Accelerating the Green Transition

Investigating the Feasibility of E-Fuel Production Connected to a CHP Plant

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Sammanfattning

Syftet med den här masterupstasen är att undersöka möjligheterna för produktionen av elektrobränslen från koldioxid (CO_2) och vätgas (H_2) integrerat med ett kraftvärmeverk utrustad med koldioxidinfångning (CCS). Detta gjordes genom att undersöka produktionen av e-metan, e-metanol och e-fotogen från infångad CO_2 och H_2 producerad genom elektrolys. Varje process designades och analyserades i Aspen HYSYS. Från Aspen HYSYS togs energiåtgången och produktkraven fram för varje process. Dessa reulstat användes för att bygga produktionsmodellen integrerat med vätgasproduktionen och kraftvärmeverket Filbornvaverket i programvaran Energy Optima 3. Både ett mindre system som använde en del av den infångade CO_2 och ett fullskaligt system som använde all infångad CO_2 modellerades. Alla simuleringar gjordes också baserat på spot priser i SE4 under åren 2021 och 2022.

Den genomsnittliga energiåtgågnen for e-bränslena var 28.8 kWh/kg för e-metan, 9.97 kWh/kg för e-metanol och 37.6 kWh/kg för e-fotogen. Energiåtgången inkluderar prodktionsprocessen och vätgasproduktionen.

Produktionskostnaden var lägst för bassystemet år 2021, 8.9, 2.2 and 16.4 $\text{SEK/kg}_{\text{bränsle}}$ för e-metan, e-metanol och e-kerosene. Högst produktionskostnad erhölls för det storskaliga systemet år 2022. Då blev kostnaderna 31.8, 10.8 and 49.9 $\text{SEK/kg}_{\text{bränsle}}$ för e-metan, e-metanol och e-fotogen. Både för åren 2021 och 2022 var porduktionskostnaden högst för den storskaliga systemet. Den huvudsakliga orsaken bakom detta är att kraftvärmeverket inte kan stå för lika hög andel av elektrisitetsbehovet för produktionsprocessen för det storskaliga systemet. Detta gör att kostanden för elektrisiteten blir väldigt hög.

Resultaten visar att integreringen av e-bränsleproduktionen med kraftvärmeverket kan leda till lägre produktionskostnad och energibehov. Fler aspekter från detta arbetet behöver dock undersökas för att kunna klargöra hur mycket lägre det kan bli. Den huvudsakliga faktorn som påverkar produktionskostnaden är kostanden för elektricitet och, den huvudsakliga faktorn som påverkar energiåtgången är produktionen av vätgas. Störst reduktion kan därmed fås genom att maximera mängden elektrisitet som kan levereras av kraftvärmeverket och att undersöka andra effektivare tekniker för produktionen av vätgas. Det kan dock konstateras att det finns stor potential för integrering av e-bränsleproduktionen med ett kraftvärmeverk.

Abstract

The overall purpose of this thesis is to investigate the feasibility of producing electrofuels from CO_2 and H_2 in connection to a CHP plant equipped with carbon capture technology. This is done by investigating the production of e-methane, e-methanol and e-kerosene from captured CO_2 and H_2 produced from electrolysis. Each of the processes is designed and analyzed in Aspen HYSYS. From this, the energy and product requirements for each process are obtained. With these results, a production model including the electrofuel and hydrogen production, integrated with the CHP plant Filbornaverket, were modelled in the software Energy Optima 3. Both a smaller system using only part of the captured CO_2 and a system at full scale using all the captured CO_2 are developed. Furthermore, the simulations were done for spot prices in SE4, for both 2021 and 2022.

Average energy demands for the e-fuels were 28.8 kWh/kg for e-methane, 9.97 kWh/kg for e-methanol and 37.6 kWh/kg for e-kerosene. This includes the manufacturing process and hydrogen production.

Production costs were lowest for the base case 2021, where e-methane, e-methanol and e-kerosene had production costs of 8.9, 2.2 and 16.4 $\text{SEK/kg}_{\text{fuel}}$ respectively. The highest production costs were for the full case 2022, where the costs were 31.8, 10.8 and 49.9 $\text{SEK/kg}_{\text{fuel}}$, following the same order. For both 2021 and 2022, the production costs were higher for the full scale case than the base case. The main reason for this is that the CHP plant could not supply the processes with as much electricity, meaning the electricity costs for production quickly became high.

The findings showed that integration of e-fuel production with a CHP plant could result in a lower production cost and energy demand. However, there are still many aspects of this project that needs to be further investigated to be able to say to which extent. The main factor affecting the production cost was electricity prices. And, the main factor affecting the energy demand was hydrogen production. Maximizing the amount of electricity contributed to the e-fuel production from the CHP plant as well as researching other hydrogen production techniques are therefore the largest reduction possibilities. From this, it can still be concluded that there is great potential in integrating e-fuel production with a CHP plant.

Keywords: CCU, CHP plant, e-fuels, e-methane, e-methanol, e-kerosene

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Nomenclature

Abbreviations

AEC	Alkaline Electrolysis Cell
ASF	Anderson-Flory-Schulz
CAPEX	Capital Expenses and Expenditure
CCS	Carbon Capture and Storage
CCU	Carbon Capture and Utilization
CHP	Combined Heat and Power
DAC	Direct Air Capture
EO3	Energy Optima 3
ETS	Emissions Trading System
FT(S)	Fischer-Tropsch (Synthesis)
GHG	Greenhouse Gas
HTFT	High-Temperature Fischer-Tropsch
IMPCA	International Methanol Producers and Consumers Association
LHV	Lower Heating Value
LTFT	Low-Temperature Fischer-Tropsch
O&M	Operation and Maintenance
PEMEC	Polymer Electrolyte Membrane Electrolysis Cell
PM	Particular Matter
PtX	Power-to-Fuel
RED	Renewable Energy Directive
rWGSR	Reverse Water Gas Shift Reaction
S/C	Steam-to-Carbon
SAF	Sustainable Aviation Fuel
SMR	Steam Methane Reforming
SNG	Synthetic Natural Gas

Chemical Compounds

C_2H_5OH	Ethanol
$C_{8-16}H_n$	Kerosene
CeO_2	Cerium Dioxide
CH_3OCH_3	Dimethyl Ether
CH_3OH	Methanol
CH_4	Methane
CO_2	Carbon Dioxide
CO	Carbon Monoxide
Co	Cobalt
Cu	Copper
Fe	Iron
H_2	Hydrogen Gas
KOH	Potassium Hydroxide

NaOH	Sodium Hydroxide
Ni	Nickel
NO_x	Nitrogen Oxides
O_2	Oxygen Gas
SiO_2	Silicon Dioxide
ZnO	Zink Oxide

Symbols

$\dot{m}_i$	Mass Flow Rate of Species *i*
η_i	Efficiency of i
α	Chain Growth Probability
h	Enthalpy
M_i	Molecular Weight of Species *i*
m_i	Mass of Species *i*
S_{C5+}	Selectivity of Hydrocarbons Longer than 5 Carbon Atoms
x_i	Mole Fraction of Species *i* in the Liquid Phase
y_i	Mole Fraction of Species *i* in the Vapour Phase

Chapter 1

Introduction

Today, humankind faces an enormous challenge: to stop global warming before the earth becomes uninhabitable. It is now widely accepted that global warming is real and caused by humans' excessive burning of fossil fuels in the latest century. In 2015, a historic deal was made called the Paris Agreement, which included the 1.5 °C target stating that all signing countries should contribute to limiting the temperature increase to 1.5 °C. Many measurements have been taken since then to limit global warming, but the realization is that today, in 2023, it seems like this target will be exceeded (United Nations 2022). There is a need for fast acceleration in the transition to limit climate change, and it needs to start now. The EU has been and still is one of the world's highest polluters. In the last three decades, however, the EU has put much effort into climate and energy policies. This has resulted in a reduction of greenhouse gas (GHG) emissions from all sectors except for transport. EU recently adopted the European Green Deal, which states that a 90 % reduction, compared to levels in 1990, of GHG emissions from the transport sector is needed by 2050 to reach climate neutrality (EEA 2021).

To accomplish this reduction the general agreement is that the main solution is electrification of the transport sector. Electrification is the most suited solution for smaller vehicles and short transportation, such as buses in rural areas. For larger vehicles and long-distance transport, electrification will be more difficult. The biggest problem is that the required batteries would merely be too heavy. To cope with decarbonisation, other alternatives need to be considered for vehicles such as large ships and aviation. One alternative is bio-based fuels produced from waste or non-edible crops. There is however not enough feedstock to meet the demand, and so other alternatives are also needed (Gross 2020).

It is also clear that only mitigating efforts will not be enough. To accelerate towards net zero emissions, carbon dioxide (CO_2) also needs to be removed from the atmosphere (IEA 2020a). This can be done by carbon capture and utilization or storage (CCUS) technologies. Via a range of different technologies, CO_2 can be captured from the air or point sources such as exhaust gases from a combined heat and power (CHP) plant. CO_2 can then be stored or utilized and recycled (IEA 2021).

One promising alternative in using captured CO_2 is for the production of fuels produced with hydrogen (H_2). These types of fuels are referred to as electric fuels, or e-fuels since they are produced with renewable electricity. E-fuels have many advantages compared to electricity in terms of easier storage possibilities, higher energy density and possibilities in using existing infrastructure (Soler and Yugo 2019). As the production of bio-fuels is more expensive than their fossil counterpart and e-fuels tend to have an even higher production cost, much is still needed in terms of research to investigate the production possibilities (Schemme et al. 2020; Fagerström et al. 2022; Brynolf et al. 2018).

1.1 Problem Statement

Today, high prices for e-fuel production are the main limiting factor for rapid production up-scaling. As mentioned, emission reduction in the transport sector needs to accelerate and electrification in heavy transport will be hard. E-fuels offer a green alternative and can be used directly or with slight modifications by vehicles (IRENA and Methanol Institute 2021). Fagerström et al. (2022) found in their work that significant energy reductions could be made when the production of e-kerosene was integrated with a CHP plant in Sweden. This approach was therefore chosen to address the problem stated and apply to local conditions in Skåne to investigate the feasibility of e-fuel production in the area.

1.2 Aim

The overall purpose of this thesis is to investigate the feasibility of producing electrofuels from CO_2 and H_2 in connection to a CHP plant equipped with CCS. The aim is to investigate if any synergies can be made by integrating the production with a CHP plant. This is done to provide knowledge to the industry sector to help accelerate the implementation of e-fuel production, mainly in Skåne. Which will also contribute to the green transition in the energy sector.

1.3 Research Questions

To answer the aim, this work was based on three research questions:

- To what cost can e-fuels be produced from integrated production with a CHP plant?
- How much energy will the production of e-fuels require?

- What positive synergies - if any, are there with integrating the production of e-fuels with a CHP plant?

1.4 Method

In this master thesis, the integration of e-fuel production process with a CHP plant is investigated. This was done to investigate the possibilities of e-fuel production in Sweden, Skåne. The work was conducted together with Energy Opticon and in collaboration with Öresundskraft. First, a literature study was done to investigate which e-fuels seemed most useful to explore. Which type of production process was most suited was also conducted from the literature, based on applicability and technical matureness.

In Figure 1.1, the model that was built and investigated for this work is shown as an overview. First a small literature study was conducted to investigate which e-fuels would be most fit to include in the work. Three e-fuels were chosen to include in this thesis, e-methane, e-methanol and e-kerosene. However, from now on they will be referred to as methane, methanol and kerosene except for when there needs to be a distinction between them and their conventional counterparts. Methanol and kerosene were chosen based on their possible application as fuel for larger vehicles and methane was chosen for the chance to investigate whether the natural gas used in Helsingborg can be exchanged for locally produced e-methane. Then the e-fuel production processes were modelled in Aspen HYSYS provided by the Faculty of Engineering, LTH. This was done to obtain all energy and product requirements that were needed for each process. The next step was to model the e-fuel production integrated with the CHP plant, Filbornaverket, in Energy Optima 3 (EO3). More information about Filbornaverket can be found in Section 2.3.2. The production was optimized over a year for both a base case and a full scale case. This was done to obtain the production prices for the fuels and to investigate if any synergies could be found between the CHP and the production process. A more thorough method description of how the model was built in Aspen is described in Chapter 5 and the model in EO3 is described in Section 6.2.

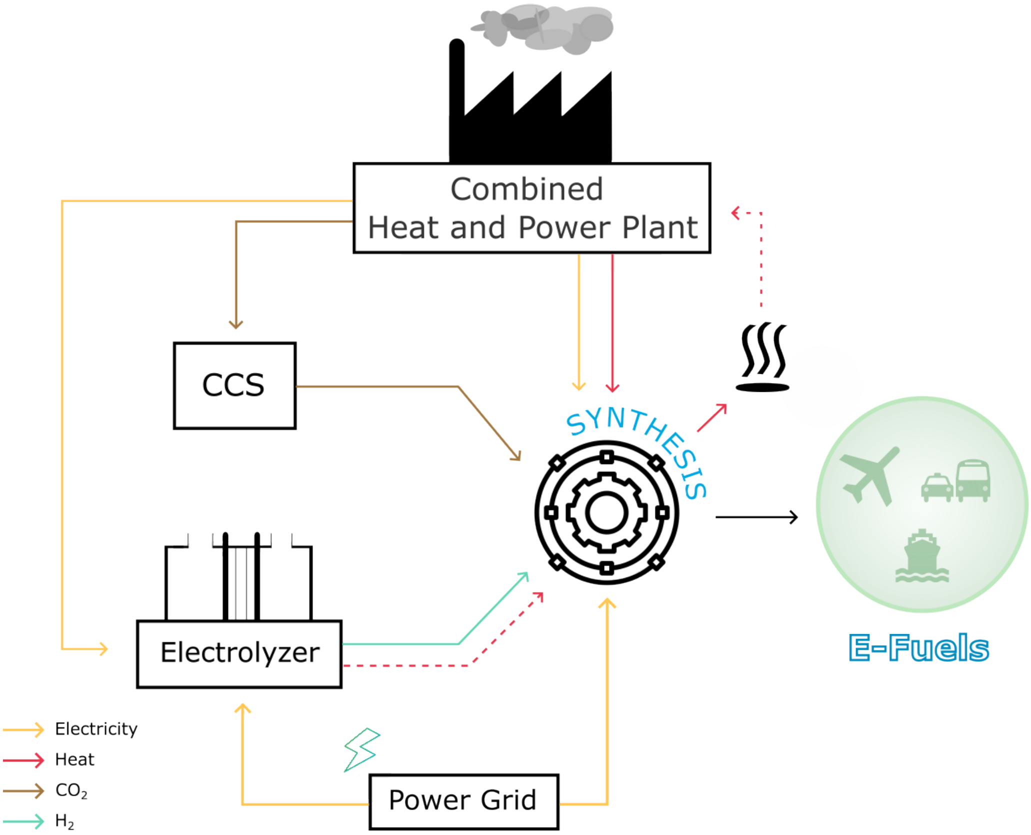


Figure 1.1: A schematic picture of the integrated system developed in this work. Arrows are displayed in different colours depending on the energy type.

This master thesis was, as mentioned, conducted together with the company Energy Opticon. Energy Opticon offers software, EO3, as an IT solution for energy companies. The software can model and optimize most energy systems and aims at reducing total production and operational costs. More in detail about the software and how it was used in this work can be seen in Section 6.2. Energy Opticon provided this work with the possibility to model the e-fuel processes in integration with the already existing CHP plant, Filbornaverket. They also provided real condition parameters for the optimization, such as the district heating load of Helsingborg and the spot price for electricity in SE4 in Sweden.

1.5 Delimitations

Some delimitations were established to define the scope of the work. These are listed below:

- The exploration of the use of CO_2 is limited to the production of three e-fuels: methane, methanol and kerosene.

- Focus of the work is on utilization and the carbon capture process was excluded.
- No consideration was taken to the limits of the power grid in Helsingborg.
- Minimal consideration was taken to size limits for the CCU facility.
- No pumps for circulation or cooling water are included in the model.
- Legal permits and safety measurements for building this type of facility in connection to a CHP plant are not included.
- No investigation on the possibilities of utilizing oxygen from the electrolyser is included.
- No deep investigation on the possibilities of using the waste heat of low temperatures from the CCU process is included.
- No other technology than electrolysis for producing hydrogen is included.
- The feasibility of this project is based on Swedish spot prices in SE4 from 2021 and 2022, and has only been explored in connection to Filbornaverket.
- No electricity grid taxes were included in the model.
- Operation and maintenance (O&M) costs for the production of e-fuels were not included in the model.
- The model for the CCS process was attained from Öresundskraft and was not studied in detail.

1.6 Division of Work

Both authors have been included in all parts of the thesis. Alice has been most in charge of the modelling done in Aspen HYSYS while Johanna has been most involved in the writing of Chapters 3 and 4. Johanna was in charge of the modelling in EO3. Alice has been in charge of making the schematic figures. Both have been equally involved in writing Chapters 2, 5, 6, 7, 8 and 9.

1.7 Ethics

Some ethical aspects should be raised regarding this master thesis. The main goal of this thesis is to contribute to the green energy transition of the future by providing new information to the industry sector regarding e-fuel production integration with a CHP plant. In the processes, there is a need for metals as catalysts, that are rare and mined during questionable ethical conditions. Cobalt (Co), for example, is a rare metal used in lithium-ion batteries that are present in almost all modern-day electronics. The Democratic Republic of Congo is one of the largest exporters of Co in the world and there are frequent reports of miserable mining conditions and child labour (Davie 2022). Extraction of metals can also cause emissions of GHG, as well as irremediably change the local environment. These problems are not discussed or taken into consideration in this work.

1.8 Disposition

Here, a summary of each chapter will be presented to get an overview of the master thesis. In this first chapter, *Introduction*, the subject is presented together with the problem statement and the research questions. The method used in this work to answer the research questions is also described.

Chapter 2, Background, provides relevant background information for the understanding of the subject.

Chapter 3 and 4, Hydrogen and Manufacturing process of e-fuels, explains the theory behind hydrogen production and the production of e-fuels together with data from other sources examining similar topics. Literary values used in this work regarding investment costs and efficiencies are also presented.

Chapter 5, Process Modelling, explains how the model was designed in Aspen HYSYS, along with all parameters used in the software.

Chapter 6, System Modelling, first presents the results from Aspen HYSYS as these results are used as input parameters for the model in EO3. The model built in EO3 is then explained along with all parameters used. The different cases are also presented in detail.

Chapter 7, Results, shows all results from the model in EO3, as well as total results from both Aspen HYSYS and EO3. Numbers for efficiencies and investment costs are also presented.

Chapter 8, Discussion, provides a discussion and analysis regarding the results along with the methods used in this work.

Chapter 9, Conclusion, presents the conclusions of the thesis, answers to the research questions along with recommendations for future work.

Chapter 2

Background

2.1 Carbon Capture and Utilization (CCU)

Carbon capture and utilization (CCU) is a term for a wide range of technologies that involve capturing CO_2 and using it. Either directly or as a feedstock (IEA 2021).

2.1.1 Carbon Capture and Storage (CCS)

There are several different technologies for capturing CO_2. One procedure is capturing it directly from the air, referred to as direct air capture (DAC). It can also be captured at point sources, e.g. in exhaust gases released from a power plant. When storing the captured CO_2, it is called carbon capture and storage (CCS). There are several different storage possibilities. Commonly CO_2 is injected in deep geological formations, often empty oil reserves or porous rock below an impermeable layer. If the captured CO_2 has a biogenic origin it is referred to as bio-CCS or in terms of CCS connected to energy production from biomass, BECCS (IEA 2021).

2.1.2 Using Carbon

Additional to storing captured CO_2, it can also be repurposed. There are several opportunities for this usage. Typically it is divided into two categories, direct use or feedstock for other products. Direct use includes using CO_2 in the food and beverage industry as a solvent, heat transfer fluid and yield-boosting biomass growth. When used as feedstock, CO_2 can be used to make fuels, building materials or chemicals (IEA 2021).

2.1.3 Synthetic Fuels

Synthetic fuels are artificially produced and designed to mimic the properties of fossil fuels. They can be used in many of the same areas as fossil fuels, including transportation. Since synthetic fuel production is more sustainable and flexible, in terms of storage and transportation, it is worth exploring the potential of synthetic fuels as a substitute for fossil fuels. These fuels could potentially lead to a more reliable source of energy (Vishal and Salkuti 2023).

Synthetic fuels are produced from syngas, a mixture of CO and H_2. There are various types of synthetic fuels, and the type of fuel produced depends on the feedstock and which production processes are used. These processes are also often referred to as power-to-fuel (PtX), power-to-liquid (PtL) or power-to-gas (PtG). Two kinds of fuels are biofuels, fuels produced from biomass, and e-fuels, fuels produced using renewable energy sources (Diab et al. 2022). Some of the more common fuels are described next.

Methane

Methane (CH_4) is the lightest hydrocarbon, also known as natural gas if the gas is of fossil-based origin. Methane can also be synthesized using biological or catalytic renewable processes and is then referred to as synthetic natural gas (SNG) (Fagerström and Nyberg 2022). Methane is used in many areas, as a fuel and in the chemical industry (Konsumenternas energimarknadsbyrå 2020).

Methanol

Methanol (CH_3OH) is an alcohol widely used in the industry sector, mainly for producing other chemicals. Methanol can be produced both from fermenting biomass and through catalytic processes. To a certain degree, it is possible to mix methanol with gasoline and use that mixture as a fuel in conventional engines. In the EU, the maximum amount that is allowed is 3 % of methanol. It is possible to run vehicles on blends with 50–80 % methanol, however, the engine then needs to be modified (IRENA and Methanol Institute 2021).

Ethanol

Ethanol (C_2H_5OH) is an alcohol used in many areas. In the chemical industry, ethanol can be used as a solvent or to synthesize other chemicals. There are two main production processes for ethanol: fermentation and hydration (Britannica 2022b). Similarly to methanol, ethanol can also be used as a fuel when mixed with gasoline. Ethanol can not be added in high ratios with gasoline without engine modification. Currently, in Sweden, gasoline is mixed with up to 10 % ethanol. (Transportstyrelsen 2022).

Dimethyl Ether (DME)

Dimethyl ether (CH_3OCH_3) has similar properties to methanol, and the chemical formula is almost the same. DME is used as a solvent, refrigerant and as an intermediate in the synthesis of other chemicals. It can also be used as a fuel since it has good combustion properties. DME can be produced from methanol synthesis or direct synthesis of syngas. DME can not be blended directly with diesel and used in a diesel engine. That is because of the properties of the DME special tank and the ignition modifications that are required (Semmel et al. 2021).

Kerosene

Kerosene ($C_{8-16}H_n$) is a hydrocarbon mixture that is used as lamp oil, solvent, insecticide and jet fuel components. Kerosene is conventionally produced from oil by distillation or cracking (Britannica 2022a). Another kerosene production possibility is through Fischer-Tropsch synthesis (FTS) (Pearson and Turner 2014).

2.1.4 Sustainable E-fuels

For an e-fuel to be considered renewable, or green, the CO_2 must be obtained through DAC or from exhausted gases from burning biomass (IRENA and Methanol Institute 2021). Together with green hydrogen, it can then be synthesized into green e-fuels. Hydrogen is considered ”green” when produced from electrolysis using renewable electricity. Otherwise, if produced from fossil fuels, it is called grey hydrogen. However, if produced from fossil sources accompanied by CCS, it is labelled blue hydrogen (IRENA 2020). The most environmentally damaging type of hydrogen is brown hydrogen, which is produced using coal. Although there is no established classification system for e-fuels, they can be classified in the same way as hydrogen, see Figure 2.1.

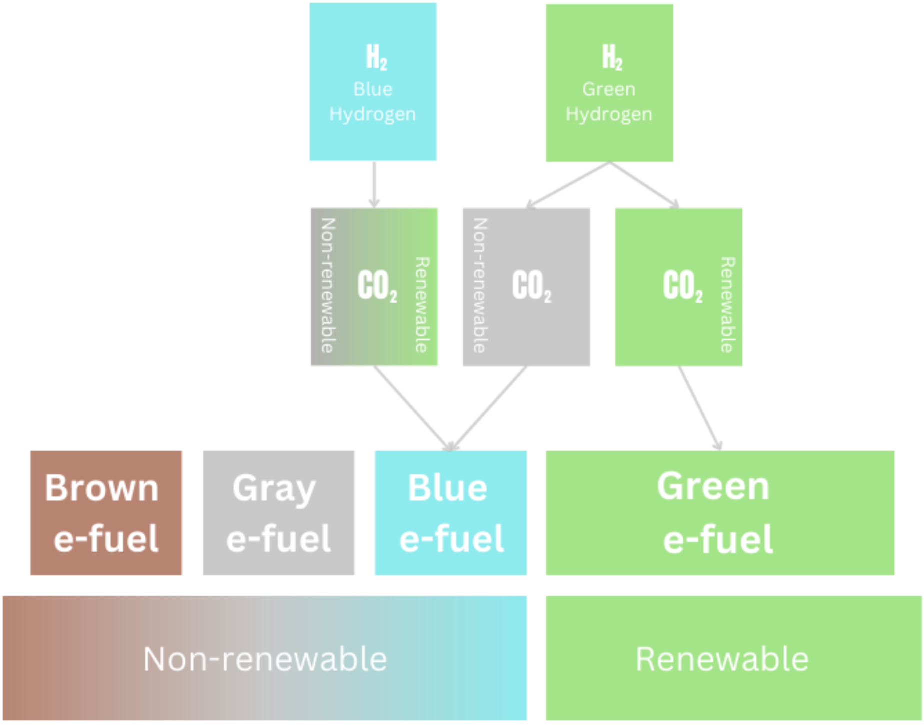


Figure 2.1: Types of e-fuels. Inspired by IRENA and Methanol Institute (2021).

Using green hydrogen and renewable CO_2 is not the only thing that establishes whether an e-fuel is green. In section, 2.2, legislation concerning the use and production of e-fuels is discussed.

2.1.5 Chosen E-fuels

The production of three e-fuels will be studied in this thesis: e-methane, e-methanol and e-kerosene. As already mentioned, they will be referred to without their e-prefix. Methane was chosen because there is a methane demand from the industry sector in Helsingborg in the form of natural gas. Natural gas is used as fuel in many applications such as fuel for vehicles, in the industry sector and for heating and cooking. Natural gas has fossil origin and is found dissolved in oil or gas caps above the oil (Carruthers et al. 2023). A green alternative to natural gas is biogas, a mixture containing mainly methane but also CO_2 and small amounts of other gases. Biogas is produced from digestion by microorganisms under anaerobic conditions (IEA n.d.). Prices for natural gas increased by more than 100 % between 2021 to 2022 in Sweden and Europe due to the Russian war in Ukraine. Before the war, natural gas prices were low, below 20 €/MWh, and reached their all-time high, 320 €/MWh in August 2022. Since then, prices have dropped again

(Trading Economics 2023b; Sheppard 2023). Biogas prices followed the natural gas prices and rose from around 60 €/MWh in early 2021 to 300 €/MWh in August 2022 (Öresundskraft n.d.). Current market and production prices for natural gas and biogas are compiled in Table 2.1.

Methanol was chosen because it is a very promising fuel for marine ships, among various other interesting areas of application. Already today, there are large ships and ferries powered by methanol. Methanol has no sulphur content compared to conventional diesel bunker fuel in this sector. It also has very low emissions of particular matter (PM) and nitrogen oxides (NOx) during combustion. Methanol produced today mainly stems from fossil fuels such as natural gas or coal. The main use for methanol, as for now, is in the chemical industry. 2019, the yearly production was around 98 million tons. This amount emits 0.3 Gt of CO_2 annually in life-cycle emissions. Producing fossil-based methanol costs between 100–250 USD/t (see Table 2.1) (IRENA and Methanol Institute 2021).

Kerosene was picked because of its application as aviation fuel. The aviation sector stands for 2.5 % of today's global emissions, and emissions from this sector are increasing fast (EASA 2022). It is currently highly uncertain to what extent batteries will be able to support longer transports, e.g. by, airplanes or trucks. Therefore, electro- or bio-based fuels are an option for the aviation sector to reduce its GHG emissions. With conventional bio-based fuels, there is the limitation of available biomass. Aviation fuel can instead be produced from captured CO_2 and green hydrogen. Then no pressure is added on land use and production of biomass (Fagerström et al. 2021). A group term for jet fuels produced from biomass or through synthesis processes is sustainable aviation fuels (SAF). Production cost and market price for fossil-based and bio-based jet fuel can be seen in Table 2.1 (IEA 2022).

Table 2.1: Market and production prices for Methane, Methanol and Kerosene.

Fuel	Price [SEK/kg]	Comment	Source
Natural gas (fossil)	10.3	Market price February 2023, Sweden	[1]
Methane (bio-based)	18.8	Market price February 2023, Sweden	[1]
Methane (bio-based)	8.29	Production cost 2020	[2]
Methanol (fossil)	0.86 - 2.15	Production cost	[3]
Methanol (bio-based)	2.75 - 6.61	Production cost	[3]
Jet-fuel (fossil)	1.54 - 4.10	Production costs 2010-2020	[4]
Jet-fuel (fossil)	5.36	Market price 2021	[4]
Kerosene (bio-based)	9.65 - 13.9	Production cost 2021	[4]

[1] Öresundskraft n.d., [2] IEA 2020b, [3] IRENA and Methanol Institute 2021, [4] IEA 2022,

2.2 Legislation

Multiple legislations apply to the production of e-fuels. On the highest level, e-fuel-production in Sweden follows EU legislation. For the production of e-fuels, it is mostly classification rules that are important from the EU level. Introduced in 2009 and legally binding since 2021, the renewable energy directive (RED) determines whether a fuel is considered sustainable. This directly affects the possibility of allocating the CO_2 used. The RED is currently under review, and a new version will be available soon. In this new version, there will be higher demands for which type of biomass can be labelled sustainable. The reason is to make it harder to use high-quality wood for energy reduction and to favour biodiversity in forests. Most recently, on the 30^{th} of March 2023, a provisional agreement was made within the RED. Raising the renewable energy target for 2030 from 32 % to a minimum of 42.5 %, but preferably 45 % (European Comission 2022; Personlig komunikation, Öresundskraft 2022).

EU has a package of legislative proposals called "Fit for 55". One of those proposals is a 2035 ban on sales of conventional cars, i.e., by 2035, there will be 100 % CO_2 emission reductions on new vehicles. The proposal passed in March of 2023. When it went through, the proposal brought with it the most recent update on the status of e-fuels since it came with a somewhat last-minute demand from Germany: that the ban should exclude e-fuels. The proposal was said to raise the production of, among other things, electric- and hydrogen cars (Council of the EU 2023; Autovista Group 2023). Now this will presumably be the case for e-fuel-driven ones too.

Another proposal from this package is the ReFuelEU Aviation proposal. That proposal passed in March 2023 as well. This now means aviation fuel must have a minimum share of 2 % SAF, at EU airports, by 2025. By 2050, that number should be 70 % (European Commission 2023).

At the end of 2022, Öresundskraft wrote a paper about CCU as an alternative to CCS. The main question was whether allocating CO_2 from waste flue gases to CCUS would be possible. The conclusions from this compilation were:

- There are no specific regulations concerning this issue, neither on national nor international levels.
- Looking at the current regulations, it seems to require physically measured CO_2 composition, even if allocation gives the same climate benefit.
- The amount of CO_2 that counts as renewable from waste incineration depends, and can be anything between 0–100 %. It can vary because of regulations, stakeholder agreements and interpretation.

(Öresundskraft 2022)

Their findings show how unclear the regulations concerning which kinds of CO_2 are allowed to count as green are for CCUS processes. Vague rules make it harder to get into the CCU industry. However, CCU is still very much under development, as are the associated regulations and legislations.

2.2.1 Price on CO_2-Emissions

To push and encourage society and the industry sector to emit less CO_2, different taxes have been implemented in Sweden since early 1990. Today there are taxes for emitting CO_2, energy taxes for producing electricity and taxes for fuels (Rydner 2022). On top of this, EU regulations also apply in Sweden. 2005, the EU launched the emissions trading system (ETS). ETS puts a cap on emissions for all involved parties, that are reduced gradually every year. Industries included in the system stand for around 45 % of the EU's CO_2 emissions. Heavy industries, energy suppliers and aviation are the ones included in the CO_2 emissions cap. The emission cap is divided between countries and industries as emissions allowances. This puts a price on carbon since allowances can be bought and sold on the ETS market (European Comission n.d.). Historically, the cost per allowance has been low, around 5–20 €/t_{CO_2} in the years 2005-2020. Since 2020 prices have increased fast and are now around 80 €/t_{CO_2} (Trading Economics 2023a).

Most actors currently included in the ETS in Sweden don't pay extra taxes for CO_2 emissions, or they pay a reduced price. CHP plants were charged from 2019 until 2022 with a CO_2 tax of 91 % compared to the full CO_2 tax. From the 1^{st} of January 2023, this tax was removed for CHP plants and thermal power plants (Rydner 2022; Finansdepartementet and Skatte- och tullavdelningen 2022). This means that the price for emitting CO_2 from a CHP plant in Sweden is only dependent on the price for emission allowances.

2.2.2 Product Requirements for E-fuels

There are not yet any set specifications for e-methane on the market or in Sweden. There are specifications (EN 16723) for bio-methane that is to be injected into the natural gas grid. These conditions are that the gas can contain a maximum of 2.5 % CO_2 at injection and the methane number should be a minimum of 65. There are several ways to calculate the methane number. To comply with the European standard, the calculation should be performed according to standard EN 16726 (Swedish Institute for Standards 2018; Swedish Institute for Standards 2016).

Not either for e-methanol is there a specific European standard but there is for methanol sold on the market. International methanol producers and consumers association (IMPCA) have conducted a standard specification that covers methanol but can apply to e-methanol as well. Conditions for methanol according to this standard is purity of 99.85 wt%/wt% on a dry basis and water content of a maximum of 0.1 wt%/wt% (IMPCA

2021). For methanol that is blended with conventional petrol, only 3 % methanol is allowed in the mix according to the standard EN 228 (Swedish Institute for Standards 2017b). There is also a standard for fuels with a 70–85 % blend of methanol, ASTM D5797-07 and for pure methanol, ASTM D-1152/97, which also complies with the IMPCA standard. Cars that run on fuels with high blends of methanol need special engines since it has lower ignition properties than conventional petrol and diesel (IEA - AMF n.d.; Swedish Institute for Standards 2017a).

More can be found about e-kerosene and SAF as the aviation fuel community has included specifications for a range of aviation fuels from non-fossil sources. One specification is based on the standard for fossil aviation fuels and is called ASTM D7566 - ”Standard Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons”. ASTM International Aviation Fuel Subcommittee has conducted this standard and specific criterion for non-fossil-based aviation fuel. E-kerosene still has to meet the same requirements as conventional aviation fuel such as the most important criteria of a freezing point at -40 °C and maximum viscosity of 8 mm^2/s at -20 °C. In ASTM D7566 specific requirements can be found such as the maximum blend limit for e-kerosene with conventional aviation fuel of 50 % for e-kerosene produced with Fisher Tropsch with an aromatic content of 8–20 % (Rumizen 2021).

2.3 Combined Heat and Power Plant

A CHP plant or cogeneration plant is a power plant that produces both heat and electricity. In most CHP plants, electricity is generated through a turbine. First, a pressurized heat transfer fluid, typically water, is heated by combustion. This forms overheated steam, which is transferred to the turbine. In the turbine, heat is converted to mechanical energy and the gas pressure drops. The steam leaving the turbine is still extremely hot and needs to be cooled down again before being circled back into the system. The remaining heat in the steam can be utilized for district heating. It is transferred to the district heating network through a condenser where the gas is condensed to water. Additionally, the mechanical energy is generated into electrical energy in the generator (Fredriksen and Werner 2014, pp. 147–159).

Big CHP plants are more complex than this simplified description, but they all work from this principle. A CHP plant can operate on a variety of fuels if the combustion is located outside of the closed circle with the turbine. For example; a CHP plant with a steam turbine (Fredriksen and Werner 2014, pp. 147–159).

CHP plants produce both steam and electricity which is required in the e-fuel production process (see Chapter 4), steam for heating and electricity for compressors and pumps. This gives possibilities for positive synergies between the production of e-fuel in integration with a CHP plant.

2.3.1 Swedish Context

Around the world, there is a strong correlation between the share of electricity generated from CHP plants in a country and how large of a district heating network the country has. In Denmark, for example, CHP plants stood for around 60 % of the country's electricity production (TWh) in 2005 but have since decreased due to Denmark's fast implementation of wind power. District heating in Denmark also stood for around 50 % of the heat market in 2005. This is, however, not the case in Sweden. Even though district heating in Sweden has around 60 % of the heat market (TWh) since 2006, electricity generated from CHP plants only stood for around 5 % (TWh) in 2006 and it has not increased drastically. This can be explained by the extensive access to other cheap electricity sources in Sweden, such as hydropower (Fredriksen and Werner 2014, pp. 35–149; Danish Energy Agency 2023; Energimyndigheten 2023).

Today the fuel mix for CHP plants in Sweden consists of more than 90 % renewable and recycled fuels. This fuel is mostly biomass from the forest, such as branches, leaves and trunk pieces. The rest is waste from the industry sector or households (Energiföretagen 2017). Despite this, the district heating industry has condemned going even further in its work for climate neutrality. By 2030 the district heating industry has set a target to be entirely carbon neutral. After this, the target is to be a carbon sink by 2045 (Fossilfritt Sverige 2020).

2.3.2 Filbornaverket

Filbornaverket is a CHP plant located in Helsingborg, Sweden. As mentioned in Section 1.4, this work will be based on the power system of Filbornaverket. Filbornaverket is a relatively new facility that was taken into operation at the beginning of 2013. It was built and is owned by Öresundskraft and Helsingborg City. Fuels used are mainly waste and small amounts of forest residues, and the CHP plant has a nominal district heating effect of 72 MW and 18 MW of electricity. The CHP plant is also equipped with state-of-the-art flue gas cleaning, that ensures that emissions from the plant are far below legal boundaries (Öresundskraft n.d.[a]). In 2015 the district heating network between Lund, Landskrona and Helsingborg was connected via the EVITA pipeline. This means higher delivery dependability of district heating in all connected cities. It also means higher possibilities of balancing the load in the network (Landskrona Energi n.d.). Öresundskraft has ongoing plans to equip Filbornaverket with a carbon capture unit that will be in place in 2027. This is to contribute to Skånes and the Swedish environmental goals to be climate neutral by 2045 (Öresundskraft n.d.[b]).

Waste as fuel

In Sweden, waste that is incinerated is waste that can not be recycled in other ways. It constitutes around half of the municipal waste. Burning waste with very high energy efficiency is according to the EU framework directive almost as good as recycling (Avfall Sverige 2022), even though energy recovery from waste is below recycling on the waste hierarchy (European Commission n.d.). Swedish waste that is incinerated with energy recovery today contains around 12 % plastic. This number is probably even higher since Sweden also imports a lot of waste from neighbouring countries (Andersson 2022). As mentioned in Section 2.2, the plastic content in waste that is incinerated in Sweden is problematic since it has fossil origin. But plastic also contains a lot of energy and when the plastic content is removed from the waste, the energy content of the waste will decrease (Energimyndigheten 2021).

2.4 The Swedish Energy Sector

2.4.1 Electricity Mix

In this work, hydrogen is produced by water electrolysis. The model and technique for that are described in Section 3. Water electrolysis requires electricity which will be provided by the electricity grid or the CHP plant. Electricity from the grid in Sweden is produced from a range of sources. The largest part of electricity produced in Sweden comes from renewable and nuclear sources. Looking over the whole year, Sweden has a net export of electricity of 25 TWh in 2020. Despite this, looking at the hourly values Sweden also imports electricity from its neighbouring countries. The highest import is from Denmark and Norway but Sweden also imports small amounts of electricity from Finland, Germany, Lithuania and Poland (Statistikmyndigheten 2022; Energimyndigheten 2023). These countries do not have the same electricity mix as Sweden and especially Germany and Poland has very high GHG intensity in their electricity production. This is due to that these countries are still using a lot of coal-fired power plants (European Environment Agency 2022). This makes labelling the produced H_2 tricky since the electricity used will be mostly green but sometimes electricity from non-renewable sources will be used. Electricity from the CHP plant itself can also be used and this electricity comes from burning waste or biomass. It is not clear if this can be labelled green either, as discussed in Section 2.2.

2.4.2 Electricity Prices 2021 and 2022

The optimizations in this work will be run on data from the years 2021 and 2022. There are a lot of differences between these years in terms of prices for electricity for example.

In 2021, the extreme electricity prices in Sweden had not yet arrived even though the average price of the year (0.63 SEK/kWh) at Nord Pool Spot was 0.52 SEK higher than in 2020. Hourly electricity prices varied a lot during the year from -0.08 öre/kWh in October to 4.33 SEK/ kWh in December. There were also large differences between the prices in the four price areas of Sweden (SE1-4). In SE4, the southernmost part the price was on average 0.39 SEK/kWh higher than in SE1 in the most northern part of Sweden. The spot price for SE4 as a daily average for the year 2021 can be seen in Figure 2.2 (Eva Rydegran 2021).

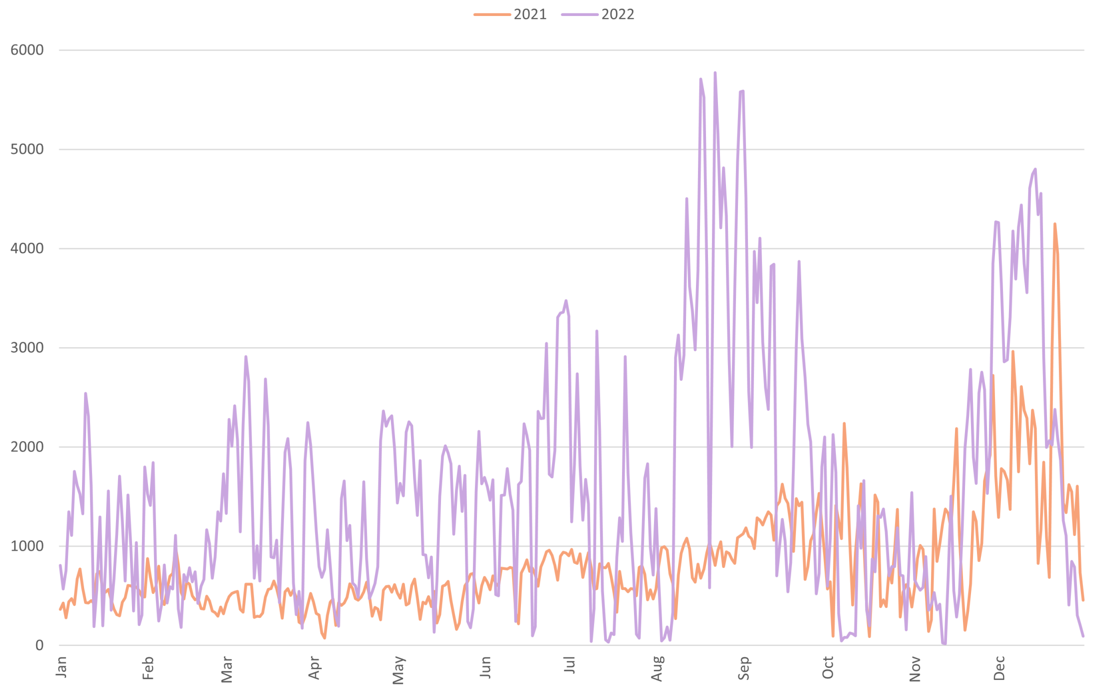


Figure 2.2: Electricity spot price as an average over 1 day for the years 2021 and 2022 in SE4 in Sweden.

Electricity prices in 2022 rose high above average as Russia started the war in Ukraine. The average price on Nord Pool Spot was 1.45 SEK/kWh which is 0.81 SEK higher than in 2021. The most contributing factor to these high prices was the Russian limit on natural gas deliveries to Europe. This made the price of natural gas skyrocket, as mentioned in Section 2.1.5. This year there was also a huge difference in prices between the areas in Sweden. On average the price in SE4 was 0.99 SEK/kWh higher than in SE1. There were also large variations during the year between the lowest and highest price for electricity. In SEK the highest hourly price of the year was 8.51/kWh and the lowest hourly price was -2.3 öre/kWh. The spot price for SE4 as an average per day for the year 2022 can be seen in Figure 2.2 (Eva Rydegran 2022).

2.5 Current CCU Projects

Even though CCU technology development is not as advanced as CCS, ex: Norway's CCS plant Sleipner which began operation in 1996 (Furre et al. 2017), there are several CCU projects worldwide. The first successful industrial-scaled CCU plant began production in 2016 (The Guardian 2017). It is located in the South of India and converts CO_2 into soda ash, a very common and useful industrial chemical. Focusing only on the plants producing e-fuels; there are, at the time of writing this, 18 facilities that are in production or have been announced (eFuel alliance 2022). Most of which are located in Europe.

CPC Finland and Prime Capital have plans to build a 200 MW green hydrogen/e-methane plant. The product will mainly be sold on the German market and used as fuel for heavy vehicles (Yle n.d.). There is also a partnership between Osaka Gas Australia and Santos to commence the production of e-methane. The plan is to open a plant in Australia and export the fuel to Japan to help reach their net-zero 2050 goal. Osaka Gas are also exploring other potentially suitable locations for e-methane production, such as North America, South America, the Middle East and Southeast Asia (Osaka Gas Co. 2023).

In Sweden, a commercial-scaled e-methanol plant: FlagShipONE, is currently under development in Örnsköldsvik, with production expected to begin in 2023. This will be the largest e-fuel plant in Europe, with a production of 50 000 $\mathrm{t_{e-methanol}}$/yr. Their goal is to establish ten e-fuel plants by 2030 (Liquid Wind 2022a) and they are already in the planning phase for the third one (Liquid Wind 2022b).

Recently, there has been a lot of discussion about aviation e-fuels. Atmosfair in Germany opened a kerosene-production facility that aims to produce enough e-kerosene to meet 20 % of the country's PtL-target by 2026. That would mean the plant could produce 0.5 % of the country's aviation fuel demand. There are plans to expand the plant further; however, it is unclear when or by how much (Reuters n.d.).

2.6 Future Prospects for E-fuels

Per the 1.5 °C target, Sweden has put up environmental goals to be carbon neutral in 2045. These goals are also in line with the EU goals that in 2050 all of Europe should be climate neutral. Last year (2022), the EU also increased the target for 2030 to a 55 % reduction compared to 1900 levels in their new target plan Fit For 55 (IEA 2021; Sveriges Miljömål 2023; European Comissionl 2023). According to the Sustainable Development Scenario produced by the IEA; CCUS needs to account for 15 % of the cumulative reduction in emissions for the energy sector to reach net zero by 2070. In that scenario, green hydrogen production also needs to increase by a factor of 7–520 Mt per year in 2070 to sustain the need from the industry sector, transport sector and buildings (IEA 2021). To reach these goals large investments are needed in CCS facilities and new production facilities for e-fuels. As mentioned before in Section 1, the transition to electrification in some sectors will be hard and slow, leaving e-fuels as the best solution. Together with the proposals from the EU explained in Section 2.2 the future for e-fuels is secured for many years to come.

Chapter 3

Hydrogen

In this chapter hydrogen and how it can be produced via water electrolysis will be presented. Some of the most usual electrolyzers and storing methods will also be presented along with additional information about safety and the by-product, oxygen (O_2).

Hydrogen is the first and the lightest element in the periodic table. It has a very high lower heating value (LHV) but since hydrogen is a gas at room temperature it has much lower energy content per volume than other fuels. Some parameters for hydrogen can be seen in Table 3.1 (Sundén 2019b).

Table 3.1: Properties of hydrogen at 25 °C and atmospheric pressure, 101 kPa (Sundén 2019a; Sundén 2019b).

Property	**Unit**	**Value**
M_{H_2}	[g/mol]	2.02
Density	[kg/m^3]	0.0824
LHV	[MJ/kg]	120
LHV	[kWh/kg]	33.3
Energy density	[MJ/m^3]	10

If compared with, for example, gasoline, hydrogen has a much higher LHV but much lower energy density. Values for gasoline are LHV = 47.3 MJ/kg and energy density = 716 MJ/m^3 (Sundén 2019a). To store hydrogen in sufficient ways, the volume needs to be reduced. Along the mechanical storage types, compression is the most common, mostly because compression techniques are already commonly used today in the industry sector. Compression of gas cost energy and for hydrogen to be a competitive energy carrier the compression will have to be as effective as possible. By using multistage compressors with intermediate cooling it is possible to achieve a reduction in the energy required for compression to around 12 % of the energy content in the hydrogen gas (Sundén 2019b). The energy required for compression varies greatly between manufacturers and compressor techniques. For this work, a value of 1.31 kWh/kg$_{H_2}$ will be used since this value is the average from measurements made between 2014-2020 from a retail station (NREL 2021).

3.1 Electrolysis

Electrolysis is the process of splitting water molecules into O_2 and H_2 with electricity in an electrolyzer. Since green electricity can be used as an energy source, this is one of the most promising ways of producing green hydrogen. There are several different electrolyzers on the market. Polymer Electrolyte Membrane Electrolysis Cells (PEMEC) and Alkaline Electrolysis Cells (AEC) are both technically mature and used commercially. These electrolyzers work differently but involve the same overall occurring reaction, seen in Reaction 3.1 (Sundén 2019b).

$$H_2O + \text{electricity} \longrightarrow H_2 + \frac{1}{2}O_2 \tag{3.1}$$

3.1.1 Alkaline Electrolysis Cell (AEC)

Alkaline electrolyzers are the oldest type of electrolyzer and the cheapest on the market which makes them the most commercially used in the industry sector. This electrolyzer is composed of two metallic electrodes usually made of steel, nickel (Ni) or Ni-plated steel. The electrodes are immersed in an alkaline aqueous electrolyte with sodium hydroxide (NaOH) or potassium hydroxide (KOH) of 20–40 wt%. KOH has higher conductivity than NaOH and is thereby preferred. The electrodes are separated by a porous material, to avoid the mixing of H_2 and O_2. AEC can work under pressures between atmospheric and 3000 kPa. By using the electrolyte at higher pressure the compression for storing the produced hydrogen can be decreased. Efficiency for an AEC is between 50–80 % and operating temperature is between 60–90 °C (Edvall, Eriksson and Rosen 2022; Grigoriev, Fateev and Millet 2022). Minimum load is required to be 10–20 % since operating on low load increases the risk of hydrogen gas diffusing over and contaminating the oxygen side (Edvall, Eriksson and Rosen 2022). For more parameters of the AEC see Table 3.2.

3.1.2 Polymer Electrolyte Membrane Electrolyzer Cell (PEMEC)

Polymer electrolyte membrane electrolyzers are a newer technology, but still a mature technology that is used in the industry sector today. PEMEC consists of solid polymer membranes and does not have a liquid electrolyte such as the AEC (Götz et al. 2016). The solid membrane makes these electrolyzers more compact and gives them a faster response time. The solid membrane is acidic and requires the electrodes to be made from noble metals. For the anode, iridium is used and for the cathode, platinum is used. Use of noble metals is expensive and the solid membrane is also more expensive on the market than the electrolyte used in the AEC. This makes PEMEC more expensive than AEC even though they are more compact and have higher energy density. Advantages whit the PEMEC is that it has a low cross-permeation which leads to a hydrogen production of 99.99 % purity (Buttler and Spliethoff 2018). PEMEC can operate up to 7000 kPa, which is one of the greatest advantages with PEMEC since it minimises the work for compression. Reported efficiency of PEMEC varies between sources, Carlson et al. (2021b) reports 60 % efficiency while Buttler and Spliethoff (2018) reports a range between 55–68 % and Edvall, Eriksson and Rosen (2022) reports 50–80 %. More parameters for PEMEC can be seen in Table 3.2.

3.1.3 Solid Oxide Electrolysis Cell (SOEC)

Solid Oxide Electrolysis also known as high temperature electrolysis is a new type of electrolyzer that in recent years has been commercialised by for example Bloom Energy. This new cell is however very promising since it has high efficiency and lower electricity demand. The working temperature is around 800–1000 °C which leads to fast degradation of the material (Corigliano, Pagnotta and Fragiacomo 2022; Götz et al. 2016). The electrolyte is composed of a solid ceramic material and the electrodes are usually nickel or of perovskite-type (Chatenet et al. 2022).

3.1.4 Comparison of Electrolyzers

In Table 3.2 some parameters are presented for the 3 types of electrolyzers presented in Section 3.1.1 - 3.1.3. As seen PEMEC has the fastest start time of all three and SOEC has the highest efficiency. SOEC is also working in considerably higher temperatures than both AEC and PEMEC. All three electrolyzers produce hydrogen with high purity.

Table 3.2: Some key parameters for three types of electrolyzers, AEC, PEMEC and SOEC.

Parameter	**Unit**	**AEC**	**PEMEC**	**SOEC**	**Source**
Efficiency (LHV)	[%]	50-85	50-80	75-85	[1] [2] [3]
Lifetime	[10^3 hours]	60-90	50-80	<20	[4] [5] [3]
Working pressure	[kPa]	<3000	<7000	100	[3] [5]
Working temp	[$^\circ C$]	60-90	50-80	700-1000	[2] [3] [6]
Cold start time	[-]	1-2 h	5-20 min	10 h	[7] [3]
Warm start time	[-]	1-5 min	10 sec	15 min	[3]
Hydrogen purity	[%]	99.9-99.9998	99.9-9.9999	99.9	[3]

[1] Carlson et al. 2021a [2] Grigoriev, Fateev and Millet 2022, [3] Edvall, Eriksson and Rosen 2022,
[4] Krishnan et al. 2020, [5] Chatenet et al. 2022, [6] Corigliano, Pagnotta and Fragiacomo 2022,
[7] Götz et al. 2016

3.2 Oxygen as a By-Product

Hydrogen is not the only product from the electrolyzer. O_2 is also gained as seen in Reaction 3.1. Oxygen can be used in various ways such as in oxygen-enriched combustion. Increasing the oxygen content in combustion (oxy-fuel combustion) can lead to higher energy efficiency and higher concentrations of CO_2 in the flue gases. Higher concentration of CO_2 in the flue gases makes CO_2 capture more efficient (Mittal, Saxena and Mohapatra 2020; Feng et al. 2022). Oxy-fuel combustion also leads to fewer impurities in the flue gas of CO and NOx and higher flexibility in operation (García-Luna et al. 2022). Oxygen is also used in the industry sector for various applications, such as in the glass industry to increase oxygen content in the furnace and the hospital for helping people with breathing issues. Oxygen used in the industry sector and in the health care system have very different characterisations in terms of purity and quality (Rao and Muller 2007; World Health Organization n.d.).

3.3 Storage and Safety of Hydrogen

There are more alternatives than compression when it comes to storing hydrogen. Available methods, besides mechanical storage, are divided into two groups, physical-based and material-based. Physical-based includes compressed gas, cold/cryo compressed and liquid H_2. Material-based includes adsorbent, liquid organic hydrogen carriers, interstitial hydrides, complex hydrides and chemical hydrogen. Cryogenic storage means lowering the temperature below the boiling point of hydrogen (-252.6 °C at 101 kPa) making it liquid. Even at liquid state, hydrogen occupies 3 times more space than gasoline for the same energy content. Liquefaction and keeping the temperature of the hydrogen below boiling point also costs 35 % of the energy content in the hydrogen. Cryo-compressed storage also pressurizes the liquid hydrogen. Chemical storage means storing the hydrogen atoms in chemical bonds. Chemical reactions are used to bind hydrogen to different compounds such as ammonia, metal hydrides and liquid organic hydrogen carriers. Often, heat is required to activate the reaction where the hydrogen is released again. Compressed hydrogen gas is the most common technique and thereby it is also well-known (Sundén 2019b). Hydrogen can be stored at different pressures depending on the material of the storage vessels. Ranges are between 20–100 MPa, but to withstand the highest pressures expensive carbon fiber materials have to be used. In the industry sector, hydrogen is most often stored at pressures between 20–30 MPa which requires metal vessels, often made out of steel (Langmi et al. 2022).

Some safety measures need to be considered when working with hydrogen. Hydrogen gas is easily ignited when mixed with air in a range of concentrations. Since hydrogen also is odour- and colourless it is important to have sensors that detect leakages. However, hydrogen is non-toxic which is not the case for other fossil-based fuels such as gasoline (Sundén 2019b).

Chapter 4

Manufacturing Process of E-fuels

In this chapter, the manufacturing process of synthetic fuels (e-fuels) will be described along with parameters for the synthesis processes found in the literature. The models in Aspen HYSYS were then based on the processes described in this chapter.

4.1 CO_2 Hydrogenation

Through CO_2 hydrogenation it is possible to produce renewable fuels. Firstly, the CO_2 will undergo hydrogenation, producing CO through a Reverse Water Gas Shift reaction (rWGSR) (Reaction 4.1). Fuels can then be produced. As an example, CH_4 can as a next step be produced either by undergoing further hydrogenation (Reaction 4.2) or by direct methanation of CO_2 via the Sabatier reaction (Reaction 4.3).

$$CO_2 + H_2 \rightleftharpoons CO + H_2O \tag{4.1}$$

$$CO + 3H_2 \longrightarrow CH_4 + H_2O \tag{4.2}$$

$$CO_2 + 4H_2 \rightleftharpoons CH_4 + 2H_2O \tag{4.3}$$

CO_2 hydrogenation can proceed via three different catalyses:

- **Thermal catalysis** yields high efficiency when regarding CO_2 conversion and production rate. It can also support high mass flows, favouring scale-ups and industrialization. Because of the high stability of CO_2 and activation energy a high temperature is required to overcome the energy barrier. This will result in higher energy consumption.
- **Photocatalysis** solely depends on solar radiation to drive the reaction. While that makes it favourable from an environmental aspect, it also means that the reaction is dependent on light access and that the conversion efficiency is low.
- **Photo-thermal catalysis** can utilise both procedures and is, therefore, more cost-effective than thermal catalysis and has greater conversion efficiency than

photocatalysis.

CO_2 hydrogenation is broadly discussed in regards to two procedures; methanation and FTS. When it comes to producing renewable fuels, such as e-fuels, photo-thermal catalysis is gaining traction. Which catalyst hydrogenation of CO_2 is best suitable for a specific process will depend on several factors, such as which type of reactor is used and what the desired end-product is (Fana and Tahir 2022).

4.2 Methanation

Methanation is the reaction where CO_2 reacts with H_2 to produce methane (CH_4) which can be seen in Reaction 4.4, same as Reaction 4.3. The reaction is exothermic and requires high temperatures to be favoured. Reactor temperatures are often around 250–450 °C. There are also side reactions occurring at the same time, such as the rWGSR (Reaction 4.1). By choosing a catalyst that has high selectivity the side reaction is limited and the production of CO is minimised. Ni-based catalysts are the most common and are used in the industry sector. They have high CH_4 selectivity, high activity and low cost. The commercially used catalyst is a Ni-based catalyst on SiO_2 support. SiO_2 support has a large surface area, low costs and stable chemical properties (Zhang et al. 2022).

$$CO_2 + 4H_2 \rightleftharpoons CH_4 + 2H_2O \tag{4.4}$$

Falcinelli et al. (2021) found in their experiment with a commercial Ni-based catalyst that almost a 100 % CH_4 yield was achieved at a temperature of 300 °C, 200 kPa and a H_2/CO_2 ratio of 4. This, along with other literature-based reaction parameters can be seen in Table 4.1.

Table 4.1: Reactor parameters for methanation from literature.

Temp [°C]	**Pressure [kPa]**	$\mathbf{R_{H_2/CO_2}}$	**Source**
300	200	4	[1]
300	500	4	[2]

[1] Falcinelli et al. 2021, [2] Schaaf, Grünig and Andreas Orth 2014

A fixed-bed reactor is the most common reactor type for methanation. The fixed bed reactor is used in large scale systems and is the most mature technique. To avoid thermal constraints on the catalyst, the reactor should be fed continuously. Typically, the minimum load that this type of system can operate on is 40 % of the maximum load. Additionally, the load change can go from minimum to maximum load within one hour (Graf et al. 2014; Gorre, Ortloff and van Leeuwen 2019).

4.2.1 Methane Distillation

After methanation, a distillation step is required. First, water is removed by separating gas from liquid. Then the temperature is decreased to below the boiling point of methane to liquefy it. The methane can then be distilled from left-over gases, mostly hydrogen and some CO_2. Xiao and Chen (2021) conducted a study on the distillation of liquefied methane and found that a pressure at the top of the distillation column of 319 kPa and the bottom 320 kPa worked best. At an inlet temperature of -172 °C the top temperature was set to -181 °C and at the bottom to -142 °C for the highest purity of the methane. These conditions gave a purity over 99 % (Xiao and Chen 2021).

4.3 Methanol Synthesis

Methanol production is today done at a commercial scale. In the industry sector, methanol is produced by synthesis from syngas. Today it is most common to produce syngas from fossil sources (Mäyrä and Leiviskä 2018). Methanol synthesis is done either with conventional gas-phase or liquid-phase processes. Reactions that occur during these processes are Reaction 4.5, 4.6, 4.7. Here reaction 4.7 is the water gas shift reaction, the same as reaction 4.1 but not reversed (National Energy Technology Laboratory n.d.).

$$2H_2 + CO \rightleftharpoons CH_3OH \tag{4.5}$$

$$CO_2 + 3H_2 \rightleftharpoons CH_3OH + H_2O \tag{4.6}$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \tag{4.7}$$

All three reactions are exothermic. Temperatures and pressures vary depending on the catalyst but are usually around 200–320 °C and 4–11.7 MPa in the gas-phase process. In the commercial process, the common reactor type is a fixed-bed reactor and the catalyst are mixtures of copper, zinc oxide, aluminium and magnesia (National Energy Technology Laboratory n.d.). Methanol production is favoured over the other reactions when lower temperatures and high pressure are used (Buttler et al. 2020).

Producing methanol with catalytic hydrogenation is also one of the more common production processes. The most common catalyst used in the process is also a copper-based catalyst (Mäyrä and Leiviskä 2018). Multiple studies have conducted that the commercial copper catalyst ($Cu/ZnO/Al_2O_3$) has high selectivity. Some mixtures also favour CO_2 over CO in the reaction, making it favourable when using captured carbon (Schemme et al. 2020; Mäyrä and Leiviskä 2018). If the feed with byproducts is recycled high selectivity can be received with the commercial copper catalyst, up to 99.9 % (Schemme et al. 2020; Saito 1998). Bukhtiyarova et al. (2017) showed in their study that the commercial copper catalyst also works for direct synthesis with CO_2. In their work, the catalyst was tested at a pressure of 3000 kPa and temperatures between 200–260 °C. When performing hydrogenation from CO_2 and H_2, parameters for the reactor found in the literature can be seen in Table 4.2.

Table 4.2: Parameters for direct methanol synthesis with CO_2 from literature.

Temp [°C]	Pressure [kPa]	R_{H_2/CO_2}	kg_{CO_2}/kg_{CH_3OH}	kg_{H_2}/kg_{CH_3OH}	Source
250	8000	4	1.37	0.19	[1]
250	8000	3	-	-	[2]

[1] Otto 2015, [2] Pontzen et al. 2011

4.3.1 Methanol Distillation

After the reaction step there needs to be a separation and distillation step. In the feed that is coming from the reactor, there is usually some water and some unreacted cases such as CO, CO_2 and H_2. The light gases can be separated after a condensation step which condensates H_2O and CH_3OH. The water is then removed by distillation (Pérez-Fortes et al. 2016). In the distillation column, a pressure of around 100 kPa is usually used and the distillation feed is around 70 degrees. From these conditions, it is possible to retrieve methanol at a 99.99 % purity (Otto 2015).

4.4 Kerosene Production

4.4.1 Reverse Water Gas Shift Reaction

From the rWGSR, CO is gained, which is needed to produce kerosene via the FT process, (Reaction 4.1). In this step, the CO yield should be maximized. To favour the formation of CO, temperatures need to be above 700 °C since it is an equilibrium reaction. Reaction 4.3 can for example be an undesired side reaction (González-Castaño, Dorneanu and Arellano-García 2021). Syngas has been used in the industry sector for a long time and is typically produced through steam reforming of natural gas (Cheng et al. 2017). The rWGSR proposes an alternative to producing syngas from renewable sources by using CO_2 and H_2 as feedstock. There are many proposed conditions regarding the choice of reactor and catalyst type. In the literature, many propose a fixed-bed reactor (König et al. 2015; González-Castaño, Dorneanu and Arellano-García 2021). A range of different catalyst types has also been proposed in the literature. Sala (2022) found in his work that a $Cu{-}Fe/CeO_2$ (Copper and Iron supported cerium dioxide) catalyst performed well over a long period and with high stability in the catalyst at 700 °C. This high temperature is otherwise tricky for catalysts as they tend to decay. González-Castaño, Dorneanu and Arellano-García (2021) modelled the rWGSR under the temperature range of 200–800 °C and a CO_2/H_2 ratio of 1 to 4. They found that the ratio 1 and 2 gave the highest CO mol fraction, but at the ratio of 1 all hydrogen was reacted. The rWGSR is not done at an industrial scale yet, but a lot of research is being done, and pilots are up and running.

4.4.2 Fischer-Tropsch Synthesis

Fischer-Tropsch synthesis (FTS) is a catalytic reaction which occurs according to Reaction 4.8. It converts syngas to liquid, often long, hydrocarbons. FTS is a highly exothermic reaction, which makes it attractive to reuse the induced heat in larger processes.

$$(2n + 1)\,H_2 + nCO \longrightarrow C_nH_{(2n+2)} + nH_2O \tag{4.8}$$

There is both high-temperature Fisher-Tropsch synthesis (HTFT) as well as low-temperature Fisher-Tropsch synthesis (LTFT). HTFT takes place around 300–350 °C and is favoured by Fe-catalysts. In this synthesis, low-carbon olefins and gasoline are produced. Cobalt (Co) catalysts can be utilized for LTFT, which is operated at temperatures around 230–280 °C. LTFT is suitable for producing diesel and kerosene (Klerk 2008). Fe-catalysts are also used in the industry sector and have the advantage of being cheaper than Co-catalysts. The main problem with Fe-catalysts is the unwanted side reactions: methanation and WGSR (Equation 4.2 and 4.7) which form CH_4 and CO_2. Co-catalyst form no CO_2 as a side reaction. CH_4 is formed mostly at high temperatures, therefore Co-catalyst works best for LTFT (Kaiser et al. 2013).

From the FT process, a particular product distribution is gained. This distribution is determined by using the Anderson-Flory-Schulz (ASF) model. According to the ASF model, the attained molar fraction (M_i) of a hydrocarbon product with carbon number n is dependent on the chain growth probability (a), according to Equation 4.9. The chain growth probability is in turn a function of the rates of chain growth and chain termination (Cheng et al. 2017; Ma et al. 1999). Which in turn is dependent on the H_2/CO ratio and the reactor temperature according to Equations 4.10 and 4.11 (Vervloet et al. 2012; Im-orb, Simasatitkul and Arpornwichanop 2015).

$$M_i = (1 - \alpha)\alpha^{n-1} \tag{4.9}$$

$$\alpha = (0.75 - 0.373\sqrt{-\log(S_{C5+})} + 0.25S_{C5+} \tag{4.10}$$

$$S_{C5+} = 1.7 - 0.0024T - 0.088\frac{y_{H2}}{y_{CO}} + 0.18(y_{H2} + y_{CO}) + 0.0079P_{tot} \tag{4.11}$$

Here, S_{C5+} is the selectivity of hydrocarbons longer than 5 carbon molecules and y_{H2} and y_{CO} is the molar concentration of H_2 and CO in the feed to the FT-reactor. T and P_{tot} are the temperature in K and the pressure in bar (Im-orb, Simasatitkul and Arpornwichanop 2015). α values from different literature can be seen in Table 4.3 for different parameters.

Table 4.3: Alpha values and corresponding reactor parameters from different litterateur sources.

Temp [°C]	Pressure [kPa]	$R_{H_2/CO}$	Other	α	Source
220	2500	2	-	0.85	[1]
225	2500	2.05	$x_{H2} + x_{CO} = 0.5$	0.85	[2]

[1] Kern and Meurer 2021, [2] König et al. 2015

The ASF distribution works well for all carbon chains, except the shortest ones. Production of CH_4 is deviating the most from the ASF distribution and it has been reported in several studies that the production of CH_4 exceeds the calculated product ratio (Braddock et al. 2016).

For LTFT, two types of reactors are used today: slurry bubble column reactor and fixed-bed reactor. They each have different advantages and drawbacks. The fixed-bed reactor has the advantage that it can be scaled up to industrial levels and a good yield is gained for middle distillates such as kerosene and diesel. However, if the catalyst is deactivated due to impurities, the reactor needs to be shut down for the catalyst to be replaced. Therefore fixed-bed reactors are not used with Fe-catalyst since this type of catalyst is deactivated faster than Co-catalyst. Slurry-bubble column has the advantage that it has a higher capacity per train and that the catalyst can be withdrawn and exchanged during operation. Limitations with this reactor are catalyst mechanical stress in large reactors and problems separating solids from liquid (Speight 2020). For the production of kerosene, the size of the FT-reactor for a capacity of 2500 t/d needs to be around 7 m in diameter and 30 m in height. The reactor is also operated at constant temperature and pressure, so there can be assumed to be no pressure drop in the reactor (Sie and Krishna 1999).

Hydrocracker

Chains that contain more than 16 carbons can be split into smaller chains and thereby added to the finished product. This can be done through hydrocracking, where the heavy hydrocarbons are mixed with hydrogen and a catalyst at temperatures around 300–400 °C. Hydrocracking also produces more branched iso-paraffines than the FT process, which mainly produces linear chains. Branched hydrocarbons lower the freezing point for the finished product, which needs to be below -40 °C for aviation fuels (see Section 2.2.2) (Kern and Meurer 2021; Klerk 2008). The catalyst needs to be bi-functional, which means it has to have both metal and acid sites. For LTFT unsulifided noble metal catalysts works best based on Pd or Pt on zeolitic or amorphous silica-aluminia support. Hydrocracking feed from LTFT requires lower temperature and pressure than hydrocracking of HTFT feed. Thereby a temperature of around 300–360 °C and a pressure of 3000–7000 kPa is needed. Hydrocrackers are in general operated at a space velocity of 0.3–2.0 h^{-1} and hydrogen is fed into the reactor at 800–1800 Nm^3/h per 1 m^3/h of feed. Nm^3 (normal cubic meter) is in this work defined after the reference conditions of 20 °C and 101 kPa. Space velocity means how many reactor volumes of feed can be processed in unit time (Klerk 2008). Product distribution over a bi-functional catalyst gained by Sie, Senden and Van Wechem (1991) can be seen in Table 4.4.

Table 4.4: Hydrocarbon distribution after Hydrocracking (Sie, Senden and Van Wechem 1991).

Carbon number	**Mole eq.**	**Carbon number**	**Mole eq.**
C_1	0.0188	C_9	10.3
C_2	0.250	C_{10}	9.75
C_3	2.94	C_{11}	9.75
C_4	9.75	C_{12}	7.75
C_5	11.4	C_{13}	2.75
C_6	10.4	C_{14}	0.988
C_7	11.5	C_{15}	0.250
C_8	11.0	C_{16}	0

Reformer and Recycling of Short Carbon Chains

Short hydrocarbons ($C_{1\text{–}4}$) and unreacted gases can be recycled back into the rWGSR (Klerk 2008). It is also possible to treat the shorter chains via a reformer before recycling them back to the rWGSR. With steam methane reforming (SMR) it is possible to produce syngas. By mixing hydrocarbons with steam at temperatures of 700–1000 °C and pressures of 300–2500 kPa, H_2 and CO, are produced, as well as small fractions of CO_2 (U.S. Department of Energy n.d.). The syngas can then be recycled. The reforming reaction can be seen in reaction 4.12. There is also a second reaction, 4.13, which occurs in the SMR, where some of the produced CO forms CO_2. When designing the reformer process, it is important to consider the Steam-to-Carbon (S/C) ratio. Typically, a ratio of at least 2.5 is desired as this will both favour the production of CO, as well as prevent coke formation and the thermal cracking of hydrocarbons (Vogt et al. 2019).

$$\mathrm{C_iH_n + nH_2O \longrightarrow iCO + (\frac{n}{2} + n)H_2} \tag{4.12}$$

$$\mathrm{CO + H_2O \longrightarrow CO_2 + H_2} \tag{4.13}$$

By performing hydrocracking of carbon chains longer than C_{16} as well as recycling chains shorter than C_8, the main product from the FT synthesis will be kerosene and water (Schemme et al. 2020; Klerk 2008).

4.5 Process Efficiencies

To determine the quality of the processes, there are some values that can be calculated. Equations 4.14 and 4.15 show how the plant efficiency and the PtX efficiency can be calculated (Schemme et al. 2020). Where $\dot{m}_i$ is the total mass flow rate of species i, P_{CO2} is the power associated with the CO_2 supply, and P_{Plant} is the electrical power required for the production process. Process efficiencies from literature can be found in Table 4.5.

$$\eta_{Plant} = \frac{\dot{m}_{Fuel} \cdot LHV_{Fuel}}{\dot{m}_{H_2} \cdot LHV_{H2} + P_{Plant}} \tag{4.14}$$

$$\eta_{PtX} = \frac{\dot{m}_{Fuel} \cdot LHV_{Fuel}}{\frac{\dot{m}_{H_2} \cdot LHV_{H2}}{\eta_{H_2}} + P_{CO2} + P_{Plant}} \tag{4.15}$$

Table 4.5: Literature values for plant efficiency (η_{Plant}) and PtX efficiency (η_{PtX}) for the three e-fuel production processes.

E-fuel	**[η_{Plant}]**	**[η_{PtX}]**	**Comment**	**Source**
Methane	0.780	N/A	Based on HHV, CO_2 adsorption instead of distillation	[1]
Methanol	0.859	0.576	Direct methanol synthesis	[2]
Kerosene	0.749	0.506	rWGSR, FT, reformer and hydrockracker	[2]

[1] Becker, Penev and Braun (2019) [2] Schemme et al. (2020)

4.6 Economy

Calculating the investment cost for the system includes costs for the hydrogen system, the e-fuel production plant and surrounding costs such as planning, work time and project development. Investment cost for equipment varies a lot between sources, therefore there will always be an error margin.

4.6.1 Hydrogen System

Investment costs for the hydrogen system include costs for the electrolyzer, H_2-compressor and hydrogen storage. Costs for the AEC electrolyzer can be calculated from Equation 4.16. This cost is valid for a size of 100 MW but the cost reduction is steepest for small sizes and for the larger sizes the reduction is flat (Taibi et al. 2020). The yearly O&M costs are 2.5 % (Khan et al. 2021).

$$\text{Investment Cost}_{\text{Electrolyzer}} = 3590\,\text{SEK/kW} \cdot \text{size} \tag{4.16}$$

Investment cost for the compressor can be calculated according to Equation 4.17. Here p stands for the compressor installed power expressed in kW. O&M for the compressor is 8 % of the investment cost (Lindborg et al. 2021).

$$\text{Investment Cost}_{\text{Compressor}} = 447\,000\,\text{SEK/kW} \cdot \text{p}^{0.5861} \tag{4.17}$$

Investment cost for the hydrogen storage can be calculated with Equation 4.18. That is valid for a storage of 30 MPa. O&M costs for the storage stand for 2 % of the investment cost (Lindborg et al. 2021).

$$\text{Investment Cost}_{\text{Hydrogen storage}} = 5000\,\text{SEK/kg}_{\text{H}_2}\cdot\text{size} \tag{4.18}$$

4.6.2 E-fuel Production Facility

Larger equipment needed for the different processes are reactors, flash separators and distillation columns. Beyond this heaters; heat exchangers, coolers and mixers are needed. Investment cost for a fixed bed reactor is 84.9 million SEK for the base sizing value of 2.52 scf/h (standard cubic feet per hour) (Swanson et al. 2010). Scaling the cost for equipment can be done with the six-tenth rule according to Equation 4.19. Here C_0 stands for the base cost for the parameter P_0 and P is the parameter for the scaled case. These parameters can be volume, gas flow and much more (Lundblad et al. 2022). The investment cost for the fixed bed reactor can thereby be calculated according to Equation 4.20.

$$\text{Investment cost} = C_0 \cdot \left(\frac{P}{P_0}\right)^{\frac{6}{10}} \tag{4.19}$$

$$\text{Investment cost}_{\text{fixed bed}} = 10.5 \cdot 10^6 \cdot \left(\frac{P}{2.52 \cdot 10^6 \text{scf/h}}\right)^{\frac{6}{10}} \tag{4.20}$$

The rest of the costs for equipment taken from literature can be seen in Table 4.6 where the base cost (C_0) is written as well as the corresponding base parameter (P_0).

Table 4.6: Literary values of equipment costs displayed as a base cost (C_0) with corresponding base parameter (P_0).

Equipment	Base cost [MSEK]	Base Parameter	Unit	Source
Flash drum, 3 phase	3.02	8000	[ACFH]	[1]
CO_2 compressor	1.53	220 000	[lb/h]	[2]
Distillation column	98.3	54.2	[t/h]	[3] [4]
Fixed bed reactor	85	$2.52 \cdot 10^6$	[SCFH]	[5]

[1] Dutta et al. 2015, [2] Spath et al. 2005 [3] Schemme et al. 2020 [4] Schorn et al. 2021
[5] Swanson et al. 2010

Additional costs for the plant and for constructing it can be found in Table 4.7. All costs are represented as percent cost of the total CAPEX (capital expenditures/investment costs) for the large equipment parts. Values from Albrecht and Nguyen (2020) are from a techno-economic study of a FT plant producing e-fuels in Denmark.

Table 4.7: Additional plant costs expressed in percent of CAPEX (Albrecht and Nguyen 2020).

Parameter	Percent [%] of CAPEX
Buildings	18
Construction expenses	41
Electrical systems	11
Engineering	33
Installation factor	47
Instrumentation control	36
Legal expenses	4
Extra equipment such as heat exchangers, coolers etc	1.9

4.7 Comparable Study Findings

There have been several techno-economic studies investigating CCU for e-fuel production. One conclusion that is reoccurring in all of them is that the cost of electricity for hydrogen production is the parameter that has the largest effect on the price of the fuel (Schemme et al. 2020; Fagerström et al. 2022; Gorre, Ortloff and van Leeuwen 2019). When comparing the final cost of producing e-fuels there is a range of numbers as a result of the production cost. Schemme et al. (2020) finds the cost for methanol to be 1.89 €/l_{DE}, were l_{DE} stands for the energy equivalent of 1 litre diesel. In their study, the different production processes were modelled in Aspen Plus. Methanol production was modelled as a catalytic synthesis from H_2 and CO_2 with a copper catalyst. Their estimated cost for Kerosene is 2.30 €/l_{DE}. For Kerosene, a LTFT process is used with a cobalt catalyst following an rWGSR (Schemme et al. 2020). Costs and energy requirements from additional different literature can be seen in Table 4.8.

Table 4.8: Production cost and energy demand for producing the three different e-fuels from literature.

E-fuel	**Production Cost [SEK/kg]**	**Energy Demand [kWh/kg]**	**Comment**	**Source**
Methanol	11.0	9.74	Including electrolysis and CO_2 capture	[1]
	10.6		Including electrolysis and CO_2 from biogas upgrading	[2]
	13.0		Including electrolysis and CO_2 capture	[3]
		0.28	Without electrolysis and CO_2 capture	[4]
Kerosene	28.9	29.9	Including electrolysis and CO_2 capture	[1]
	21.5	21.0	Including electrolysis and CO_2 capture	[5]
		37.3	Only RWGSR and FT-process	[6]
Methane	13.5		Including electrolysis and CO_2 capture	[7]
	31.2		Including electrolysis and CO_2 capture	[3]
	20.0		Including electrolysis CO_2 capture, liquefaction and infrastructure	[8]
		27-53	Including electrolysis	[9]

[1] Schemme et al. 2020, [2] Bongartz et al. 2018, [3] Brynolf et al. 2018, [4] Otto 2015,
[5] Fagerström et al. 2022, [6] Fagerström et al. 2021, [7] Kiani et al. 2021. [8]Korberg et al. 2021
[9] Biswas et al. 2020

There is a limited amount of published papers investigating the integration of an e-fuel production process with a CHP plant in Sweden. One of them, Fagerström et al. (2022), models the e-kerosene process including CO_2 capture with amine technology and hydrogen production with electrolysis. The e-kerosene process includes rWGSR and FT and the process is integrated with a CHP plant in Sweden. The result is that large energy savings can be made by heat integration with the CHP plant. In their study, they found that the energy savings possible were from 35.2 MW for the non-integrated case to 7.6 MW for the integrated case and a production output of 1676 kg/h. In this output, 40 % was the fraction $C_{10–15}$.

There are multiple routes for producing e-fuels than described in this work. Methane can also be synthesised from syngas according to Reaction 4.2. It can also be produced by upgrading biogas, which is a mixture of methane, CO_2 and other gases in small amounts. Upgrading biogas can be done in many ways such as chemical scrubbing, biological consumption and separation. There is also the possibility of in-situ bio methanation or combining the anaerobic digestion process with a bioelectrochemical cell to achieve higher methane yield. This is not, however, done on industrial scale jet (Dou, Dykstra and Pavlostathis 2018).

As described in Section 4.3 methanol can also be synthesised from syngas just as methane. This is the more mature method that is used on a large scale in the industry sector. Syngas can not only be produced from fossil sources it can also be produced from biogenic waste degradation. This is also the process to produce biogas. Reaction 4.5 describes methanol synthesis from syngas. This reaction is much more exothermic than Reaction 4.6 which means that there is a higher need for cooling the reactor since the reaction is favoured by lower temperatures. Methanol synthesis from syngas has some advantages compared to synthesis from CO_2, the main one being that it is already performed on a large scale. However, direct methanol synthesis from CO_2 has advantages too such as higher selectivity of CO_2 than of CO and fewer impurities are formed in the reaction (Liu, Hagelin-Weaver and Welt 2023; Buttler et al. 2020).

One other promising process is called alcohol-to-jet, which uses alcohols such as ethanol, methanol or long-chain fatty alcohols that are converted into jet fuel. The alcohols can be produced from biomass such as starch and sugar or through synthesis. The alcohol-to-jet process involves four stages: dehydration of alcohol, oligomerization, hydrogenation and separation. This process has the advantage that all four steps already are commercial and used in the industry sector. A disadvantage is that the process requires the formation of the alcohol which also stands for some losses in terms of energy and efficiency. There are also other processes for SAF such as hydropressed esters and fatty acids or direct sugars to hydrocarbons (Romero-Izquierdo et al. 2021).

Chapter 5

Process Modelling

This chapter describes how the modelling has been set up. Which parameters and technologies have been chosen for the system, as well as why they were chosen is discussed. Then, the setup in Aspen HYSYS is explained in greater detail.

Figure 5.1 shows a schematic illustration of the CCU system and how it is integrated with the other components; CHP plant, CCS and hydrogen system. Between the units, material, heat and electricity flows can be followed.

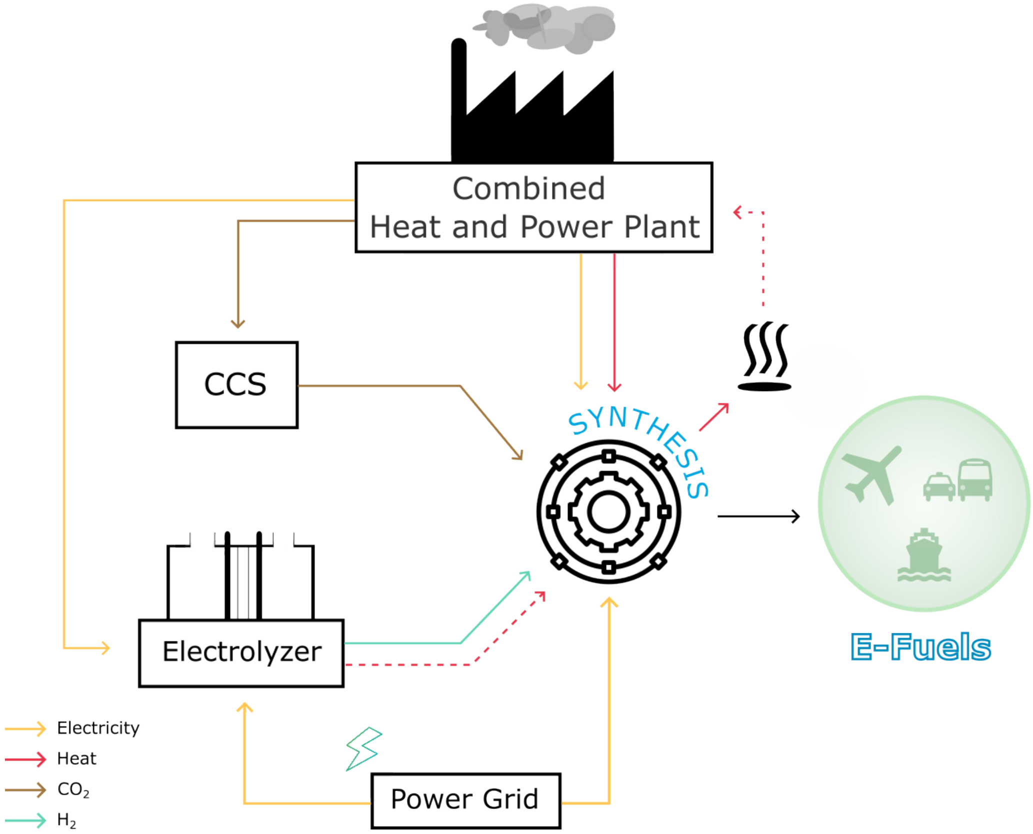


Figure 5.1: Schematic illustration of the PtX system.

5.1 Chosen Model Parameters

5.1.1 Hydrogen Production Model

Components for the hydrogen system were chosen based on current technology and their suitability with the model. Since the AEC is the most developed technique and the cheapest and most durable one, this type of electrolyzer was chosen. A faster starting time could be beneficial, but since the only requirement for the process is that enough hydrogen is produced each hour for the e-fuel production, this is not necessary. One hour's starting time is enough to optimize production after electricity prices. A storage unit will also be included in the model. This is included to be able to pause hydrogen production if electricity prices are too high. It also gives redundancy to the system if the electrolyzer breaks or needs maintenance. The chosen storage technique is compressed gas storage. This technique is also well-known and costs less energy compared to the energy content in the gas. To minimize the compression energy, the electrolyzer will be run at 3000 kPa and 60 °C. All parameters used in the hydrogen production model can be seen in Table 5.1.

Table 5.1: All parameters for the units in the hydrogen production model.

Unit	Parameter	Unit	Value
AEC	Temperature	[°C]	60
	Pressure	[kPa]	3000
	Efficiency	[%]	70
	Cold start time	[Hours]	1.5
Compressed hydrogen gas storage	Pressure	[kPa]	30 000
	Temperature	[°C]	25
	Start value	[MWh]	0.5 of max
Compressor	Auxiliary power	[%]	2.12

5.1.2 E-fuel Production

As mentioned previously, the production of methane, methanol and kerosene will be modelled in this work. There are different possible production methods for each fuel. The processes modelled in this paper were chosen based on their technical maturity and the possibility of commercial use. Meaning there could be great potential to implement this work shortly.

Methane

Methane is produced through methanation in this work, according to Equation 4.2. The feedstock is fed to a fixed-bed methanation reactor with a commercial Ni/SiO_2-based catalyst. The process requires both steam and electricity. Steam is provided by the boiler in the CHP plant, and electricity is either from the turbine or the grid.

Methanol

Methanol is, in this work, produced through catalytic hydrogenation according to Equation 4.6. This process requires one less step than methanol synthesis from CO and H_2, as it eliminates the rWGSR. The reactor for direct methanol synthesis is a fixed-bed reactor paired with a commercial Cu/ZnO-based catalyst. The whole process also requires steam and electricity, provided in the same way as for methane.

Kerosene

Kerosene production takes place through two main processes: rWGSR and FTS. The rWGSR takes place in a fixed-bed reactor with a Cu−Fe/CeO_2-based catalyst. The FT reactor is also a fixed-bed reactor. The reaction will be a LTFT with a Co-based catalyst, which will favour the production of hydrocarbons in the kerosene range. Steam and electricity are supplied as in the other cases.

5.1.3 Production Volume

The e-fuel productions will be modelled for two different production volumes. First, there will be a base case in which methane is produced to meet the demand of parts of the industry sector in Helsingborg. The amount of CO_2 required for this will serve as a benchmark for modelling the production of methanol and kerosene. Subsequently, a full-scale simulation will be conducted in which the entire amount of CO_2 planned to be captured in the CCS process will be used in each production case. As discussed in Section 2.6, the demand for e-fuels is expected to continue to increase. Therefore, a full-scale plant will be investigated. Since it takes several years from the initiation of the planning phase to the start of production, it is reasonable to assume that stakeholders will favour a larger plant that not only meets their current needs but also anticipates future demands and potential sales in an expanding market. Both cases will be described in more detail in Section 6.3.

5.2 Aspen HYSYS Modelling

As a first step, the e-fuel productions are modelled in Aspen HYSYS, a chemical process simulator used to simulate both small unit properties and full-scale plants. This is done to estimate the energy and feed streams required for respective processes. Subsequently, the design of each e-fuel production process is presented.

The feedstocks are identical for each case. It is made up of a H_2 stream and a CO_2 stream which also contains 18 wt% water. However, before mixing with the H_2 stream, it is led through a flash drum to minimize the water content. All stream parameters and which H_2:CO_2 ratio is used for each process are compiled in Table 5.2.

Table 5.2: Feedstock composition and ratio for each process

Feed	T [°C]	P [kPa]	Composition	Process	H_2:CO_2 ratio
CO_2	60	102	$x_{CO2} = 0.99$	Methane	4
H_2	60	3000	$x_{H2} = 1$	Methanol	3
				Kerosene	2

5.2.1 Methane Production

Figure 5.2 shows a simplified schematic of the process. Initially, the feedstock is brought to the methanation reactor's operating parameters of 300 °C and 600 kPa (Stream 1, Figure 4.1). To keep the reaction isothermal, the reactor is cooled with a cooling stream. After the methanation reaction (Reaction 4.3), the gaseous share of the mixture (Stream 2, Figure 4.1) is separated and recycled into the methanation reactor again. The rest is cooled to -162 °C, which is below methane's boiling point, before it continues to a distillation column. It should here be noted that this cooling was disregarded due to the delimitations. In the distillation column, methane is separated from unreacted gases and water and extracted as methane gas. In Aspen, the distillation column was modelled as a reboiled absorber. As a last step, this stream is cooled off so that the fuel is in liquid form, with a purity of 98.7 mol%. If the methane is going to be used only as an alternative to natural gas, this last cooling step is unnecessary. Parameters used for the reactor and distillation column are compiled in Table 5.3. For the detailed Aspen model, see Appendix A.

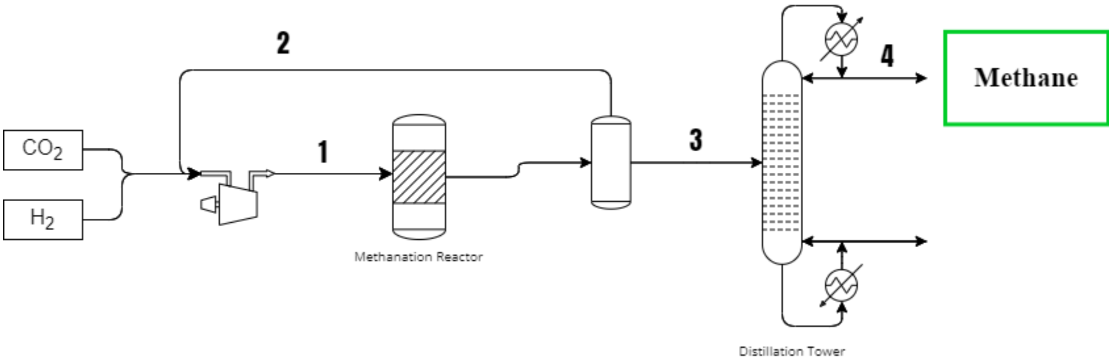


Figure 5.2: Simplified flowsheet of the Methane production process

Table 5.3: Reactor and distillation column parameters for the methane production.

Unit	T [°C]	P [kPa]	Reaction
Methanation Reactor	300	600	$CO_2 + 4H_2 \rightleftharpoons CH_4 + 2H_2O$
Distillation Column	-97.8-237	2790-3100	-

Optimizing the Model and Energy Reduction

To optimize the yield, the tool Case Studies were used in Aspen HYSYS. One or multiple variables, such as temperature or pressure, can be varied to observe the effect on another variable, such as e.g., methanol yield. To get accurate results, the recycle stream should be disconnected before conducting the case studies. Both the temperature and the pressure of the feed are examined. However, since the varying values show little to no difference, they are kept the same. The tested case studies are listed in Table 5.4. Additionally, an adjusting unit is used to correctly set the amount of CO_2 that is needed to reach the production target.

Table 5.4: Case studies conducted on the methane production process.

Case study	Varying Parameter	Interval	Optimal
1	Feed Temperature [°C]	240-450	Little to no difference
2	Reactor Pressure [kPa]	100-800	600

Aspen HYSYS has multiple tools for optimization. Aspen Energy Analyzer can for example give suggestions on where heat exchangers can be integrated. However, for the methane production, not much could be done regarding energy reduction within the model. Three cooling streams are used in the process that results in excess heat that could be utilized with other processes. These are presented later in Table 6.3, in Section 6.1.

5.2.2 Methanol Production

In Figure 5.3, a simplified flowsheet of the methanol production is shown. First, the feedstock is compressed to a pressure of 8000 kPa. As an effect of this, the gas also needs to be cooled off. The gas mixture (Stream 2, Figure 5.3) is fed into a fixed bed reactor where it will be subjected to direct methanol synthesis (see equation 4.6). As a simplification, the reactor is modelled as a Gibbs reactor. The reactor parameters are 8000 kPa and 200 °C. Since the reaction is exothermic, the reactor is cooled to keep the reactor isothermic. The heat in the stream out from the reactor is used in a heat exchanger which heats the feed to the reactor from 95 °C to 200 °C and cools the reacted feed from the reactor to 100 °C. The product stream is then cooled to 80 °C via a second heat exchanger and a cooler. Once cooled, the product stream is separated into a liquid stream and a gaseous stream. The gaseous one is recycled and reintroduced along with the product stream to the direct methanol synthesis. Before distillation, the liquid feed from the separator is depressurized in a valve. Here, the pressure is lowered from 8000 kPa to 100 kPa. The distillation is performed under atmospheric pressure and a product stream with a mole fraction of 99 % methanol is obtained. Parameters for the reactor and distillation column can be seen in Table 5.5. For the full model, see Appendix B.

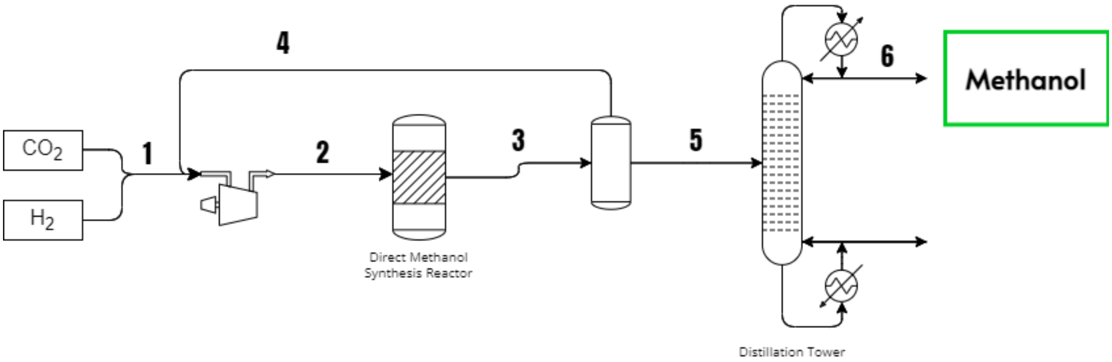


Figure 5.3: Simplified flowsheet of Methanol Production Process

The process model for methanol is based on Otto (2015).

Table 5.5: Reactor parameters for the methanol production process.

Unit	T [°C]	P [kPa]	Reaction
Methanol Synthesis Reactor	200	8000	$CO_2 + 3H_2 \rightleftharpoons CH_3OH + H_2O$
Distillation Column	64-100	100	-

Optimizing the Model

To get an optimized model with as high a yield as possible, some alterations were made. Three case studies were done for the methanol process, each with one changing variable to see if this had any effect on the methanol yield. The parameters were temperature, pressure and H_2:CO_2-ratio. The results from the case studies can be seen in Table 5.6.

Table 5.6: Case studies conducted on the methanol production process.

Case study	Varying Parameter	Interval	Optimal
1	Reactor Temperature [°C]	200-245	200
2	Reactor Pressure [kPa]	6000-12000	Little to no difference
3	H_2:CO_2-ratio in feed	1-5	3

As the pressure had very little difference on the methanol yield, the pressure of 8000 kPa was chosen since it was found to be a good pressure in the model and the literature (see Section 4.3). A small increase in the methanol yield by 0.5 % could be seen at a pressure of 12 000 kPa. This small increase in yield was considered not motivated due to higher energy demand from the compressor. For this pressure a temperature of 200 °C gave the highest yield. A ratio between H_2 and CO_2 of 3 was also found to be most optimal. After the alterations from the optimization, the molar fraction of methanol before distillation was 0.491 which is in the same range as the process developed by Otto (2015).

Energy Reduction

To minimize the energy required in the process some alterations were made. First possible heat exchangers were investigated and two were incorporated as seen in the model (Appendix B). This was done using the Aspen Analyser tool which finds possible solutions for heat exchangers in the model. Then one more heater was included which uses the excess heat from the cooler before the flash drum for circulation to pre-heat the feed to the distillation column which saves the energy needed for the distillation column. After this, the composition and temperature of the feed were compared with the composition and temperature of the trays in the distillation column to find the best feed position. The best feed position was found to be tray number 3 from the top. There was a desire to incorporate pre-heating before the reboiler in the distillation column but due to lack of knowledge of the software and time, this was not possible. Instead, this will be calculated in theory where the heat from the first cooler (see Appendix B) is used to pre-heat the stream before the reboiler in the distillation column. This is done by calculating the heat that is possible to utilize in the reboiler and transferred through a heat exchanger. The inlet stream to the reboiler is 99.5 °C (Figure 5.4) and in a good heat exchanger the temperature difference between the cold side of the warm stream and the inlet temperature can be 5 °C. The temperature difference between the cold side of the warm stream and the inlet in a gas/water heat exchange needs to be a bit higher, 15 °C. The heat that can be utilized can then be calculated with Equation 5.1

$$m_1h_1 + m_4h_4 - m_2h_2 - m_3h_3 = 0 \tag{5.1}$$

Since the mass, m_1 is equal m_2 and the mass, m_3 is equal m_4 Equation 5.1 can be written as Equation 5.2

$$m_1(h_1-h_2) + m_4(h_4-h_3) = 0 \tag{5.2}$$

Both temperatures of stream 1 and 2 (Figure 5.4) are known which means that the energy that can be utilized can be calculated. This energy was then subtracted from the energy required in the reboiler. Here h stands for the enthalpy of the fluid or gas and m stands for the mass.

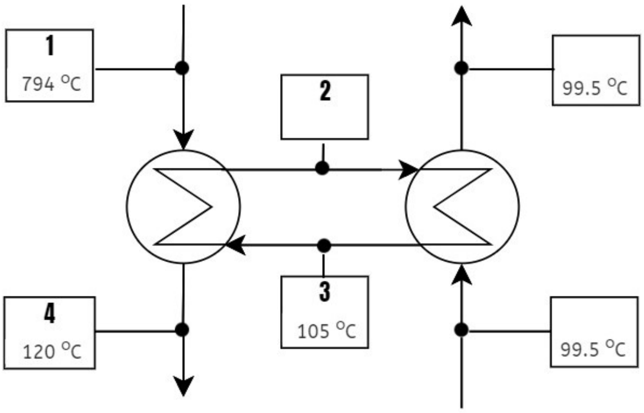


Figure 5.4: Simplified picture of heat exchangers in the methanol process.

5.2.3 Kerosene Production

A simplified flowsheet of the Kerosene production process can be seen in Figure 5.5. First, the feedstock is heated to 1000 °C before being fed to an rWGSR. The resulting syngas is then purged of water and led through a multistage compressor. When the desired pressure and temperature are reached, in this case: 220 °C and 4.15 MPa, the syngas is introduced to a FT-reactor. It is desirable to have a H_2:CO ratio of two for the FT-feed to ensure high CO conversion. It will therefore be necessary to also introduce more H_2 to the syngas-feed to reach the desired composition.

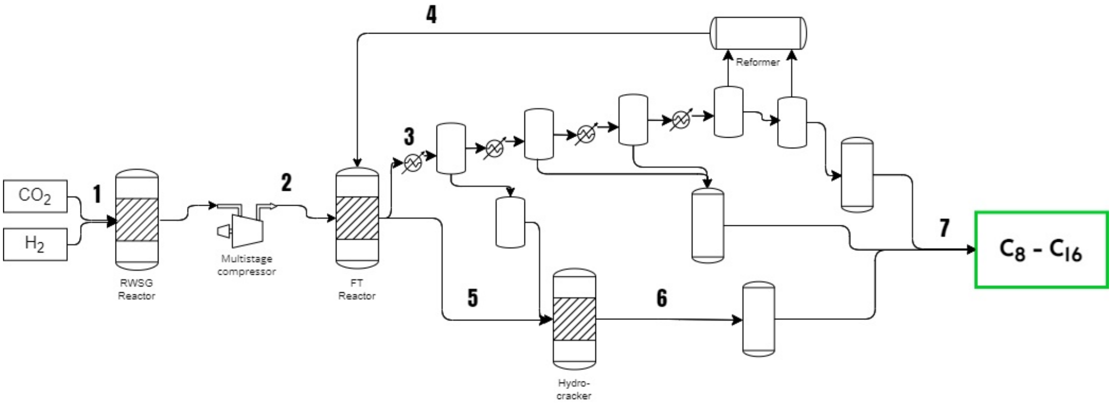


Figure 5.5: Simplified flowsheet of Kerosene production process.

It is assumed that the product distribution from the FT process follows the ASF distribution model. Equations 4.10 and 4.11, along with the operating conditions of 220 °C and 4.15 MPa, are used to calculate α (Table 5.7). Equation 4.9 can be used with this value to determine the mole equivalent of each carbon number component. The initial 30 values are calculated with the aforementioned equation, see Table 5.8. The reaction has also been normalized by assuming that the remaining products consist of C_{30+}.

Table 5.7: Values used to determine the ASF distribution.

α	S_{C5+}	T [°C]	P [MPa]	y_{H2}	y_{CO}
0.858	0.840	220	4.15	0.663	0.332

Table 5.8: ASF Distribution from the parameters in Table 5.7.

Carbon number	**Mole eq.**	**Carbon number**	**Mole eq.**
C_1	0.0203	C_{17}	$1.74 \cdot 10^{-3}$
C_2	0.0174	C_{18}	$1.50 \cdot 10^{-3}$
C_3	0.0149	C_{19}	$1.28 \cdot 10^{-3}$
C_4	0.0128	C_{20}	$1.10 \cdot 10^{-3}$
C_5	0.0110	C_{21}	$9.40 \cdot 10^{-4}$
C_6	$9.40 \cdot 10^{-3}$	C_{22}	$8.06 \cdot 10^{-4}$
C_7	$8.06 \cdot 10^{-3}$	C_{23}	$6.91 \cdot 10^{-4}$
		C_{24}	$5.93 \cdot 10^{-4}$
	$\sum_{n=1}^{7} x_{C_iH_n} = 66.6\,\%$	C_{25}	$5.08 \cdot 10^{-4}$
		C_{26}	$4.36 \cdot 10^{-4}$
C_8	$6.92 \cdot 10^{-3}$	C_{27}	$3.74 \cdot 10^{-4}$
C_9	$5.93 \cdot 10^{-3}$	C_{28}	$3.21 \cdot 10^{-4}$
C_{10}	$5.09 \cdot 10^{-3}$	C_{29}	$2.75 \cdot 10^{-4}$
C_{11}	$4.36 \cdot 10^{-3}$	C_{30}	$2.36 \cdot 10^{-4}$
C_{12}	$3.74 \cdot 10^{-3}$		
C_{13}	$3.21 \cdot 10^{-3}$		$\sum_{n=17}^{\infty} x_{C_iH_n} = 7.49\,\%$
C_{14}	$2.75 \cdot 10^{-3}$		
C_{15}	$2.36 \cdot 10^{-3}$	H_2O	2.18
C_{16}	$2.03 \cdot 10^{-3}$		
	$\sum_{n=8}^{16} x_{C_iH_n} = 25.9\,\%$		

This distribution is incorporated in the model by inserting Reaction 5.3 in the FT-reactor.

$$CO + (3 - \alpha^{[1]})H_2 \rightleftharpoons m_n^{[2]}C_nH_i + H_2O \qquad (5.3)$$

[1] According to Reaction 4.10. [2] According to Reaction 4.9.

The hydrocarbon mixture mainly consists of $C_{1-7}H_n$, more precisely 66.6 %. These are shorter hydrocarbons which can be passed through a reformer to be broken down back to CO, to be able to recycle them to the FT-reactor. $C_{8-16}H_n$ make up 25.9 % of the mixture and are the products of interest, which has been denoted as kerosene. The longer hydrocarbons: $C_{17+}H_n$ will be hydrocracked, and then further separated. Additional hydrogen needs to be added before the hydrocracker as this is a highly hydrogen-demanding process. 800 Nm^3/Nm^3 liquid feed is introduced.

Two product streams are generated by the FT-reactor: one with gaseous syncrude and unreacted syngas (Stream 3, Figure 5.5), and another with heavy waxes (Stream 5, Figure 5.5). Stream 3 is separated in four different flash drums, operating at temperatures of 120, 60, 25 and −25 °C. Since the product stream is to contain several different hydrocarbons, these differing flash drum temperatures will favour the desired carbon number products. The separated gas containing the shorter hydrocarbons is led through a reformer and then recycled into the FT reactor (Stream 4, Figure 5.5). To ensure the reformation proceeds as desired, steam is introduced until a S/C-ratio of 2.5 is reached.

The liquid streams containing longer hydrocarbons, C_{17+}, are treated in a hydrocracker (Stream 6, Figure 5.5). Finally, the liquid streams with the desired carbohydrates are extracted as e-fuels (Stream 7, Figure 5.5). Parameters for the reactors are compiled in Table 5.9. For the full model, see Appendix C.

Table 5.9: Reactor parameters for the production process of Kerosene.

Unit	T [°C]	P [kPa]	Reaction
rWGSR Reactor	1000	102	$CO_2 + H_2 \rightleftharpoons CO + H_2O$
FT Reactor	220	4150	$CO + (3 - \alpha)H_2 \rightleftharpoons m_nC_nH_i + H_2O$
Hydrocracker	360	500	see Table 4.4
Reformer	800	3500	$C_iH_n + nH_2O \rightleftharpoons nCO + (n/_2 + n)H_2, 1 \leq i \geq 4$ (1) $CO + H_2O \rightleftharpoons CO_2 + H_2$ (2)

The process model for kerosene is based on Daniel H. König and Wörner (2015).

Optimizing the Model and Energy Reduction

A heat exchanger was introduced for heat integration, where stream 3 is used to pre-heat stream 1 which needs to be at 1000 °C for the rWGSR to take place. A second heat exchanger has been added to bring stream 4 to the FTS reacting temperature of 220 °C.

In addition to these changes, several case studies have been done (see Table 5.10). The pressure of the hydrocracker also showed little to no difference and was therefore not changed.

The temperature at each separation step was shifted ± 10 % and then adjusted to maximize the mass flow and selectivity of the end product. Lastly, the valve pressure (of a valve located right before the last separation step), was varied between 100–2000 kPa, and showed a favourable outcome at 375 kPa.

Table 5.10: Performed case studies on the production process of Kerosene.

Case study	Varying Parameter	Interval	Optimal
1	Hydrocracker Pressure [kPa]	3000 - 7000	Little to no difference
2-9	Separator Temperatures [% units]	± 10	
10-11	Valve-pressure [kPa]	100 - 2000	375
		25 - 300	250

5.2.4 Assumptions

Some assumptions were made in the models. These are all listed and sorted in this section according to small and large assumptions, depending on their impact on the model.

Small Assumptions

- A Ni/SiO_2-based catalyst is used for the methanation synthesis.
- A Cu/ZnO-based catalyst is used for the methanol synthesis.
- A Cu−Fe/CeO_2-based catalyst is used in the rWGSR.
- A Co-based catalyst is used in the FTS.
- A bifunctional (acid/metal) catalyst is used in the hydrocracker.
- No other contaminants than water in the stream of CO_2 is considered.
- No catalysts were included in the Aspen model but reaction parameters were chosen based on the catalyst.
- Hydrogen gas from the electrolyzer is assumed to be 100 % pure.
- The pressure drop is zero throughout the process. This entails the reactors, heat exchangers, condensers, distillation reboilers, heaters, coolers and pumps.

Large Assumptions

- Heat losses were neglected.
- All chosen catalysts are assumed to have 100 % selectivity, leading to no side reactions.
- Tray efficiency in the distillation columns is 100 %.

- Cooling of reactors with exothermic reactions has 100 % efficiency.
- Distribution after the hydrocracker is assumed to follow the literature without deviation.
- Concentration of CH_4 is assumed to follow the ASF distribution.
- The energy consumption of the hydrocracker is negligible.
- Cooling of the stream to the methane distillation column was disregarded.

Chapter 6

System Modelling

This chapter presents the results obtained from the Aspen HYSYS models since these values serve as input data for the EO3 model. The EO3 model will be explained next. The final results are presented in the following chapter (Chapter 7).

6.1 Output Parameters from Aspen HYSYS

6.1.1 Methane

Table 6.1 compiles the stream compositions for the streams indicated in Figure 5.2. As seen, stream 4: Methane, the product stream, is obtained with a purity of 98.7 mol%.

Table 6.1: Stream composition and parameters for the methane base case.

Stream	T [°C]	P [kPa]	Composition, x_i			
			CO_2	CH_4	H_2	H_2O
1. Feed	300	600	0.0622	0.124	0.813	0.0015
2. Recycle	-160	700	-	0.181	0.819	-
3. Distillation Feed	-162	2780	-	0.892	0.0031	0.105
4. Methane	-90.6	2790	-	0.987	0. 0034	0.0092

Table 6.2 shows the energy and product requirements for the methane process model in Aspen. It shows parameters both for the base case and the full scale case. The full scale case requires slightly less energy in terms of steam and electricity. The product demand for CO_2 and H_2 is the same for both cases.

Table 6.2: Energy and product requirements for methane production.

Parameter	**Unit**	**Value**	
		Base Case	Full scale
Steam	[kW/kg$_{CH_4}$]	0.863	0.424
Electricity	[kW/kg$_{CH_4}$]	2.92	2.58
CO_2 demand	[kg$_{CO_2}$/kg$_{CH_4}$]	2.80	2.80
H_2 demand	[kg$_{H_2}$/kg$_{CH_4}$]	0.53	0.53

Table 6.3 shows the energy streams that were not integrated into the model. These streams either had too low temperature to be integrated into the process or too low heat flow. These streams still have the potential to be integrated with the CHP plant or be upgraded and added to the district heating network, but this was not done in this work.

Table 6.3: Non-integrated energy streams in the methane production process model.

Stream type	**T_{in} [°C]**	**T_{out} [°C]**	**Heat flow [10^6kJ/h]**		**Comment**
			Base case	Full scale	
Cooler	60	20	1.61	7.43	
Reactor cooling	300	300	24.6	114	Cooling to keep the reactor temp at 200 °C.
Cooler	300	35	28.5	117	

6.1.2 Methanol

Stream compositions and parameters for the methanol base case are presented in Table 6.4 for the streams seen in Figure 5.3. From the distillation (Stream 5), methanol is produced with a purity of 99 mol%.

Table 6.4: Stream composition and parameters for the methanol base case.

Stream	**T [°C]**	**P [kPa]**	**Composition, x$_i$**			
			CO_2	H_2	H_2O	CH_3OH
1. Initial mixture	20.3	102	0.244	0.750	0.0058	-
2. Methanol Synthesis Feed	200	8000	0.0022	0.983	0.0035	0.0114
3. Methanol Synthesis Outlet	200	8000	0.0001	0.981	0.0057	0.0135
4. Recycle	95	8000	0.0005	0.985	0.0035	0.0115
5. Distillation Feed	91.8	100	-	0.0027	0.506	0.491
6. Methanol	64.8	100	-	0.0055	0.0045	0.99

Table 6.5 shows the energy and product requirements for both the methanol base case and full scale case. The full scale case requires more energy in terms of electricity but less in terms of steam. The H_2 demand is the same for both cases, but the CO_2 demand is higher for the full scale case.

Table 6.5: Energy and product requirements for methanol production.

Parameter	**Unit**	**Value**	
		Base Case	Full scale
Steam	[kW/kg$_{CH_3OH}$]	0.715	0.549
Electricity	[kW/kg$_{CH_3OH}$]	0.778	0.945
CO_2 demand	[kg$_{CO_2}$/kg$_{CH_3OH}$]	1.14	1.38
H_2 demand	[kg$_{H_2}$/kg$_{CH_3OH}$]	0.195	0.195

Table 6.6 shows energy streams that were not integrated with the model or the CHP plant. These streams have too low a temperature for any integration in the model, but they have the potential to be utilised.

Table 6.6: Non-integrated energy streams in the methanol production process model.

Stream type	**T$_{in}$ [°C]**	**T$_{out}$ [°C]**	**Heat flow [10^6kJ/h]**		**Comment**
			Base case	Full scale	
Cooler	60	20	1.65	7.37	
Reactor cooling	200	200	10.0	37.8	Cooling to keep the reactor temp at 200 °C.
Condenser	63.4	63.4	36.5	134	Condenser before the reflux in the distillation column.

6.1.3 Kerosene

The compositions of the kerosene streams are compiled in Table 6.7. These streams can also be seen in Figure 5.5. The final stream (Stream 7, E-fuels) consists of 57.3 mol% $C_{8-16}H_n$.

Table 6.7: Stream compositions and parameters for the kerosene base case

Stream	**T [°C]**	**P [kPa]**	**Composition, x_i**						
			CO_2	H_2	H_2O	CO	C_1-C_7	C_8-C_{16}	$C_{17}+$
1. rWGSR-Feed	1000	102	0.326	0.667	$7.8 \cdot 10^{-3}$	-	-	-	-
2. FT-Feed	220	4150	$9 \cdot 10^{-4}$	0.673	$6.9 \cdot 10^{-3}$	$3.4 \cdot 10^{-3}$	-	-	-
3. Gaseous Syncrude	225	4150	0.0576	0.741	0.178	-	0.316	$1 \cdot 10^{-4}$	-
4. Recycle	800	3500	-	0.670	$6.8 \cdot 10^{-3}$	$9 \cdot 10^{-4}$	0.322	$1 \cdot 10^{-4}$	-
5. Heavy Waxes	583	4150	-	0.396	0.522	-	0.0649	0.0129	$4.1 \cdot 10^{-3}$
6. Cracked Hydrocarb.	360	5000	-	0.977	-	-	$5 \cdot 10^{-4}$	$2.6 \cdot 10^{-3}$	0.0197
7. E-fuels	22.5	100	-	$3 \cdot 10^{-4}$	$5.8 \cdot 10^{-3}$	-	0.29	0.573	$7.3 \cdot 10^{-3}$

Table 6.8 shows the energy and product demands for kerosene base case and full scale production. The full scale case requires minimally less steam than the base case. Apart from that, however, the demands are equal.

Table 6.8: Energy and product requirements for kerosene production.

Parameter	**Unit**	**Value**	
		Base Case	Full scale
Steam	$[kW/kg_{C_{8-16}H_n}]$	1.03	0.99
Electricity	$[kW/kg_{C_{8-16}H_n}]$	21.7	21.7
CO_2 demand	$[kg_{CO_2}/kg_{C_{8-16}H_n}]$	1.12	1.12
H_2 demand	$[kg_{H_2}/kg_{C_{8-16}H_n}]$	0.31	0.31

Table 6.9 shows the energy streams that were not integrated into the model. Here, numerous streams can potentially be used for the district heating network or integration with the CHP plant. In contrast to the methane and methanol productions, the stream temperatures differ slightly from the base and full-scale cases.

Table 6.9: Non-integrated energy streams in the kerosene production process model.

	Base case			**Full scale**		
Stream type	**T$_{in}$ [°C]**	**T$_{out}$ [°C]**	**Heat flow [10^6 kJ/h]**	**T$_{in}$ [°C]**	**T$_{out}$ [°C]**	**Heat flow [10^6 kJ/h]**
Cooler	60	20	1.60	60	20	7.37
Cooler	60	20	3.69	60	20	17.1
Cooler	229	220	13.0	229	220	62.2
Cooler	465	220	345	459	220	1720
Reactor cooling	220	220	21.6	220	220	107
Cooler	220	120	128	220	120	654
Cooler	116	60	68.8	116	60	347
Cooler	60	25	0.424	60	25	215
Cooler	95	25	0.829	95	25	4.1
Cooler	1900	800	2460	1850	800	12100
Reactor cooling	800	800	4.30	800	800	13.1
Cooler	800	225	863	800	225	4460
Cooler	3300	360	9.01	3310	360	44.2
Cooler	360	30	6.57	360	30	32.2

6.2 Energy Optima 3 Modelling

EO3 is used to model the CCU process and the hydrogen production process, together with the CCS-equipped CHP plant. This is a software that is used as a tool to model energy systems, optimize them and make thorough prognostics for energy consumption and costs. The program is used by various energy companies within Sweden and the EU. Instead of considering the processes taking place within specific units, the units are modelled as a block diagram with energy flows going in and out. The block diagram can be optimized according to various factors, for instance, production cost. Optimizations are built on input data which can include: prices, efficiencies, district heating loads and weather forecasts. The modelling can also be further developed by special programming, where the user can customize it to their specific system detailing. Figure 6.1 shows the modelled CCU system in EO3.

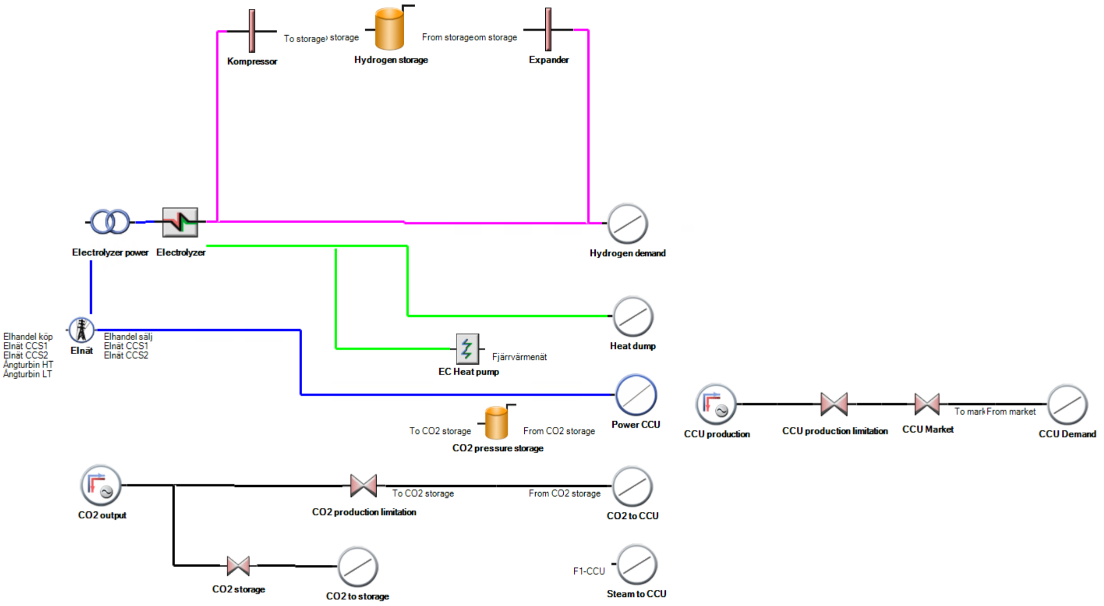


Figure 6.1: The modelled of the CCU process in EO3. Each energy type has a colour, pink is hydrogen, green is heat, blue is electricity and black is CO_2 or e-fuels.

6.2.1 Hydrogen System

The hydrogen system is modelled in EO3 in direct connection to the CHP plant, Filbornaverket. This system includes an electrolyzer, a compressor and a storage (see Table 5.1). Input data for these units to the model for the base case can be seen in Table 6.10 and 6.11. Parameters that are changed for the full scale case can be seen in Section 6.3, where the cases are described.

Table 6.10: Electrolyzer-parameters for the base case.

Parameter	Unit	Value	Comment
Size	[MW]	113	130 MW for Kerosene
Load change	[MW/h]	75.3	
Efficiency	[%]	70	
Maintenance cost	[SEK/MWh]	10.7	[1] [2], 12.1 SEK/MWh for Kerosene
Start/Stop cost	[kSEK]	212	[1] [2], 238 kSEK for Kerosene

[1] Taibi et al. 2020, [2] Khan et al. 2021

Table 6.11: Compressor- and hydrogen storage parameters for the base case.

Parameter	**Unit**	**Value**	**Comment**
	Compressor		
Auxiliary Power	[%]	3.93	
Pressure difference	[MPa]	3-30	
Load change	[MW/h]	75.3	Same as for electrolyzer
	Hydrogen storage		
Size	[MWh]	120	
Size	[m^3]	214	
Pressure	[MPa]	30	

6.2.2 CCU System

A finished model over Filbornaverket with CCS was provided by Energy Opticon and Öresundskraft. The CCS parameters used in this work correspond to an amine CCS process. The model was then extended with hydrogen- and e-fuel production. In EO3 the e-fuel production will be modelled as flows of energy and products to the production, with flows of energy (e-fuels) leaving the production. Flows that are needed are heat energy (steam), electrical energy, hydrogen and CO_2. Steam comes directly from the boiler or the turbine in the CHP plant, electricity can come either from the grid or the CHP plant, hydrogen comes from the hydrogen system and CO_2 comes from a CO_2 flow that is based on the CCS process, see Figure 6.1. The results from the Aspen models (Section 6.1) will be used as input parameters to model the e-fuel production in EO3. To control the production of e-fuels the model was built so that a production target for the whole optimization period could be set. The different optimization cases and how they are modelled in EO3 are described in the next Section.

6.3 Optimization Cases

12 cases will be run in the finished model in optima, plus two reference cases. A compilation of all cases can be seen in Table 6.12. It was decided to run all cases on data from both the years 2021 and 2022. This was decided since the data between the years differ a lot in terms of electricity prices. Here 2021 represents a normal year and 2022 represents an extreme year (see Section 2.4.2). It is worth noting that no one knows how the prices will be in the future and 2022 could for all we know be a good representation of how the new normal is. Each case was run with 1 hour time steps. The one hour time step was chosen since the electricity data are given in this time step and the spot price for electricity is decided on an hourly basis. The reference cases are run to have something

to compare with and represent the scenario when Filbornaverket is running with the CCS but without any production of e-fuels or hydrogen.

Table 6.12: All cases optimized in Energy Optima 3.

Product	**Base case 2021**	**Base case 2022**	**Full scale 2021**	**Full scale 2022**	**2021**	**2022**
Methane	x	x	x	x		
Methanol	x	x	x	x		
Kerosene	x	x	x	x		
Ref case					x	x

A small optimizing test was performed before deciding on the size of the electrolyzer and storage for the base case. These were done by optimizing the production of methane over a month with different sizes on the electrolyzer and storage. All optimization cases can be seen in Table 6.13. The conclusion from these tests resulted in the base case.

Table 6.13: Parameters for the small optimizing test to decide the optimal size for electrolyzer and hydrogen storage.

Case	**Electrolyzer [MW]**	**Storage [MWh]**	**Comment**
1	87	61	Minimum size for production target
2	87	120	
3	113	61	30 % bigger than minimum
4	113	120	
5	131	61	50 % bigger than minimum
6	131	120	
7	174	120	100 % bigger than minimum
8	113	250	One try with around 100 % bigger storage

The base case was designed around the methane need of part of the industry sector in Helsingborg. The demand is 250 GWh per year of natural gas and approximately 25 to 45 MW per hour. From this data, the case was scaled to meet the yearly supply of natural gas. The electrolyzer was scaled to fit the maximum production of 45 MW methane per hour, and the hydrogen storage was scaled to hold 1.5 hours of full production of hydrogen from an electrolyzer of the size 113 MW. This size is smaller than 4000 kg of hydrogen gas which is easier to get a permit for (Lindborg et al. 2021). All parameters for the base case can be seen in Table 6.14. As already mentioned, methanol and kerosene were then scaled after the same CO_2 demand that was required for the methane case.

Table 6.14: Parameters for the base case optimization.

Parameter	Unit	Value	Comment
Electrolyzer size	[MW]	113	130 MW for Kerosene
Hydrogen storage	[MWh]	120	
CH_4 max production per hour	[kg/h]	3240	LHV methane 13.9 kWh/kg
CH_4 min production per hour	[kg/h]	1300	(40 % of max)
CO_2 demand per hour	[kg/h]	6300	
Fix power CO_2 comp	[MW]	9	CO_2 compressor to storage
Relative auxiliary power	[%]	2.12	CO_2 compressor to storage

Another parameter for the optimization was that the load of the production was set to a minimum of 40% of the full scale (see Section 4.2). The production could also be off. To simplify the model and prevent long optimization times no restraints were put on how long the production could be off. To prevent the production from being of a very short time, such as an hour, which would not be realistic, a high cost was included for starting and stopping the process. Another simplification that was made was that the optimization was run over all hours of the year (8760 h) without a maintenance stop. To account for this, the yearly production target was scaled to match the full scale hours of Filbornaverket, 8200 hours per year.

The full scale case is designed around the possibility to use all CO_2 that is captured at Filbornaverket. The captured amount is around 28 t_{CO_2}/h. To use all this CO_2 for the production of methane, an electrolyzer of 252 MW is needed. To have flexibility in the system, and be able to adjust production volumes, a CO_2 storage is included in the optimization. Also, for this reason, the electrolyzer size is set to 327 MW. All parameters for the full scale case can be seen in Table 6.15. The ones not already mentioned have been scaled up using the same principles as for the base case.

Table 6.15: Parameters for the full scale case optimization.

Parameter	**Unit**	**Value**	**Comment**
Electrolyser size	[MW]	327	565 MW for Kerosene
Hydrogen storage	[MWh]	345	1.5 h of maximum production
Maintenance cost	[SEK/MWh]	4.6	[1] [2], 8.0 SEK/MWh for Kerosene
Start/Stop cost	[kSEK]	251	[1] [2], 434 kSEK for Kerosene
CO_2 demand	[kg/h]	28200	
CH_4 production per hour	[kg/h]	10100	Average production per hour
CH_3OH production per hour	[kg/h]	20400	Average production per hour
Kerosene production per hour	[kg/h]	25100	Average production per hour
CO_2 storage	[tons]	3000	

[1] Taibi et al. 2020, [2] Khan et al. 2021

For the full scale case, some additional simplifications were made to simplify the model and shorten the optimization time. Therefore, the possibility for the production to be off, as well as the start and stop time for the electrolyzer and compressor, were removed. Also for the full scale case, the maintenance stop was only included in the scaling and not in the optimization. Since all CO_2 was to be used no production target was used and the only constraint was that the production could vary between minimum and maximum and that all CO_2 was used at the end of the year. Therefore, instead of accounting for the maintenance stop by scaling the production target, the hourly CO_2 production was scaled after the CHP plant's 8200 full scale hours. This resulted in a CO_2 flow of 26.4 t_{CO_2}/h.

In both the base case and the full scale case, the excess heat from the electrolyzer was connected to the district heating network via a heat pump. Since the CHP plant runs on full scale all the time the district heating load that was included in the model could always be met. Thereby, no heat was sent to the district heating network and this possibility was therefore switched off.

6.4 Assumptions

Some assumptions were made in the model in EO3. They are listed below, and divided into small and large assumptions, depending on their impact on the model.

6.4.1 Small Assumptions

- The boiler is constantly running at full capacity.

- No cost for water or purification of water to the electrolyzer is included in the model.
- Changed efficiency for the electrolyzer depending on load was not included.
- For each case, the load change in the production of the e-fuels was assumed to be linear.
- The minimum load of 40 % for e-fuel production was based on the methane process and used for all cases.

6.4.2 Large Assumptions

- Steam from the boiler is assumed to be used directly in the e-fuel production. Additionally, whether the steam is low- or high-pressure has not been taken into consideration.
- The optimal electrolyzer size for the methane production was assumed to fit the methanol case as well.
- The optimal hydrogen storage size for methane production was assumed to fit all cases.

Chapter 7

Results

In this Section, the results from the modelling in EO3 will be presented. The calculated efficiencies and investment costs will also be presented.

EO3 optimizes the production to meet the included demands while at the same time minimizing the cost as mentioned before. The constraints put on each case can be seen in Section 6.3. The production prices for each case can be seen in Table 7.1. As seen, the base cases for each fuel have a lower production cost both in 2021 and 2022. A lower price is also obtained for all cases in the year 2021 compared to 2022, no matter base case or full scale case.

Table 7.1: Production costs for each e-fuel for every case. Here B stands for base case and F stands for full scale case.

e-Fuel	**B 2021 [SEK/kg]**	**B 2022 [SEK/kg]**	**F 2021 [SEK/kg]**	**F 2022 [SEK/kg]**
Methane	8.9	20.7	17.4	31.8
Methanol	2.2	6.2	5.9	10.8
Kerosene	16.4	28.7	26.9	49.9

Table 7.2 shows the required energy to produce each fuel for both the base case and the full scale case. The energy demand includes both the electrolysis and the e-fuel production process and is different for the two different volume productions since the process dynamics slightly change for each case. That includes the hydrogen fuel dimension, seen in Table 6.2, 6.2 and 6.8. Figure 7.1 shows the amount of energy that is supplied to the process from the CHP plant as a share of the total process energy demand.

Table 7.2: Total energy requirements to produce 1 kg of e-fuel including the synthesis process and hydrogen production.

e-Fuel	**Energy requirements base case [kWh/kg]**	**Energy requirements full scale [kWh/kg]**
Methane	28.8	28.0
Methanol	9.13	10.8
Kerosene	37.6	37.6

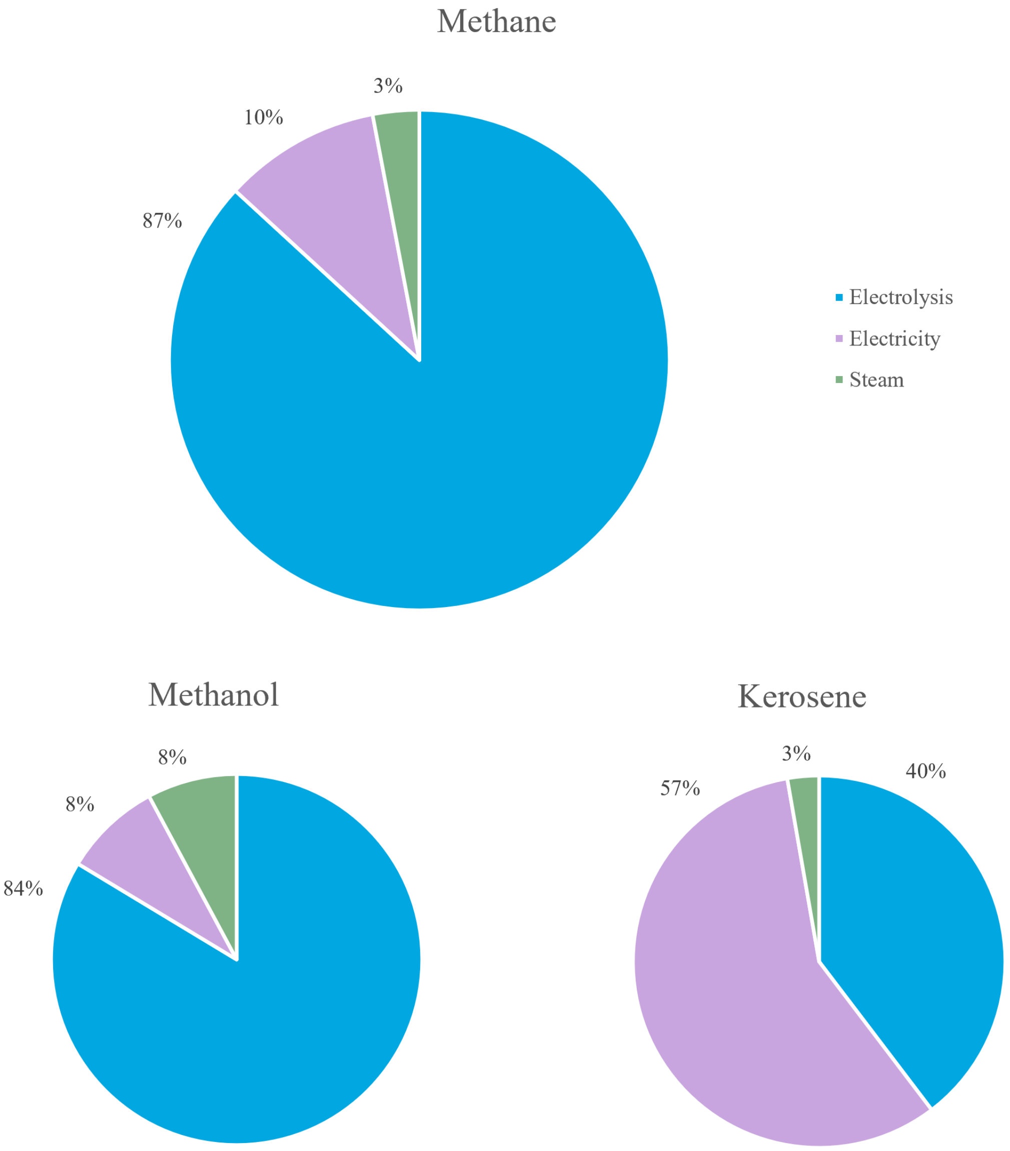


Figure 7.1: Share of energy-supply to the e-fuel production, shown as percent of the total energy demand seen in Table 7.2

In Table 7.3 the size of the installed capacity for a plant producing each e-fuel can be seen. The numbers include electricity for the electrolyzer, compressors and the production process. Numbers for steam demand include the steam that is needed for the production process of the e-fuels. As seen, large amounts of electricity are needed for full scale sized plants. Methane requires the smallest amount of electricity and steam and Kerosene requires the most.

Table 7.3: Installed capacity size that will be needed for a production plant for each e-fuel.

e-Fuel	**Plant size base case [MW]**		**Plant size full scale [MW]**	
	Electricity	Steam	Electricity	Steam
Methane	133	2.79	366	6.32
Methanol	130	5.83	356	16.5
Kerosene	323	8.33	1380	30.4

Table 7.4 shows the plant size in terms of output of e-fuels in MW for each fuel and case. The capacity for the full scale case is lower for methanol compared to methane since they were both scaled on a maximum output of 45 MW. For kerosene the average output per hour was higher than 45 MW therefore the maximum output was set to the same ratio as for methane. However, the values follow the same pattern.

Table 7.4: Plant size in terms of maximum production of fuel per hour in MW.

e-Fuel	**Plant size base case [MW]**	**Plant size full scale [MW]**
Methane	45	208
Methanol	45	166
Kerosene	96.3	445

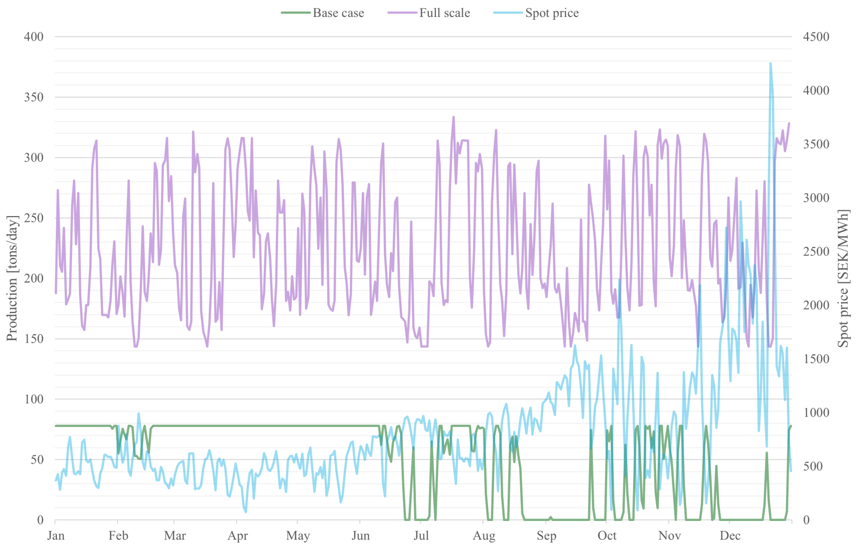
Table7.5 shows the plant efficiencies and PtX efficiencies calculated with Equation 4.14 and 4.15. The values are deviating for the two cases of methanol. For methane and kerosene, the values are nearly identical.

Table 7.5: Plant efficiency and PtX efficiency for the production of each e-fuel in the base case and full scale case.

e-Fuel	**Plant efficiency [η_{Plant}]**		**Power-to-X efficiency [η_{PtX}]**	
	Base case	Full Scale	Base case	Full Scale
Methane	0.681	0.692	0.472	0.478
Methanol	0.902	0.743	0.612	0.503
Kerosene	0.372	0.372	0.321	0.321

7.1 Methane

In Figure 7.2, the average daily production of methane for the base case and full scale case can be seen for both the year 2021 (Figure 7.2a) and 2022 (Figure 7.2b). The average spot price per day for each year is also included in the figure for comparison. Here it can be seen that the production in the base case could be switched off. For the full scale, this was not possible and instead, the production fluctuates between the maximum and minimum load.

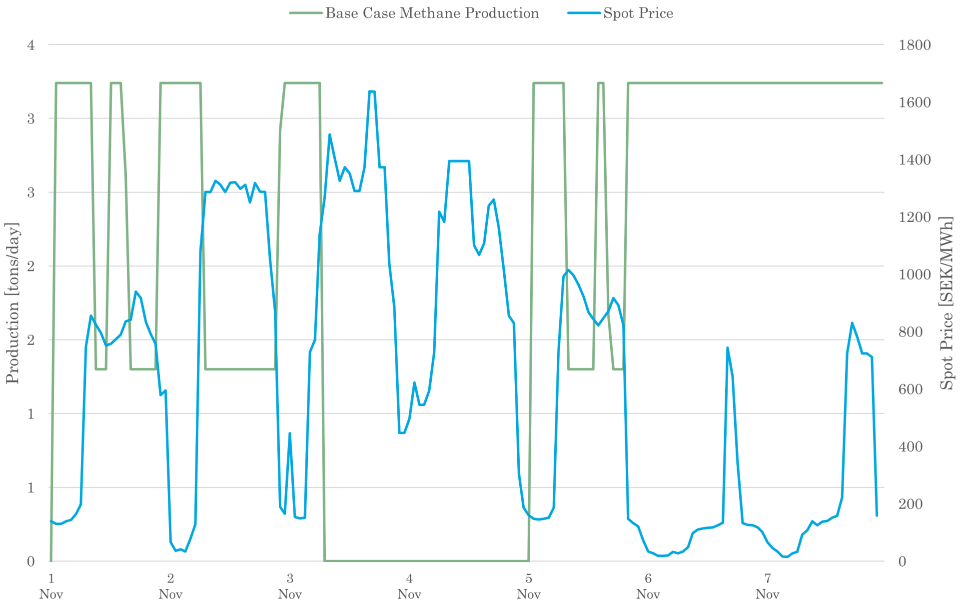


(a) Methane production for the year 2021.

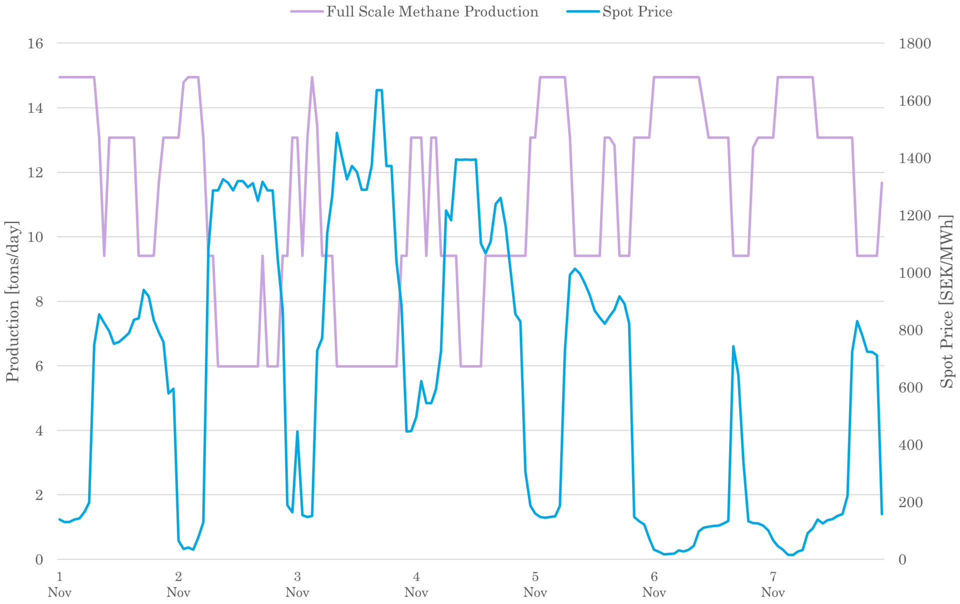
(b) Methane production for the year 2022.

Figure 7.2: Methane production for base case and full case simulations for the years 2021 and 2022, compared with the respective yearly electricity spot prices.

Figure 7.3a shows the production of methane for each hour during one week in November 2021 (base case). The correlation between how the production fluctuates because of the spot price can be seen more clearly here. When the spot price is high, production is turned off, or runs at a minimum and when the spot price is lower, the production reaches its maximum capacity.



(a) Fluctuations for base case production.

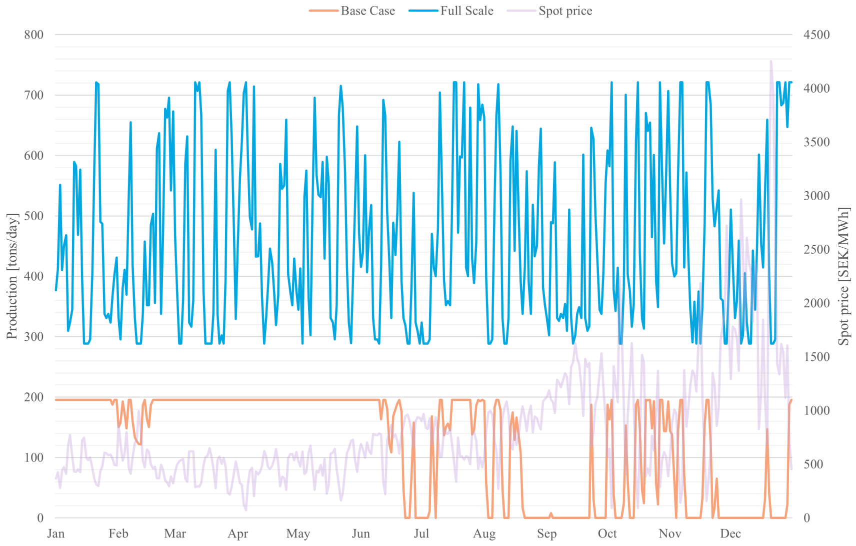


(b) Fluctuations for full scale production.

Figure 7.3: Correlation between the production of methane and the spot price for each hour during one week in November 2021.

7.2 Methanol

In Figure 7.4 the average daily methanol production for both the base case and the full scale case is shown for the year 2021 (Figure 7.4a) and 2022 (Figure 7.4b). For each year, the average spot price per day is also shown in the figure. Just as for methane, the production of methanol could only be switched off for the base case.



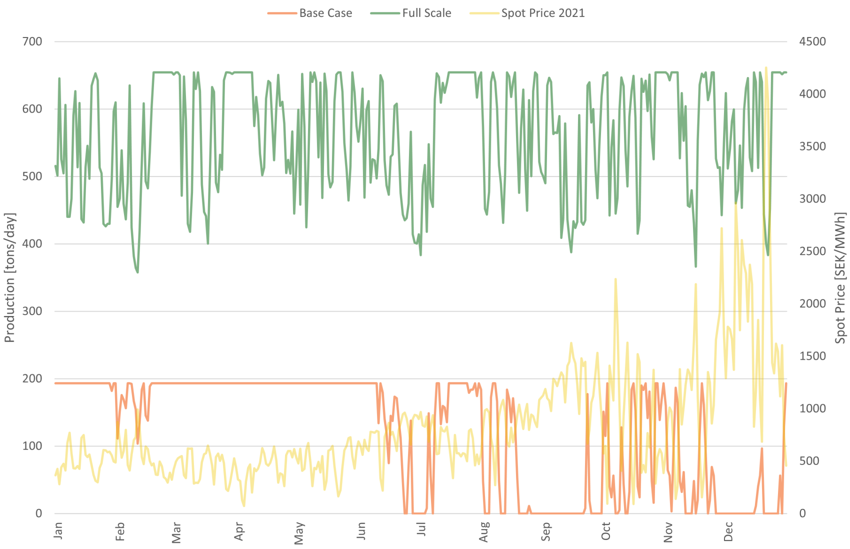
(a) Methanol production for the year 2021.

(b) Methanol production for the year 2022.

Figure 7.4: Methanol production for base case and full case simulations for the years 2021 and 2022, compared with the respective yearly electricity spot prices.

7.3 Kerosene

In Figure 7.5 the average daily production can be seen for both the base case and the full scale case for the years 2021 (Figure 7.5a) and 2022 (Figure 7.5b). It can be seen that the production follows the same pattern for both methane and methanol.



(a) Kerosene production for the year 2021.

(b) Kerosene production for the year 2022.

Figure 7.5: Kerosene production for base case and full case simulations for the years 2021 and 2022, compared with the respective yearly electricity spot prices.

7.4 Supply

In Figure 7.6 the power supply to the methane production for 2021 can be seen for both the base case and the full scale case. The power supply is shown as a percentage of the share that is supplied from the CHP plant. The other share is supplied from the grid. Here it can be seen that for the base case (green line) the supplied power is supplied by the CHP plant to a higher extent than for the full scale case. Later in the year, there are also long periods when there is no need for power from the grid since all of it is supplied from the CHP plant.

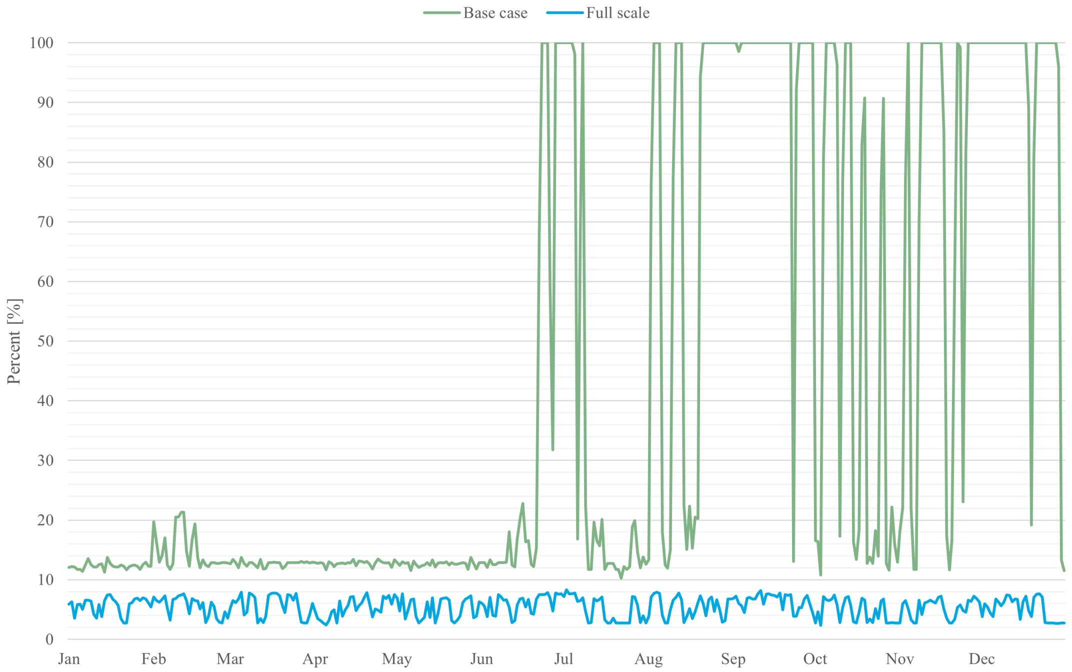


Figure 7.6: Power supply to the methane production for both the base case and the full scale case 2021 and 2022 as an average percent of how large share is provided by the CHP plant.

The average share of power supplied by the CHP plant over the year 2021 can be seen for all cases in Table 7.6. As seen, the largest share is gained in the methanol production and the smallest in kerosene production.

Table 7.6: The average share of power supply that is covered by the CHP plant for all cases the over the year 2021.

e-Fuel	Base case 2021 [%]	Full scale 2021 [%]
Methane	15.3	3.90
Methanol	18.5	4.28
Kerosene	4.87	0.25

7.5 Investment Costs

Total investment costs for the hydrogen system and the production facilities can be seen in Table 7.7 and 7.8. The costs were calculated based on Equations 4.16, 4.17, 4.18 and the values in Table 4.6 and 4.7 in Section 4.6. All investment costs are rough estimates and deviation from reality is possible.

Table 7.7: Total investment cost for the Hydrogen system of different sizes, including electrolyzer, H_2 compressor and storage.

Case	Electrolyser size [MW]	Total Cost [MSEK]
Base case	113	816
Full scale	327	1990
Base case Kerosene	130	877
Full scale Kerosene	565	3750

As seen, the total cost for each hydrogen system in Table 7.7 is higher compared to the cost of the entire production facility for each e-fuel (Table 7.8). Even at full scale.

Table 7.8: Total investment cost for the production facilities for each e-fuel, both for the base case and full scale case.

E-fuel	Total cost base case [MSEK]	Total cost full scale [MSEK]
Methane	87.5	202
Methanol	165	1000
Kerosene	560	1410

Chapter 8

Discussion

In this chapter, the results will be discussed, along with how the model was built and the assumptions made in the work.

8.1 Method

The chosen method was to first model the production processes of the e-fuels in Aspen HYSYS to gain all process requirements in terms of energy and reactant ratios. This was a good option to gain exact requirements for the processes and to understand how the production dynamics are behaving. The limits of this were mostly knowledge of the software and the extra time it took to learn the software. Another method could have been to use literature values for the process requirements as input parameters for the model in EO3. This would have allowed more time to be spent on energy integration with the CHP plant. However, all process requirements are often not given in the literature and values are also deviating between sources depending on how the process is designed. By using Aspen HYSYS a result is gained for these exact process designs that were modelled.

As this work was done in cooperation with Energy Opticon, their optimization software EO3 was used for modelling the e-fuel production process integrated with the CHP plant, Filbornaverket. As the production of e-fuels is not the main application for which EO3 is designed, some limitations were seen. These resulted in simplifications in the model to reduce optimization times. However, EO3 provided the possibility the integrate the process on real conditions such as the CHP, Filbornaverket, district heating loads and spot prices.

8.2 Aspen Models

Several factors in the Aspen modelling were not considered, which could have impacted the resulting values. As stated: heat losses, pressure drops and side reactions are disregarded. Considering heat losses would have resulted in greater energy demand for the process. The same thing goes for including pressure drops. Including side reactions in the simulation would mean that the purity of the e-fuel would be lower since other chemicals would be present in the process. It would also lead to a lower yield, meaning the process would not be as favourable as it is currently.

The CO_2 stream comes from the CCS process and contains some amounts of other substances from the flue gases, such as nitrogen, oxygen, and water. Except for water, which stood for 18 wt% of the stream, the other components were negligible. Hydrogen gas from the electrolyzer is assumed to be 100 % pure. This is a minor assumption since hydrogen from an AEC electrolyzer is 99.99 % pure, (as mentioned in Section 3.1.4).

Catalysts for the processes were also not included in Aspen. However, reaction parameters and other reactor conditions were modified after the chosen catalysts. If included in the modelling, the reaction extent could have been greater. Catalysts are assumed to have 100 % selectivity. This is another reason side reactions, even though small, are negligible.

One could argue that distillation columns would be preferable with kerosene production (model shown in Appendix C). Including a distillation column would lead to a less complicated separation process, with less intermediate cooling and heating. However, it is unclear what this would entail for the process energy demand since a distillation reboiler demands a great deal.

One delimitation of this paper is the disregard for cooling, meaning the energy demand of the processes is underestimated. However, from those cooling streams (Tables 6.3, 6.6 and 6.9), there is available heat at various temperatures that could either be integrated with the process or led to the district heating network. As no excess heat is gained when a stream is cooled to degrees below zero, the cooling of the stream to the methane distillation column will have a larger impact. This means that the energy requirement for the methane production will be higher.

The tray efficiency of the distillation columns is assumed to be 100 %. That applies to an ideal distillation column. In reality, the column would not be as effective as it is in the modelling. Additional trays would be required to reach the same purity.

The products from the FTS are calculated according to the ASF model. However, the CH_4-fraction in the ASF distribution is known to be underestimated. The modelling does not account for that. But if it would, it would result in higher energy demand and lower product purity. The component distribution following the hydrocracker is assumed to follow the literature values perfectly. Realistically, this would not be the case, bringing the reaction extent to a lower value.

8.2.1 Energy Demand

The energy demand for all three fuels in this work is in the same range as the found literature values. Energy demands for the methane process of 28.8 kWh/kg and 28 kWh/kg for the base case and full scale case, respectively, were required. These values are in the lower range of the literature value, 27.0–35.0 kWh/kg (see Table 4.8). For methanol, the energy demand was 9.13 kWh/kg for the base case and 10.8 kWh/kg for the full scale case. This is close to the literature values of 9.74 kWh/kg. The same goes for the kerosene production, where the energy demand came to 37.6 kWh/kg for both cases. This is in the upper range of the literature values of 21.0–37.3 kWh/kg. In Table 4.8, one of the literature values for methanol and two for kerosene also include the CO_2 capture. This means that these energy demand values include the required energy for the capturing process as well. However, the largest energy demand from the literature does not include CO_2 capture or electrolysis. This shows how much the values can deviate and that the acquired results are extremely process-dependent. The literature values for methane energy demand only include electrolysis and the production process, just like the ones presented in this work. It is also worth noting that the values found in the literature are based on similar production processes for e-fuels, but the structure can deviate. The type of electrolyzer is not the same for each of the references, which, of course, will affect the results.

The difference in energy demand between the base case and the full scale case can be seen in Table 6.2, 6.5 and 6.8. There is not a large difference between the cases for any of the fuels. The slight deviations depend on the changed characteristics in the process when the production volume is changed. Higher magnitudes result in higher energy demand for compressors and reboilers. Pressurising gases is not a linear process in the case of hydrogen. Heat is also generated during compression, which needs to be cooled for efficient compression. The differences in total energy demand between the cases are still small enough to have minimum impact on the assumption that the load change is linear for each case. This can therefore be assumed to be a valid assumption.

Looking at Figure 7.1, it is clear that hydrogen production stands for the largest share of the energy demand. For kerosene, this is not the case. Here, the electricity demand for pumps and compressors is grander than for hydrogen production. This means that the largest savings can be made in the production process for kerosene by optimizing the compressors and pumps further. The large share in electricity demand for the process is slightly high in this case, and it should not be larger than the share of electrolysis. As the total energy demand for kerosene is still reasonable, it was not investigated further due to time limitations. For methane and methanol, the largest savings can be made during hydrogen production. This step is very energy-consuming and also the hardest to optimize further. The efficiency of hydrogen production depends on the electrolyzer technique. The chosen electrolyzer was the AEC. This type of electrolyzer is the cheapest and most used electrolyzer in the industry sector. New varieties of electrolyzers are emerging on the market. For example, SOEC has shown very high efficiency (see Section

3). The technique in this area is fastly developing, and in the near future, the energy demand for hydrogen production will likely be much lower. This will contribute to a lower energy demand for e-fuel production.

8.3 Production Cost

The production cost generated in this work for producing methane is between 8.90–31.8 SEK/kg, which is in the same range compared to the literature values seen in Table 4.8, which is between 13.5–20.0 SEK/kg. The lowest production price, 8.90 SEK/kg, is gained for the base case 2021, which is lower than other literature values. For methanol, the production cost is lower compared to the literature values, 2.20–20.8 SEK/kg compared to 10.6–12.7 SEK/kg. The production price gained for kerosene is within the same range as the found literature values: 16.4–49.9 SEK/kg compared to 21.0–37.3 SEK/kg.

As seen in Table 7.1, the production costs vary between the years and the base case and full scale case. The lowest production cost for all three fuels is gained in the year 2021 for the base case. For all three fuels, the production price per kg for the base case in the year 2021 is lower than the found literature values. There is no apparent reason for this low production cost since many various parameters affect the result. The parameter that is probably affecting the most is the integration with the CHP plant. None of the values from the literature shown in Table 4.8 are derived from processes integrated with a CHP plant. For the base case, a larger share of the needed electricity power is provided by the CHP plant, as seen in Figure 7.6. When the process is supplied to a 100 %, the production is either off or on low load. This means that money is earned from selling electricity to the market. Money is also earned since the CHP plant is burning waste, which has to be taken into account if this process is to be applied to another CHP plant, or as a stand-alone process. The money earned from burning waste will decrease the production price. All steam for the production processes is also covered by the CHP plant. This means that supplying the process with steam will generate money in this model.

The production price for methanol is very low in all cases. Even with the high electricity prices in 2022, the production price is remarkably low. The model was thoroughly investigated to see if any mistakes were made. None could be found, but this result should still be considered with caution. From Table 7.6, it can be seen that the power supply to the production process in the base case for methane is supplied to 18.5 %, which is the highest percentage of all cases. This means that the production process of methanol requires the lowest share of bought electricity from the grid. This could be the reason behind the very low production price. The lowest gained production price of 2.2 SEK/kg is, however, not much lower than the production price for bio-based methanol, as seen in Table 2.1. The process for e-methanol is more energy intense, especially due to the hydrogen production, as seen in Figure 7.1. Therefore, more investigation would be needed before stating that this result is reasonable.

Parameters in the EO3 model that will affect the production price is, as mentioned, that money is gained when burning the fuel. Electricity is also sold and bought from the market, at the cost of the spot price. No cost for electricity taxes are included in the model, as well as costs for water to the electrolysis or O&M for the e-fuel processes. In the simulation, the boiler is running at full capacity for the entire year. In reality, there is a maintenance stop during the summer, lasting around three weeks. The production is scaled around this production stop, but since the boiler is running at all times in the model, money is earned all year when, in reality, no money is made during this production stop.

Despite the mentioned uncertainties, it can be concluded that there is a large possibility of producing e-fuels at competitive prices. Though it is still cheaper to produce fuels from fossil sources, as seen in Table 2.1, the production costs are comparable to the bio-based production of the respective fuels. The most compatible is the price gained for the base cases in 2021. This shows that if the production processes are designed thoroughly and integrated with a CHP plant, the production of these e-fuels could be competitive with the bio-based alternatives.

8.4 The Integrated System

Filbornaverket is, in reality, connected to the district heating network in Helsingborg, and also via EVITA, to Lund and other connecting cities (see Section 2.3.2). When running the model, no heat was sent to the district heating network from the electrolyzer in the first runs. Therefore, this possibility was switched off in all cases. In the EO3 model, Filbornaverket was disconnected from the rest of the system. However, if the model would have run in integration with the whole network, it is reasonable to assume that some heat could have been sent to the network. This could have led to averting production costs in other parts of the network.

As described in Section 6.2, the finished model of Filbornaverket in connection with CCS was retained from Energy Opticon and Öresundskraft. The required energy for the CCS is included in the model and is affecting the production from the CHP plant. As this was included in the acquired model, the energy share for the CCS is not included in the results. It will not affect the production price either since these prices were compared to the reference case of Filbornverket with CCS. This will mean that, in actuality, there will be an additional energy demand and cost for the CCS. Further integration between the CCS and e-fuel production process is, however, possible. As the CCS process requires heat, there is a possibility to supply this heat from the electrolyzer or the waste heat from the e-fuel production process.

There is also the fact that the production is optmizied on historic data. This means that perfect planning can be done about when the production should be on maximum, minimum, or off. This will not be the case in reality. Spot prices can only be predicted for the future and are not fully known. The historic data brings an almost perfect production strategy over the year leading to low production costs since times with high prices can be avoided. This means that in reality, the production price will most likely increase slightly.

8.4.1 Cases

There is a large difference between the production costs between the years 2021 and 2022. The production cost is higher for all cases in 2022 compared to 2021. This has to do with the spot price for electricity. In 2022, the average yearly spot price was much higher than in 2021 (see Section 2.4.2) leading to higher production costs. This shows that the production cost is very sensitive to the electricity costs. It is hard to say if the prices in 2022 were an anomaly or if this is the new normal. If it is, strategies for making the production of e-fuels cheaper need to be evaluated. From this work, it can be seen that if the electricity is produced by the producer, and not bought from the grid, the production price will be lower. Integration with a CHP plant is therefore favourable. It is noteworthy that if Filbornaverket would be integrated with e-fuel production, it would mean that the CHP plant would no longer be able to supply the electricity network with any electricity. Instead, it would be an electricity consumer. This will of course affect the surrounding area and the electricity network.

Some parameters also had to be changed for the full scale case to simplify the model. One of them was that the production of e-fuels had to be running at all times. This also contributes to the higher production price for the full scale case. If there would have been an option to switch off the production when the spot price is high and sell electricity instead, a lower production price could be achieved. However, large investment costs (more about that in Section 8.6) are needed for the production of these e-fuels. Due to these high costs, it is not reasonable to build a large production plant and then turn it off for long times if the electricity prices are high. Therefore the production needs to be optimized to be able to run during high electricity prices as well. This means that the full scale case might visualise a more realistic production plan.

8.4.2 Constructional Aspects

As discussed, the production costs for all full scale cases are greater than the ones for the base cases. This could be due to that the whole EO3 model is not upscaled to fit with the larger process units. It would be possible to simulate that by modifying the sheet of Filbornaverket. However, due to a lack of time and knowledge of that part of the model, this was not done. One thing that would need to be altered is the size of the heat pumps. What would it entail for the full scale case production price if it could be provided with the same ratio of electricity from the CHP plant as the base case? All of these changes would naturally be costly, in addition to the fixed costs of building the production plant.

On the contrary, there would be a larger volume of e-fuels, which depending on the market, could make these costs worthwhile. In the case of Filbornaverket, to avoid becoming an energy consumer at all times, the base case would suffice, as this would cover the industry sector demand in Helsingborg. In the case of wanting to build a full scale production, a larger CHP plant should be looked at for process integration. This could potentially affect the production costs.

8.5 Synergies with the CHP Plant

As seen from the result there are a lot of synergies that can be made when integrating e-fuel production with Filbornaverket. Steam can be provided directly from the CHP plant and in the case of Filbornaverket when waste is used as fuel the cost of steam is very low. Money can even be earned if the district heating load is low. The biggest advantage is the supply of electricity that can be provided by the CHP plant. By optimizing the whole system together, production can be run in ways that minimize the production cost. As mentioned in Section 2.4.2 the volatile electricity price can sometimes be negative. At these times when the price is negative or low it is not beneficial to sell the produced electricity from the CHP plant. If the production of e-fuels is run at these times, very beneficial production prices could be achieved.

Another factor that favours capturing the carbon and utilizing it as e-fuels is the price of CO_2 emissions. These have as described in Section 2.2.1 historically been low but are today at much higher levels. To avoid these high prices puts additional incentives to invest in CCS and e-fuel production. The cap in ETS is also reduced each year meaning that the price will only increase moving forward.

8.6 Investment Costs

From the investment costs, see Section 7.5, it can also be seen that the cost for the hydrogen system stands for the largest share. This can be explained by the fact that the prices for electrolyzers and hydrogen compressors are still very expensive. Especially the costs for the electrolyzer, since this is still considered new technology. Costs for components belonging to the e-fuel production facilities, such as reactors, distillation columns and heat exchangers, are lower since this equipment has been used and developed over a longer time. These types of components are used in multiple industrial processes and costs have been reduced over the years thanks to technology advancements and competition. This cost reduction will most likely be the case in the future for electrolyzers and H_2-compressors as well and reductions are already seen on the market. It must also be considered that costs for the components can vary. Values found in the literature deviate between sources and the price is also very dependent on the specific process design.

8.7 Efficiencies

The gained efficiencies seen in Table 4.5 are in the same range as the literature values seen in Table 7.5. The developed methane production process in this work has a plant efficiency of 0.681 and 0.692 for the base case and full scale case respectively. Compared to the value from the literature of 0.780 which is based on the HHV the gained values are in the same range. Plant efficiency for the methanol production in this work is 0.902 for the base case and 0.743 for the full scale case. Both these values are in the range of the found literature value. The difference in efficiency between the base case and full scale case is depending on the difference in energy and product requirements for the cases seen in Table 6.5. Realistically the plant efficiency for the base case is very high and this is also a sign that the base case for methanol produced here is ”too good”. This also coheres with the very low production price for methanol gained. Although, the gained efficiency for the base case is not considerably higher than the literature value of 0.859. This indicates that the developed process is not completely unrealistic. The plant efficiency for kerosene gained is much lower than the found literature value, 0.372 for both base case and full scale case compared to 0.749. This low efficiency can most certainly be addressed by the high electricity demand for the production process (see Figure 7.1). This makes it clear that the kerosene process could be optimized further.

PtX efficiency is lower than the plant efficiency since it also accounts for the energy required to capture the CO_2. This value was gained from the model in EO3. For methane, the PtX efficiency gained was 0.472 for the base case and 0.478 for the full scale case. Unfortunately, no reference value was found to compare this with. The methanol process PtX efficiency gained was 0.612 for the base case and 0.503 for the full scale case. These values are in the same range as the literature value of 0.576. For the kerosene process, the PtX efficiency of 0.321 is much lower than the found literature value of 0.506. However, it is not as low as the plant efficiency compared to the literature value. This indicates that it is the production process that is accountable for the low values.

8.8 Sustainable E-fuels

It could be debated whether the e-fuels produced from the conditions in this work can be labelled sustainable. Even though the hydrogen is produced from electricity from the Swedish electricity grid or the CHP plant, it is not considered as green hydrogen completely, as described in Section 2.1.4 and 2.4.1. Whether the CO_2 can be considered green is not clear either. Most would not think so, see Section 2.1.4. According to the summation of CO_2 laws in connection to CCU-processed made by Öresundskraft (see Section 2.2) it is not as simple as a yes or no. It seems like there are not any clear legislations regarding it, and that it varies from where what and who is part of the project. If producers do not know whether they will be able to brand their e-fuels as sustainable, that will more than likely lower their incentives in the e-fuel branch since their product will not be as sought after. The transportation sector needs to undergo big changes shortly. E-fuels can be a part of that. There need to be clearer rules as to what counts as green and how to go about it when branding e-fuels. As this work has shown, there are integration possibilities with CHP plants, and we believe that allocating CO_2 from waste flue gases should be allowed, and not hinder the opportunity of producing renewable e-fuels.

Chapter 9

Conclusion

The conclusions of this work are presented as answers to the research questions.

To what cost can e-fuels be produced from integrated production with a CHP plant? E-fuels were found to have the same production cost as their bio-counterpart. However, by further integration with the CHP, and by adapting the process volume to the CHP capacity, it would be possible to achieve lower prices. Additionally, if there is no need for a constant supply of e-fuels, the process could be even more flexible, resulting in a lower production price. This would, however, not make sense, given the vast investment costs that were appraised. The main factor affecting the cost is electricity. This is clear since all production costs were higher in 2022 than in 2021. So, the surest way of obtaining lower production costs is to contribute electricity from the CPH plant to the production.

How much energy will the production of e-fuels require? The results established that the production process of e-fuels still requires considerable energy input. Especially in terms of a full scale plant. However, large reductions are possible, and the findings in this thesis should be further investigated. It is also clear that the hydrogen demand stands for the largest energy share in production. This means the largest reductions can be made regarding better hydrogen production technologies.

What positive synergies - if any, are there with integrating the production of e-fuels with a CHP plant? It can be concluded from the results that a reduction in production price can be acquired when integrating the production with a CHP plant. The largest effect was accredited to the electricity supply. It can also be seen from the results that further integration is possible and heat from the electrolyzer and e-fuel production processes could potentially be utilized in the CCS process or supplied to the district heating network. This work also shows that, if integrated with a CHP plant, cost reductions can be made by optimizing the times when electricity is used in the production process and when it is sold to the market.

9.1 Recommendations for Future Work

For future work, recommendations are to look further into the integration between the e-fuel processes and the CHP plant. It is seen from this work that there is potential for energy savings in numerous steps throughout the process. This is worth investigating more to see how large the potential is. It would also be interesting to study the effect of different taxes on the production price. This will most likely also favor the CHP plant's electricity production, depending on how it is produced. By investigating further what effect taxation would have, it would be possible to suggest what type of taxation is needed in the future to make the production of e-fuels competitive.

It would also be valuable to investigate the e-fuel production process in other kinds of industries. That would result in knowledge about both what characteristics the CHP plant had a positive impact on and which parameters are most important for cost- and energy-sufficient e-fuel production.

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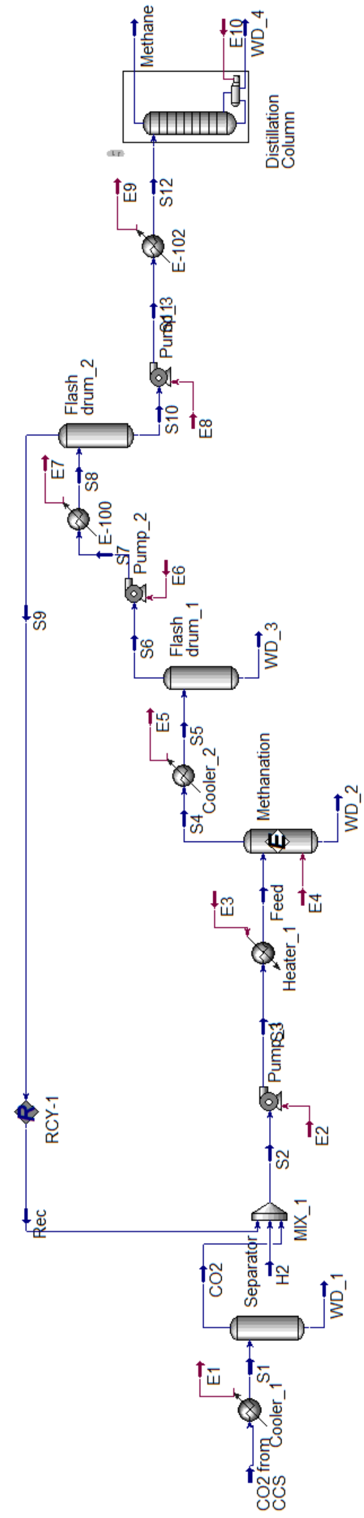
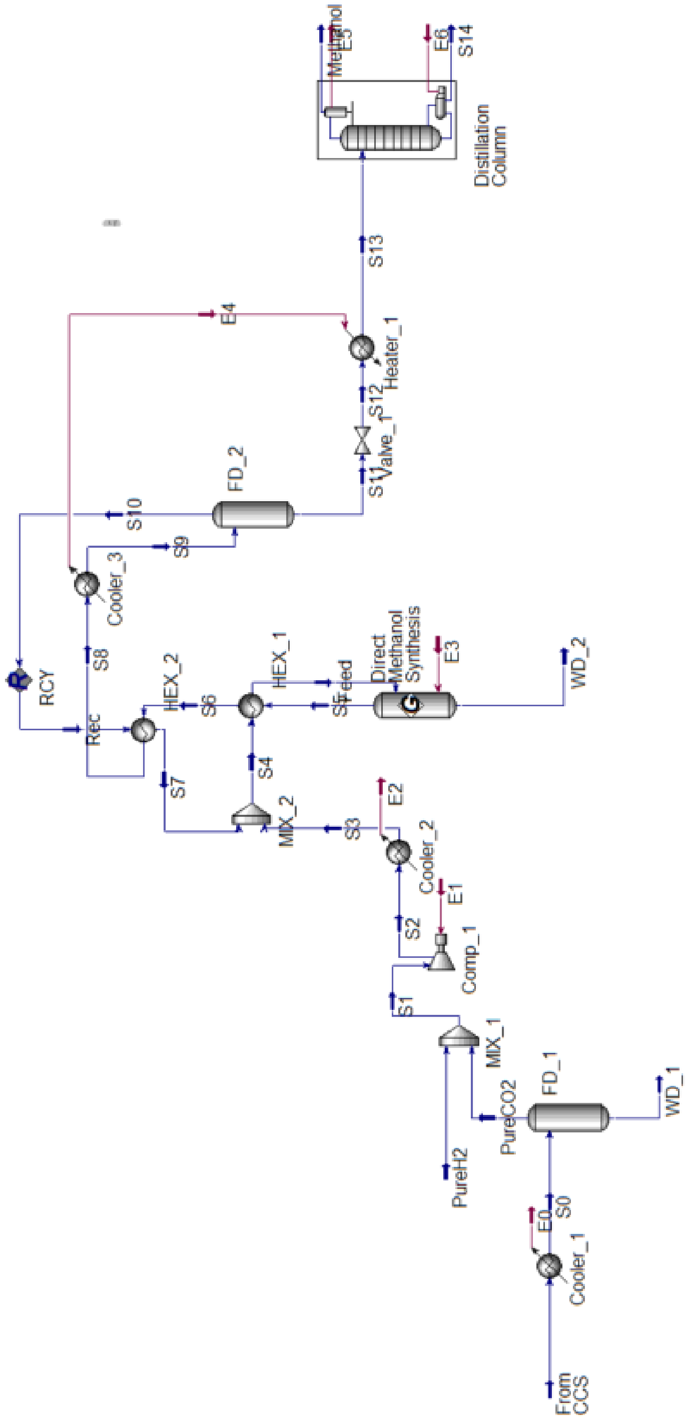
Appendix

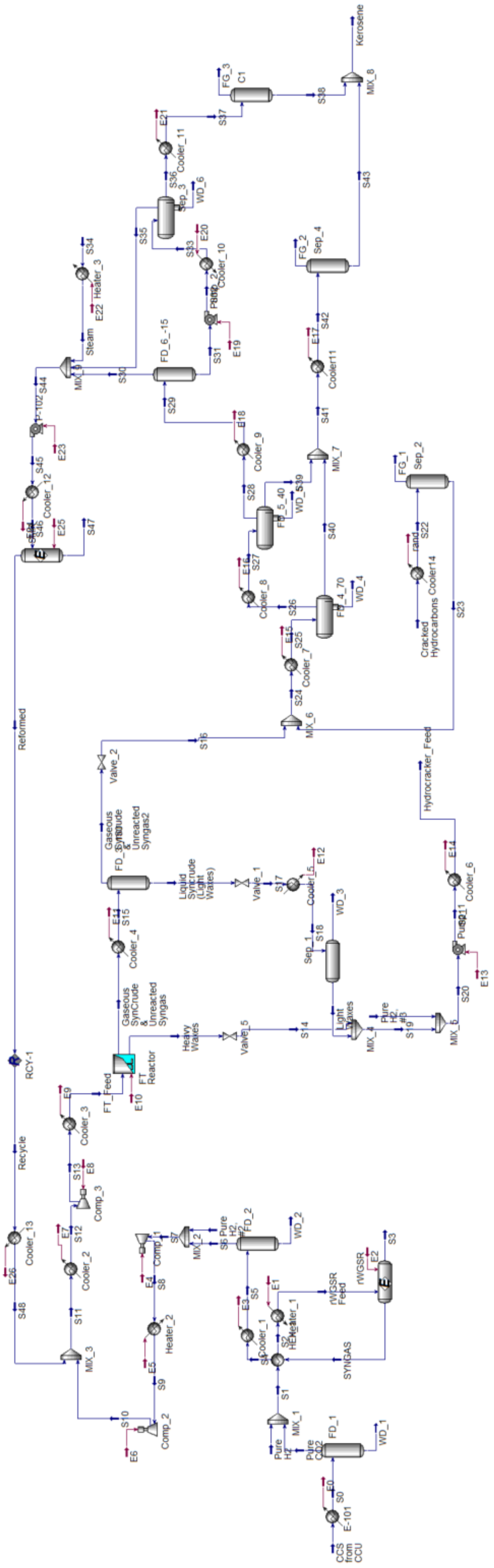
A


CO2 from CCS
Cooler_1
E1
S1
Separator
WD_1
CO2
H2
MIX_1
Rec
S2
E2
Pump_1
S3
RCY-1
Heater_1
E3
Feed
E4
Methanation
WD_2
S4
Cooler_2
E5
S5
Flash drum_1
WD_3
S6
Pump_2
E6
S7
E-100
E7
S8
Flash drum_2
S9
S10
E8
Pump_3
S13
E-102
E9
S12
Distillation Column
Methane
E10
WD_4

B


From CCS
Cooler_1
E0
S0
FD_1
WD_1
PureCO2
PureH2
MIX_1
S1
Comp_1
E1
S2
Cooler_2
E2
S3
MIX_2
S4
S7
HEX_1
HEX_2
S5
Feed
S6
Direct Methanol Synthesis
E3
WD_2
Rec
RCY
S8
Cooler_3
S9
S10
FD_2
S11
Valve_1
S12
Heater_1
E4
S13
Distillation Column
Methanol
E5
E6
S14

C


CCS from CCU
E-101
FD_1
WD_1
Pure CO2
Pure H2
MIX_1
SYNGAS
rWGSR Feed
rWGSR
FD_2
WD_2
MIX_2
Comp_1
Heater_2
Comp_2
MIX_3
Cooler_2
Comp_3
Cooler_3
FT_Feed
FT Reactor
Heavy Waxes
Valve_5
Gaseous SynCrude & Unreacted Syngas
Cooler_4
Liquid Syncrude (Light Waxes)
Valve_1
Sep_1
Light Waxes
MIX_4
MIX_5
Pump
Cooler_6
Hydrocracker_Feed
Valve_2
MIX_6
Cooler_7
Cooler_8
Cooler_9
MIX_7
Cooler11
Sep_4
Sep_2
Cracked Hydrocarbons
Cooler14
FD_6_-15
Cooler_10
Sep_3
Cooler_11
C1
MIX_8
Kerosene
Heater_3
Steam
MIX_9
Cooler_12
Cooler_13
Recycle
RCY-1
Reformed