCA-processes, modelled within this thesis, are presented. For descriptions of parameters used in functions in the openLCA-model, see Section 4.10.5.

electrolysis, PEM

Table I.1: openLCA modelling for electrolysis, PEM

electrolysis, PEM			
Flow	Amount	Unit	Provider
Input			
electricity, medium voltage	$50.07 \cdot (1 - \text{electricity_mix})$	kWh	market for electricity, medium voltage electricity, medium voltage Cutoff, U - DE
electricity, medium voltage	$50.07 \cdot \text{electricity_mix}$	kWh	market for electricity, medium voltage electricity, medium voltage Cutoff, U - NO
water, deionised	10,701	kg	water production, deionised water, deionised Cutoff, U - NO
Output			
hydrogen gas	1	kg	
oxygen gas	7,937	kg	

carbon dioxide production, liquid | carbon dioxide, liquid | Cutoff, U

Table I.2: openLCA modelling for carbon dioxide production, liquid | carbon dioxide, liquid | Cutoff, U

carbon dioxide production, liquid carbon dioxide, liquid Cutoff, U			
Flow	Amount	Unit	Provider
Input			
chemical factory, organics	4,00E-10	Item(s)	chemical factory construction, organics chemical factory, organics Cutoff, U - RER
electricity, medium voltage	0.4*(1-electricity_mix)	kWh	market for electricity, medium voltage electricity, medium voltage Cutoff, U - DE
electricity, medium voltage	0.4*electricity_mix	kWh	market for electricity, medium voltage electricity, medium voltage Cutoff, U - NO
Energy, waste	(2.87+0.507)* industrial_heat	MJ	
heat, district or industrial, natural gas	(2.87+0.507)* (1-industrial_heat)* industrial_heat_gas	MJ	market for heat, district or industrial, natural gas heat, district or industrial, natural gas Cutoff, U - Europe without Switzerland
heat, district or industrial, other than natural gas	(2.87+0.507)* (1-industrial_heat)* (1-industrial_heat_gas)	MJ	market for heat, district or industrial, other than natural gas heat, district or industrial, other than natural gas Cutoff, U - Europe without Switzerland
monoethanolamine	0,013	kg	market for monoethanolamine monoethanolamine Cutoff, U - GLO
tap water	0,026	kg	market group for tap water tap water Cutoff, U - RER
Water, cooling, unspecified natural origin	0,0164	m3	
Water, river	8,60E-04	m3	
Water, well	8,30E-04	m3	
Output			
Carbon dioxide, fossil	0,005	kg	
carbon dioxide, liquid	1	kg	
Methane, fossil	0,01	kg	
Monoethanolamine	0,013	kg	
wastewater, average	2,44E-06	m3	market for wastewater, average wastewater, average Cutoff, U - Europe without Switzerland
wastewater, average	2,64E-07	m3	market for wastewater, average wastewater, average Cutoff, U - CH
Water	0,0014	m3	
Water	0,0167	m3	

feed media blend, F2

Table I.3: openLCA modelling for feed media blend, F1

feed media blend, F1			
Flow	Amount	Unit	Provider
Input			
Confidential			
Output			
concentrated feed, F1	5	1	

fermentation, F1

Table I.4: openLCA modelling for fermentation, F1

fermentation, F1			
Flow	Amount	Unit	Provider
Input			
ammonia, anhydrous, liquid	35,659	kg	market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER
Carbon dioxide	2348.9*(1-carbon_purification)	kg	
carbon dioxide, liquid	2348.9*carbon_purification	kg	carbon dioxide production, liquid carbon dioxide, liquid Cutoff, U - NO
concentrated feed, F1	2799	l	feed media blend, F1
electricity, medium voltage	0.0*electricity_mix	kWh	electricity voltage transformation from high to medium voltage electricity, medium voltage Cutoff, U - NO
electricity, medium voltage	0*(1-electricity_mix)	kWh	electricity voltage transformation from high to medium voltage electricity, medium voltage Cutoff, U - DE
Energy, waste	0*industrial_heat	MJ	
ethanol fermentation plant	2,78E-07	Item(s)	ethanol fermentation plant construction ethanol fermentation plant Cutoff, U - CH
heat, district or industrial, natural gas	0*(1-industrial_heat)* industrial_heat_gas	MJ	market for heat, district or industrial, natural gas heat, district or industrial, natural gas Cutoff, U - Europe without Switzerland
heat, district or industrial, other than natural gas	0*(1-industrial_heat)* (1-industrial_heat_gas)	MJ	market for heat, district or industrial, other than natural gas heat, district or industrial, other than natural gas Cutoff, U - Europe without Switzerland
hydrogen gas	297.6*hydrogen_production	kg	electrolysis, PEM - NO
hydrogen, liquid	297.6*(1-hydrogen_production)	kg	market for hydrogen, liquid hydrogen, liquid Cutoff, U - RER
Output			
broth, F1, out, non-purified	47151	kg	
Energy, waste heat, water	4887,459	MJ	
tail gas, F1	0	kg	

broth purification, F1, out

Table I.5: openLCA modelling for broth purification, F1, out

broth purification, F1, out			
Flow	Amount	Unit	Provider
Input			
broth, F1, out, non-purified	1	kg	fermentation, F1
filtered liquid	1	l	membrane filtration
Output			
broth, F2, in, purified	1	kg	

fermentation, F2

Table I.6: openLCA modelling for fermentation, F2

fermentation, F2			
Flow	Amount	Unit	Provider
Input			
ammonia, anhydrous, liquid	18,4641	kg	market for ammonia, anhydrous, liquid ammonia, anhydrous, liquid Cutoff, U - RER
broth, F2, in, purified	47151	kg	broth purification, F1,out
concentrated feed, F1	0	l	feed media blend, F1
electricity, medium voltage	0*electricity_mix	kWh	electricity voltage transformation from high to medium voltage electricity, medium voltage Cutoff, U - NO
electricity, medium voltage	0*(1-electricity_mix)	MJ	electricity voltage transformation from high to medium voltage electricity, medium voltage Cutoff, U - DE
Energy, waste	12239.2*industrial_heat	MJ	
heat, district or industrial, natural gas	12239.2*(1-industrial_heat)* industrial_heat_gas	MJ	market for heat, district or industrial, natural gas heat, district or industrial, natural gas Cutoff, U - Europe without Switzerland
heat, district or industrial, other than natural gas	12239.2*(1-industrial_heat)* (1-industrial_heat_gas)	MJ	market for heat, district or industrial, other than natural gas heat, district or industrial, other than natural gas Cutoff, U - Europe without Switzerland
oxygen gas	0	kg	electrolysis, PEM - NO
oxygen, liquid	369.12* (1-hydrogen_production)	kg	market for oxygen, liquid oxygen, liquid Cutoff, U - RER
Output			
broth, F2, out, non-purified	34591	kg	broth purification, F2, out
broth, F2, out, purge	5000.0*purge	kg	
stripping gas, F2	69380*(1+(1-purge)*125/500)	kg	

broth purification, F2, out

Table I.7: openLCA modelling for broth purification, F2, out

broth purification, F2, out			
Flow	Amount	Unit	Provider
Input			
broth, F2, out, non-purified	34591	kg	
filtered liquid	34591	l	
Output			
-	-	-	

purge sink F2

Table I.8: openLCA modelling for purge sink, F2

purge sink, F2			
Flow	Amount	Unit	Provider
Input			
broth, F2, out, purge	5000	kg	fermentation, F2
electricity, medium voltage	$0.0*(1-\text{electricity_mix})$	kWh	electricity voltage transformation from high to medium voltage electricity, medium voltage Cutoff, U - DE
electricity, medium voltage	$0.0*\text{electricity_mix}$	kWh	electricity voltage transformation from high to medium voltage electricity, medium voltage Cutoff, U - NO
Output			

market for wastewater, unpolluted | wastewater, unpolluted | Cutoff, U

Table I.9: openLCA modelling for market for wastewater, unpolluted | wastewater, unpolluted | Cutoff, U

market for wastewater, unpolluted wastewater, unpolluted Cutoff, U			
Flow	Amount	Unit	Provider
Input			
wastewater, unpolluted	1	m3	
Output			
wastewater, unpolluted	1	m3	treatment of wastewater, unpolluted, capacity 5E9l/year wastewater, unpolluted Cutoff, U - NO

market for treatment of sewage sludge by anaerobic digestion | sewage sludge | Cutoff, U

Table I.10: openLCA modelling for market for treatment of sewage sludge by anaerobic digestion | sewage sludge | Cutoff, U

treatment of sewage sludge by anaerobic digestion sewage sludge Cutoff, U			
Flow	Amount	Unit	Provider
Input			
anaerobic digestion plant, for sewage sludge	6,06E-07	Item(s)	anaerobic digestion plant construction, for sewage sludge anaerobic digestion plant, for sewage sludge Cutoff, U - CH
chemical, inorganic	0,085	kg	market for chemical, inorganic chemical, inorganic Cutoff, U - GLO
electricity, low voltage	3.27*electricity_mix	kWh	market for electricity, low voltage electricity, low voltage Cutoff, U - NO
electricity, low voltage	3.27*(1-electricity_mix)	kWh	market for electricity, low voltage electricity, low voltage Cutoff, U - DE
heat, district or industrial, natural gas	58,83	MJ	market for heat, district or industrial, natural gas heat, district or industrial, natural gas Cutoff, U - Europe without Switzerland
sewage sludge	1	m3	
Output			
Carbon dioxide, biogenic	1,66	kg	
Methane, biogenic	0,056	kg	

treatment of wastewater, unpolluted, capacity 5E9l/year | wastewater, unpolluted | Cutoff, U

Table I.11: openLCA modelling for treatment of wastewater, unpolluted, capacity 5E9l/year | wastewater, unpolluted | Cutoff, U

treatment of wastewater, unpolluted, capacity 5E9l/year wastewater, unpolluted Cutoff, U			
Flow	Amount	Unit	Provider
Input			
electricity, low voltage	0.028*(1-electricity_mix)	kWh	market for electricity, low voltage electricity, low voltage Cutoff, U - DE
electricity, low voltage	0.028*electricity_mix	kWh	market for electricity, low voltage electricity, low voltage Cutoff, U - NO
heat, central or small-scale, other than natural gas	0,013	MJ	market for heat, central or small-scale, other than natural gas heat, central or small-scale, other than natural gas Cutoff, U - Europe without Switzerland
heat, district or industrial, natural gas	0,018	MJ	market for heat, district or industrial, natural gas heat, district or industrial, natural gas Cutoff, U - CH
sewer grid, 5E9l/year, 110 km	2,18E-07	km	sewer grid construction, 5E9l/year, 110 km sewer grid, 5E9l/year, 110 km Cutoff, U - CH
wastewater treatment facility, capacity 5E9l/year	5,69E-09	Item(s)	wastewater treatment facility construction, capacity 5E9l/year wastewater treatment facility, capacity 5E9l/year Cutoff, U - CH
wastewater, unpolluted	1	m3	
Output			
waste graphical paper	0,016	kg	treatment of waste graphical paper, municipal incineration with fly ash extraction waste graphical paper Cutoff, U - CH
waste plastic, mixture	0,016	kg	market for waste plastic, mixture waste plastic, mixture Cutoff, U - NO
Water	0,1	m3	
Water	0,9	m3	

water production, deionised | water, deionised | Cutoff, U

Table I.12: openLCA modelling for water production, deionised | water, deionised | Cutoff, U

water production, deionised water, deionised Cutoff, U			
Flow	Amount	Unit	Provider
Input			
aluminium sulfate, without water, in 4.33% aluminium solution state	2,41E-05	kg	market for aluminium sulfate, without water, in 4.33% aluminium solution state aluminium sulfate, without water, in 4.33% aluminium solution state Cutoff, U - GLO
electricity, medium voltage	2.6E-5*(1-electricity_mix)	kWh	electricity voltage transformation from high to medium voltage electricity, medium voltage Cutoff, U - DE
electricity, medium voltage	2.6E-5*electricity_mix	kWh	electricity voltage transformation from high to medium voltage electricity, medium voltage Cutoff, U - NO
hydrochloric acid, without water, in 30% solution state	3,79E-05	kg	market for hydrochloric acid, without water, in 30% solution state hydrochloric acid, without water, in 30% solution state Cutoff, U - RER
ion-exchanger for water treatment	9,00E-11	Item(s)	market for ion-exchanger for water treatment ion-exchanger for water treatment Cutoff, U - GLO
magnesium oxide	9,14E-06	kg	market for magnesium oxide magnesium oxide Cutoff, U - GLO
sodium chloride, powder	1,12E-04	kg	market for sodium chloride, powder sodium chloride, powder Cutoff, U - GLO
sodium hydroxide, without water, in 50% solution state	8,97E-05	kg	market for sodium hydroxide, without water, in 50% solution state sodium hydroxide, without water, in 50% solution state Cutoff, U - GLO
steam, in chemical industry	1,31E-05	kg	market for steam, in chemical industry steam, in chemical industry Cutoff, U - RER
sulfuric acid	1,91E-04	kg	market for sulfuric acid sulfuric acid Cutoff, U - RER
Water, river	5,35E-04	m3	
Water, well	5,75E-04	m3	
Output			
Aluminium	3,80E-06	kg	
Chloride	1,05E-04	kg	
Magnesium	5,51E-06	kg	
sewage sludge	2,22E-05	m3	market for sewage sludge sewage sludge Cutoff, U - NO
Sodium, ion	9,56E-05	kg	
Sulfate	6,78E-06	kg	
wastewater, unpolluted	8,03E-05	m3	market for wastewater, unpolluted wastewater, unpolluted Cutoff, U - NO
Water	1,42E-05	m3	
water, deionised	1	kg	

water production, ultrapure | water, ultrapure | Cutoff, U

Table I.13: openLCA modelling for water production, ultrapure | water, ultrapure | Cutoff, U

water production, ultrapure water, ultrapure Cutoff, U			
Flow	Amount	Unit	Provider
Input			
cast iron	4,35E-08	kg	market for cast iron cast iron Cutoff, U - GLO
copper, cathode	1,21E-08	kg	market for copper, cathode copper, cathode Cutoff, U - GLO
electricity, medium voltage	0.00546*electricity_mix	kWh	market for electricity, medium voltage electricity, medium voltage Cutoff, U - NO
electricity, medium voltage	0.00546*(1-electricity_mix)	kWh	market for electricity, medium voltage electricity, medium voltage Cutoff, U - DE
ion-exchanger for water treatment	8,89E-11	Item(s)	market for ion-exchanger for water treatment ion-exchanger for water treatment Cutoff, U - GLO
metal working, average for metal product manufacturing	4,35E-08	kg	metal working, average for metal product manufacturing metal working, average for metal product manufacturing Cutoff, U - RER
metal working, average for steel product manufacturing	3,14E-07	kg	metal working, average for steel product manufacturing metal working, average for steel product manufacturing Cutoff, U - RER
nitrogen, liquid	6,63E-06	kg	market for nitrogen, liquid nitrogen, liquid Cutoff, U - RER
seawater reverse osmosis module	1,83E-07	m2	market for seawater reverse osmosis module seawater reverse osmosis module Cutoff, U - GLO
steel, low-alloyed	3,14E-07	kg	market for steel, low-alloyed steel, low-alloyed Cutoff, U - GLO
tap water	1,5	kg	market group for tap water tap water Cutoff, U - RER
ultrafiltration module	7,78E-10	Item(s)	market for ultrafiltration module ultrafiltration module Cutoff, U - GLO
ultraviolet lamp	3,36E-07	Item(s)	market for ultraviolet lamp ultraviolet lamp Cutoff, U - GLO
wire drawing, copper	1,21E-08	kg	wire drawing, copper wire drawing, copper Cutoff, U - RER
Output			
Calcium, ion	5,99E-05	kg	
Carbon dioxide, fossil	1,25E-04	kg	
Chloride	4,13E-05	kg	
Magnesium	3,60E-05	kg	
Nitrate	9,29E-05	kg	
Phosphate	1,35E-04	kg	
Potassium, ion	5,85E-05	kg	
scrap copper	5,42E-10	kg	market for scrap copper scrap copper Cutoff, U - CH
scrap copper	1,16E-08	kg	market for scrap copper scrap copper Cutoff, U - Europe without Switzerland
scrap steel	3,97E-10	kg	market for scrap steel scrap steel Cutoff, U - CH
scrap steel	3,14E-07	kg	market for scrap steel scrap steel Cutoff, U - Europe without Switzerland
Silicon	4,06E-05	kg	
Sodium, ion	3,37E-05	kg	
Sulfate	1,44E-05	kg	
waste bulk iron, excluding reinforcement	1,11E-09	kg	market for waste bulk iron, excluding reinforcement waste bulk iron, excluding reinforcement Cutoff, U - CH
waste bulk iron, excluding reinforcement	4,24E-08	kg	market for waste bulk iron, excluding reinforcement waste bulk iron, excluding reinforcement Cutoff, U - Europe without Switzerland
wastewater, unpolluted	4,25E-04	m3	market for wastewater, unpolluted wastewater, unpolluted Cutoff, U - CH
Water	7,50E-05	m3	
water, ultrapure	xlii	1	kg

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