Oxyfuel combustion and carbon capture of a cogeneration plant for synthetic fuel production

Master's thesis in Sustainable Energy Systems

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Abstract

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This work evaluates the integration of oxyfuel combustion with an existing biomass combined heat and power plant and utilize the carbon dioxide from the flue gas to produce e-methanol. The primary objectives include determining the potential quality of e-methanol production, assessing CO_2 emissions reduction and evaluating economic viability of the system. The study was done taking Växjö Energi’s Sandvik 2 plant as the reference to dimension other components to produce methanol. The plant data used in the work is Vaxjö energi’s real-time data recorded in 2023.

Other main components involved in the process are electrolyzer to produce oxygen for the oxyfuel combustion and the methanol reactor to produce methanol. Two electrolyzer types namely alkaline electrolyzer and the solid oxide electrolyzer have been implemented and compared throughout the work, and the latest and most popular technology has been implemented for the methanol production. The study employs detailed process design, cost analysis, and sensitivity analysis to explore the feasibility of the integrated system.

The integrated system demonstrates significant CO_2 emissions reduction and efficient e-methanol production. It can produce between 0.15-0.17 megatons of e-methanol annually, depending on the electrolyzer type, while meeting a significant portion of the municipality’s heating demand of 407 GWh annually. Total annual costs range from 235-258 million EUR for the alkaline variant and 337-423 million EUR for the SOEC variant, with break-even pricing of 1486-1553 EUR/ton and 1979-2483 EUR/ton respectively. The system utilizes 68.6-72.2% of CO_2 with the alkaline variant and 73.9% with the SOEC variant.

An upgraded system can utilize up to 98.09% of CO_2 emissions to produce 0.22 megatons of methanol annually, aligning with energy targets. Nonetheless, while feasible, the overall costs are significantly higher. Further cost reductions are possible by maximizing electricity production and reducing heat production, resulting in a lower break-even price for e-methanol. Economic factors such as heating revenues, subsidies, CO_2 taxation, and fuel costs reduce the overall costs to 207-229 million EUR for the alkaline variant and 307-393 million EUR for the SOEC variant. This leads to a break-even price of 1306-1375 EUR/ton for the alkaline variant and 1800-2304 EUR/ton for the SOEC variant.

The study identifies technical risks and limitations, including component lifespan and cost inclusiveness, necessitating further research and development. Overall, the integrated system holds significant potential for contributing to climate change mitigation and supporting Sweden’s carbon neutrality goals.

Oxyfuel combustion, Power-to-X, carbon capture, green methanol, electrolysis, costs, combined heat and power, hydrogen, oxygen

Declaration of independence

We hereby declare that we have written this thesis independently, that we have not used any sources other than those indicated and that we have marked all statements taken verbatim or in spirit from other works as such, that the thesis submitted has not been the subject of any other examination procedure either in its entirety or in significant parts, that we have not already published the thesis either in its entirety or in parts, and that the electronic copy is consistent with the other copies.

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Signature Jatin Srinivas Donni	Location, Date

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Acronyms and Abbreviations

AB	Aktiebolag
AC	Alternating current
ACC	Annualized capital cost
AEL	Alkaline electrolysis
ASU	Air separation unit
atm	Atmospheric conditions
BECCS	Bioenergy with carbon capture and storage
BEP	Break-even price
BFB	Bubbling fluidized bed
BWR	Boiling water reactor
CAGR	Compound annual growth rate
CAPEX	Capital expenditure
CC	Carbon capture
CCS	Carbon capture and storage
CCU	Carbon capture and utilization
CFB	Circulating fluidized bed
CHP	Combined heat and power
CO_2PU/CPU	Carbon dioxide processing unit
DC	Direct current
DH	District heating
DME	Dimethyl ether
e-fuel	Electrofuel
e-methanol	Electro-methanol
ESP	Electrostatic precipitator
ETS	Emission trading system
EU	European union
EUR	Euro
FG	Flue gas
FGC	Flue gas condenser
FGD	Flue gas desulphurization
FGLPH	Flue gas low pressure heater
FGPU	Flue gas processing unit
FGR	Flue gas recycling
FLH	Full load hours
FM	Fluidization medium
GHG	Greenhouse gas
HE/HEX	Heat exchanger
IMPCA	The international methanol producers and consumers association
KOH	Potassium hydroxide
LCOH	Levelized cost of hydrogen
LHV	Lower heating value
LMTD	Log mean temperature difference
LPG	Liquified petroleum gas
MATLAB	Matrix laboratory

MEA	Monoethanolamine
Mio	Million
MPU	Methanol production unit
NO_x	Gases with nitrogen and oxygen (NO_2, NO_3)
OF	Oxyfuel
OPEX	Operational Expenditure
PC	Pulverized coal
PEMEL	Proton exchange membrane electrolysis
PGU	Power generation unit
PPU	Power production unit
PtX	Power-to-X
PV	Photovoltaic
R&D/RnD	Research and development
RFG	Recirculated flue gas
SC	Steam condenser
SEK	Swedish kronor
SMR	Small modular reactor
SOE	Solid oxide electrolysis
SO_x	Gases with sulphur and oxygen (SO_2, SO_3)
SRC	Steam raising converter
SSZ	Scandia stabilized zirconia
TAC	Total annual cost
TCC	Tube cooled converter
TRL	Technology readiness level
USD	American dollar
WEU	Water electrolysis unit
YSZ	Yttria stabilized zirconia

Nomenclature

Latin letters

Symbol	Unit	Description
A	m^2	Area
k	%	Interest rate
M	g/mol	Molar mass
$\dot{m}$	kg/s	Mass flow
n	mol	No.of moles
N	-	No. of modules
$\dot{n}$	mol/s	Molar flow
P	W_{el}	Power
Q	W_{th}	Heat
r	%	Share of recycled flue gas
S	-	Component size
t	year (a)	lifetime
$\dot{V}$	m^3/s	Volume flow
W	Wh_{el}	Electricity
wt%	-	Weight percent
X	-	Volumetric ratio
y	%	Share of gas

Greek letters

Symbol	Unit	Description
η	%	Efficiency
ρ	kg/m^3	Density
α	-	Ratio of excess oxygen in oxidant
Δ	-	change
Ψ	%	CO_2 conversion rate
β	-	Additional oxygen share
Y	%	Share of non-emitted flue gas

Subscripts

Symbol	Description
B	Boiler
dem	Demand
el	Electrical
f	Fuel
G	Generator
heat/th	Thermal

i	Running index
in	Input
out	Output
ox	Oxyfuel
ref	Reference
T	Turbine
tot	Total

Chemical formulae

Structure	**Description**
Al_2O_3	Aluminum oxide
C (atom)/C_2 (molecule)	Carbon
$Ca(OH)_2$	Calcium hydroxide
$CaSO_3$	Calcium sulfite
CH_3OH/MeOH	Methanol
CO_2	Carbon dioxide
Cu	Copper
CuO	Copper oxide
e^-	Electron
H (atom)/H_2 (molecule)	Hydrogen
H_2O	Water
H_2S	Hydrogen sulfide
KOH	Potassium hydroxide
N (atom)/ N_2 (molecule)	Nitrogen
NH_3	Ammonia
NH_4OH	Ammonium Hydroxide
NO	Nitrogen oxide
NO_2	Nitrogen dioxide
NO_3	Nitrogen trioxide
N_2O	Nitrous oxide
O (atom)/O_2 (molecule)	Oxygen
OH	Hydroxide
S	Sulphur
SO	Sulphur oxide
SO_2	Sulphur dioxide
SO_3	Sulphur trioxide
ZnO	Zinc oxide

1. Introduction

The contemporary world struggles with an unprecedented climate crisis, by an upsurge in the global average temperature surpassing 1.1°C above pre-industrial levels as of 2019 [1]. This alarming situation stems from heightened concentrations of greenhouse gases (GHGs) in the atmosphere, predominantly caused due to human activities [1]. Notably, carbon dioxide (CO_2), primarily emitted through the combustion of fossil fuels which in turn stands for about 84.3% of the global primary energy use and about 30.8% of Sweden's [2], accounts for a substantial portion of anthropogenic GHG emissions.

Addressing the urgency of climate change requires globally coordinated efforts aligned with the Paris Agreement's objectives to cap the global average temperature at 1.5°C above pre-industrial levels. Key to this endeavour is by decarbonizing the energy sector to reduce 45% of GHG emissions by 2030 and achieve net-zero emissions by 2050 [3], a target set by many nations, including Sweden, aiming for carbon neutrality by 2045 [4–6].

While renewable energy presents itself as a viable option to reduce CO_2 emissions, challenges such as intermittency and insufficient supply persist [7]. Furthermore, transitioning to renewable energy from the current dominance of fossil fuels in the primary energy supply, which stands at 80%, poses a formidable challenge. In this context, carbon capture and storage (CCS) technologies emerge as crucial tools for mitigating emissions. The European Climate Foundation (2010) declared that only by adding technology such CCS, it could be possible to reduce 80% of the 1990s greenhouse gas emissions in 2050 [8].

Among the different CCS technologies, oxyfuel combustion stands out. Although oxyfuel combustion has not commercially established yet, it is considered the most promising of the technologies, because it offers easy CO_2 capture and a low-efficiency penalty, slightly above 7% [9]. The principle behind oxyfuel combustion is to aid the capture of CO_2 from flue gases by eliminating nitrogen prior to combustion.

Furthermore, Bioenergy with Carbon Capture and Storage (BECCS) holds considerable potential, particularly in Sweden due to the existing forest industry and the associated carbon stock [10], leveraging biomass as a renewable carbon source for negative emissions [11]. Despite its promise, BECCS faces challenges related to cost and infrastructure.

Complementing carbon capture, Power-to-X technologies offer additional avenues for decarbonization, enabling the conversion of surplus renewable energy into various chemicals or fuels, such as e-methanol- a versatile chemical with applications across industries and as a clean energy resource.

In this report, we propose the integration of oxyfuel combustion technology into a biomass combined heat and power (CHP plant), utilizing oxygen generated by separating water using an electrolyzer. This innovative approach aims to harness CO_2 emissions from the CHP plant, combined with hydrogen – another product from the water separation in the electrolyzer, to produce methanol – a sustainable energy recourse called e-methanol. By leveraging renewable electricity and cutting-edge technologies, our initiative seeks to contribute to Sweden's transition towards carbon neutrality while addressing the challenges of climate change.

The objective of this master's thesis is to assess the feasibility and profitability of integrating oxyfuel technology into a Biomass-fuelled cogeneration plant, complemented by Power-to-Methanol. This involves utilizing an electrolyzer powered by renewable electricity to split water, providing oxygen for oxyfuel combustion and hydrogen for methanol production.
With this objective in mind, the study will investigate the following:

1. Determining the potential quantity of e-methanol that can be produced.
2. Assessing the extent to which CO_2 emissions can be mitigated.
3. Evaluating the economic viability of the entire process.
4. Identifying and analysing the challenges associated with each technology, including risks, permits, and regulatory allowances.

Summing it up, a systematic illustration on the proposed design is shown in Figure 1.

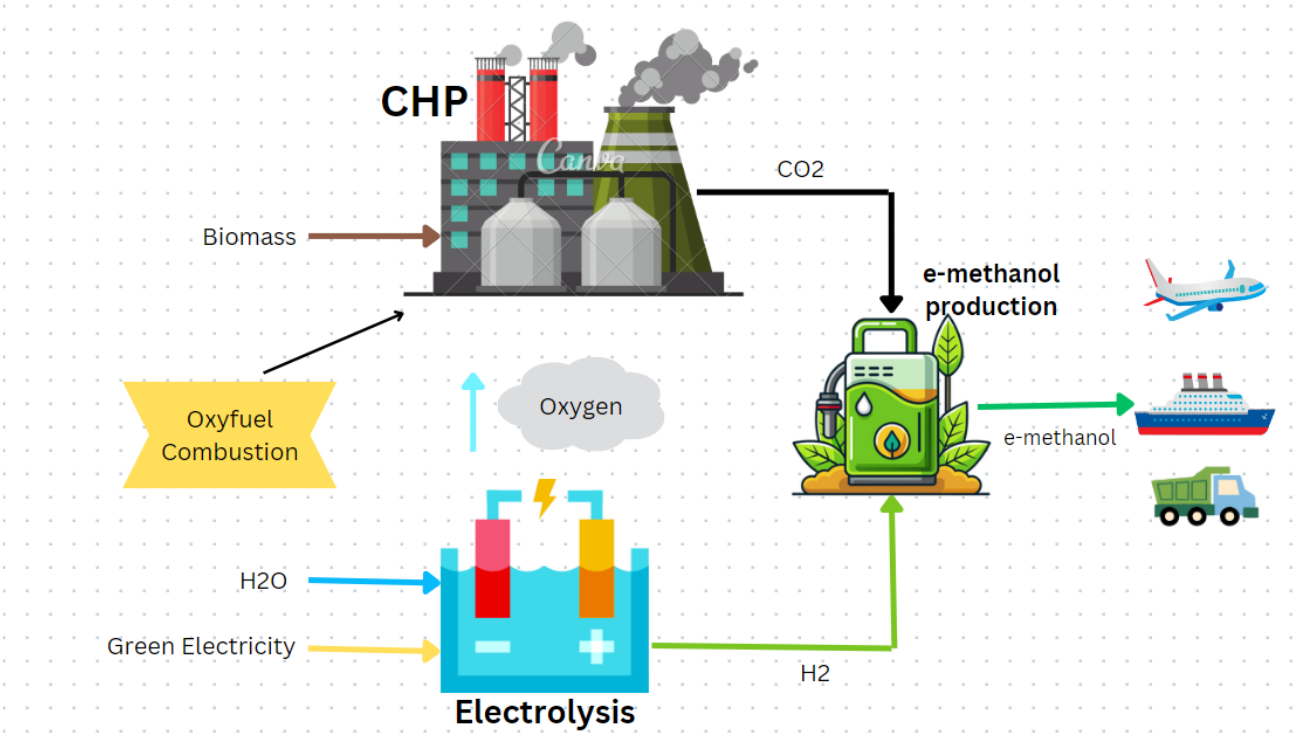


Figure 1: Illustration on proposed system including the applications and flows.

2. Theoretical Background

First, it is indispensable to have a closer look at the single technologies and key processes which are used in the later system approach of this master thesis. Starting with background knowledge on carbon capture, BECCS and Power-to-X, this chapter will cover the provision of hydrogen and oxygen for the final methanol production. The intension is to give a rough overview of which technologies have been researched and why a specific system concept was selected at the end of the day. It will also illustrate which alternatives are open for a possible system specification or adaptation.

2.1 Combined Heat and Power (CHP)

A combined heat and power (CHP) also known as the cogeneration plant is a highly efficient method of producing both heat and electricity simultaneously using a single fuel source. The main objective of a CHP plant is to maximize the duty of a fuel by utilizing the heat which would be otherwise be wasted in electricity-only generation plant [12].

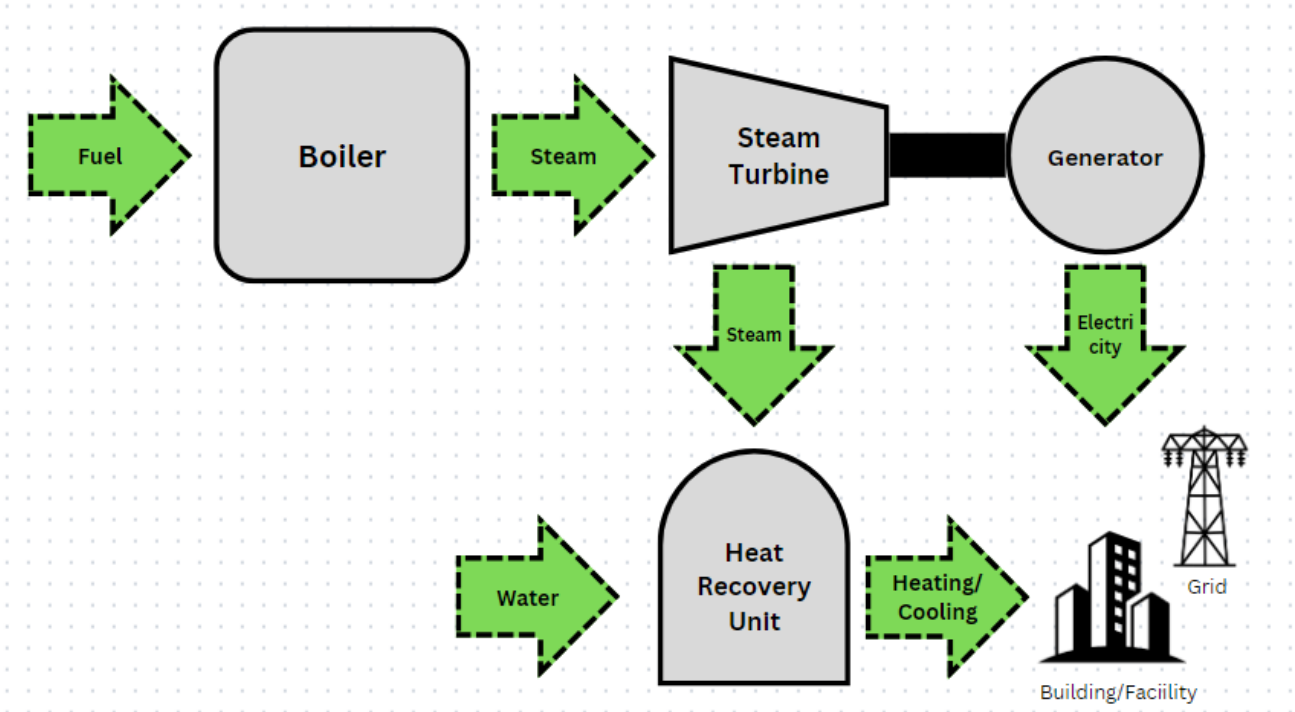


Figure 2: Functionality of combined heat and power.

Benefits of CHP [13]

- Increased efficiency
- Decreased emissions per unit fuel burnt
- Cost savings
- Improves energy security

2.2 Carbon Capture

Carbon capture is a process in which a relatively pure stream of CO_2 from industrial sources, power plants and other large-scale emitters is separated, treated and transported to a long term storage typically, geological formations such as saline aquifers and oil and gas fields, this is termed as CCS (carbon capture and storage) or in some cases, the separated CO_2 can be used for high demand applications and this is termed as CCU (carbon capture and utilization) [14].

2.2.1 Carbon Capture Methods

The carbon capture technology can be differentiated based on many factors such as the CO_2 separation method, point of capture and so on, but the three main approaches to capture CO_2 can be distinguished: post-combustion capture, pre-combustion capture, and oxyfuel combustion. Figure below presents the fundaments of the above-mentioned technologies.

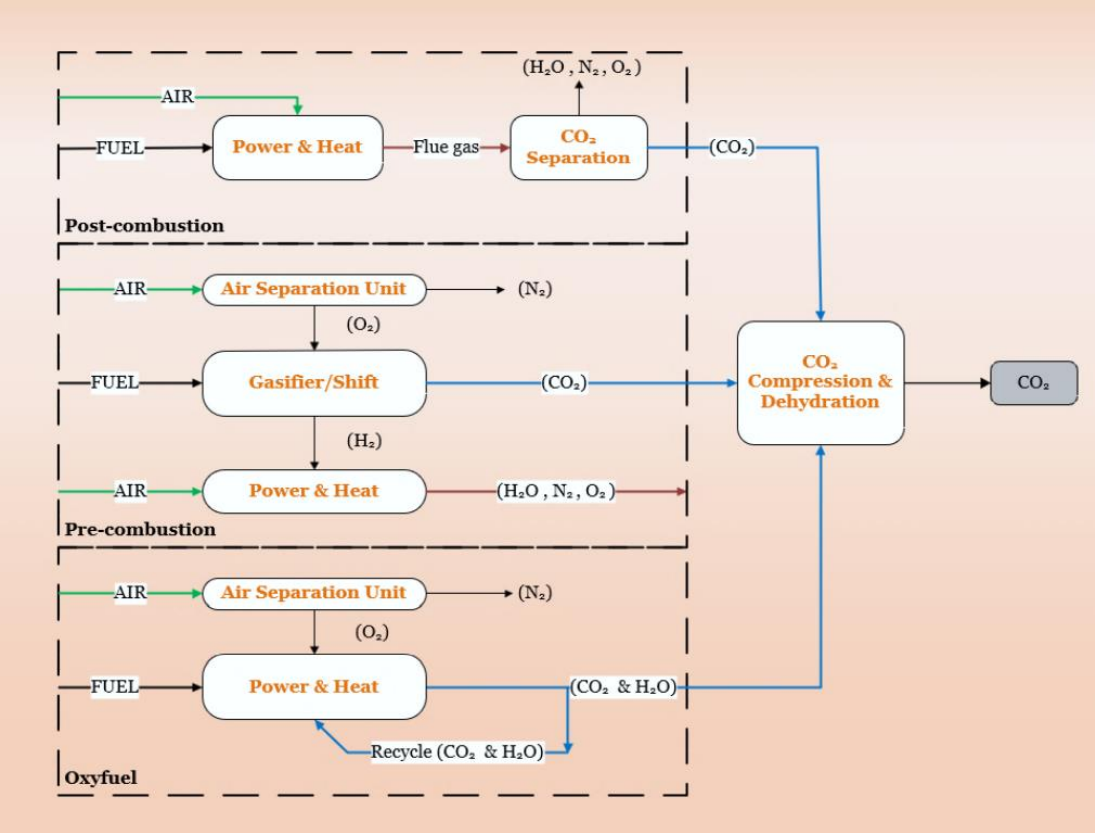


Figure 3: Scheme of different carbon capture technologies. [15]

- **Pre-Combustion**

Pre-combustion capture involves the capture of CO_2 prior to air-fuel combustion. The process primarily uses an inexpensive solvent (usually rectisol or selexol), to absorb CO_2 under high pressure. CO_2 is later separated by lowering the pressure at above atmospheric pressure and does not require heat for regeneration [16]. This method is usually implemented in natural gas combined cycle plants,

fertilizer and chemical production units [17]. Though, it has a lower efficiency penalty: less than 9% [18], yet it is expensive and requires further development [19].

- **Post-Combustion**

This process involves the separation of CO_2 from flue gases after combustion of fossil fuels. The exhaust gas after combustion is majorly composed of a mixture of nitrogen, carbon dioxide, sulfur oxides, water vapor and particulate matter and therefore requires treatment before the separation [12]. It is currently considered as the most mature capture technique and hence the most popular out of the three, though it requires a significant amount of energy at the CO_2 extraction stage with 8-12% efficiency penalty [18].

- **Oxyfuel Combustion**

The topic of interest in this thesis is the oxyfuel (OF) combustion which was discovered in 1982 [20]. The principle behind this technology is that air in the combustion process is substituted by a stream with a high vol% of oxygen content (up to 95 vol% is favorized [21]) hence eliminating nitrogen prior combustion. The resulting flue gas stream consists 80-85% of CO_2 and water [22] hence decreasing the capture cost by 30% compared to its counterparts [23]. To sustain a controllable and stable flame, the carbon dioxide rich flue gas stream is partly recycled and led back to the combustion chamber [24].

Table 1 illustrates the advantages and disadvantages of oxyfuel combustion carbon capture as opposed to air-fuel combustion with post-combustion carbon capture [25].

Table 1: Qualitative comparison of air-fuel combustion and oxyfuel combustion. Table reproduced from [25].

	Advantages	**Disadvantages**
Air-fuel combustion with pre-combustion carbon capture	✓ Frequently used in the industrial processes ✓ Lower energy requirements compared to other CO_2 capture methods ✓ Syngas can be used as a fuel for turbine cycle ✓ Requires less amount of water compared to post-combustion capture	× Significant loss of energy compared to post-combustion capture × High equipment cost × Requires extensive supporting systems × Mainly applicable to new plants × More R&D required
Air-fuel combustion with post-combustion carbon capture	✓ Applicable for existing and new power plants ✓ Extensive research is absolved related to technical behaviour and is therefore a well-known technology (sorbents, catalysts, equipment, etc.) ✓ Future developments will increase the plants total efficiency and reduce the CO_2 emissions ✓ Most used method in CO_2 capturing	× Low CO_2 partial pressure at ambient pressure × The amine technologies used results in an almost 30% loss of the net power output and an efficiency reduction of 11% × The steam extraction decreases the flow to low-pressure turbine; affecting the efficiency and reducing capability × High performance, circulation volume, and water requirements are needed for high capture levels × Constant addition of chemicals × Chemical slip from process
Oxyfuel combustion carbon capture	✓ Produce high efficiency steam cycles ✓ Low level of pollutant emissions at low costs ✓ Cost effective compared to other CO_2 capture methods. A low cost is required to capture more than 98% of CO_2 ✓ Easy to retrofit into an existing power plant, and does not require an on-site chemical operation ✓ All components are well-known technology	× High energy penalty when using an ASU × High overall cost when using an ASU × Technology needs to be proved for large scale operations (for more than 30 MW) × High risk of CO_2 leakage

2.2.2 Bioenergy with Carbon Capture and Storage

The Bioenergy with Carbon Capture and Storage (BECCS) is a derivative of CCS, in which the CO_2 is captured from processes using biomass or bioenergy as the source of combustion rather than fossil fuels, as in the case of CCS. The principle behind BECCS is, CO_2 is absorbed from the air by biomass through photosynthesis, when it grows. This biomass residues in the form of tops and branches of trees in the forest, bark and saw dust from the wood industry is later used as a fuel the power plant to produce energy, the released CO_2 after the combustion is captured using carbon capture hence resulting in negative emissions [7, 11]. Figure 4 illustrates the carbon flow of BECCS. When BECCS systems are employed, a negative carbon flow from the atmosphere into storage is created[26].

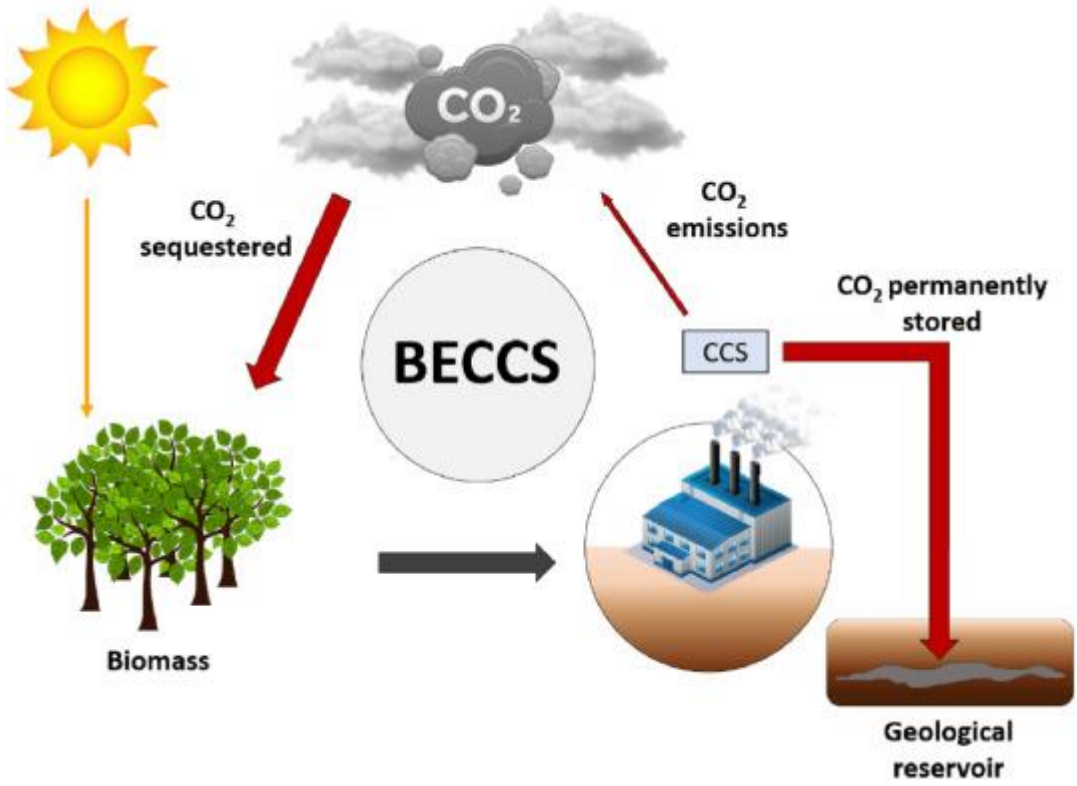


Figure 4: The carbon flow of BECCS. When BECCS systems are employed, a negative carbon flow from the atmosphere into storage is created. [26]

Sweden has high potential of implementing BECCS due to a well-developed forest industry and the net growth of carbon stock in the forest and its strong ambitions to achieve net-zero emissions by 2045 [10].

2.3 Power-to-X

Power-to-X (PtX) is a concept that converts electrical power into other forms of energy or chemical products. These technologies mainly aim to make use of excess electricity (mainly from renewable sources) produced during low demand scenarios and convert them into useful products such as hydrogen, synthetic fuels and chemicals which can be used for respective applications.

Green hydrogen is an important energy source for a future low-carbon society. It produces only water vapor when burned, yet its power can drive many of our energy systems, from vehicles to heating homes. It is also central to the PtX model because it is a hub for collecting and redistributing energy.

PtX also helps other sectors and industries to achieve carbon-neutrality. The CO_2 emissions produced in carbon-intensive industries and plants can be captured and reacted with green-hydrogen to produce useful products such as methanol (see Figure 5). This concept of methanol production is in the scope of the thesis and has further been discussed and implemented in the work.

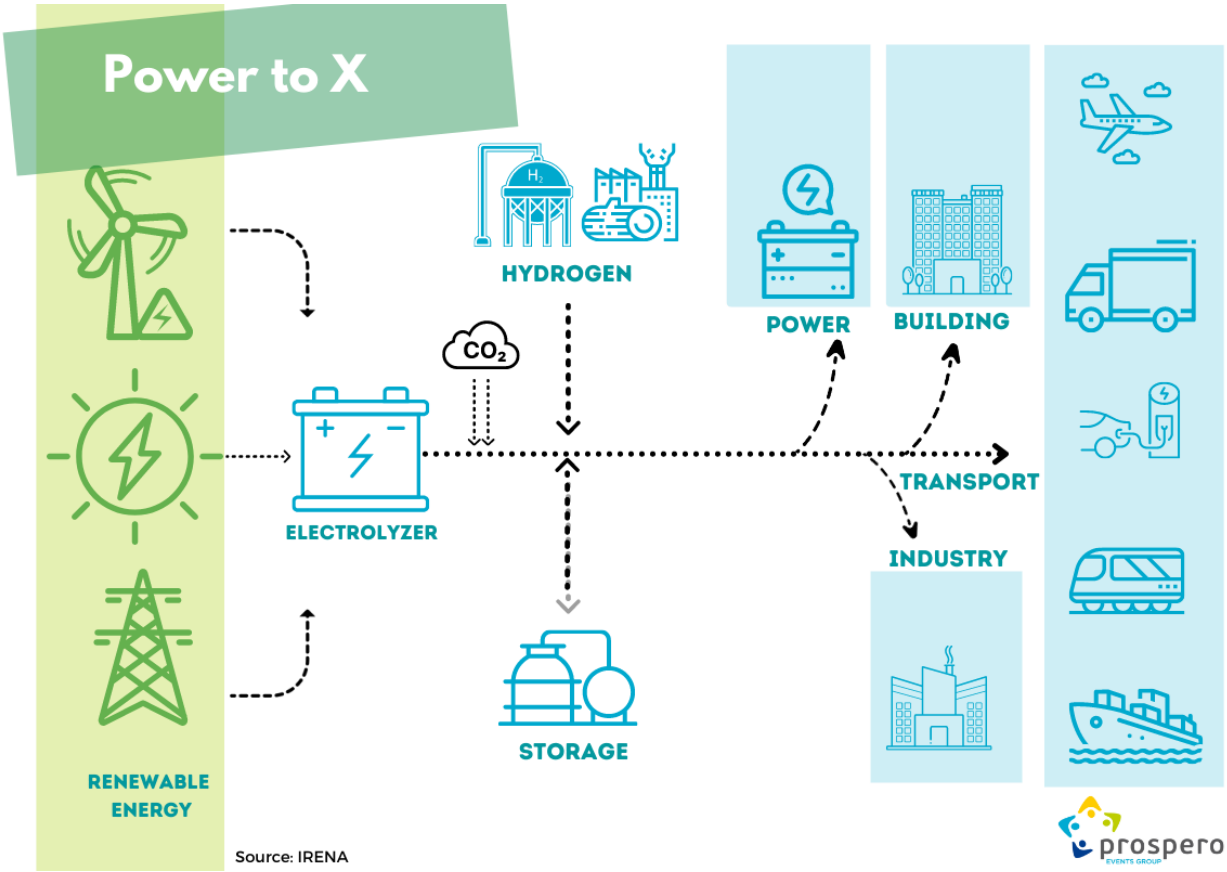


Figure 5: Illustration of the Power-to-X concept [27]

2.4 Hydrogen and oxygen supply

Because of a high low heating value (LHV) of 120 MJ/kg and its multifunctional usage in different energy sectors such as industry, heating, electricity and transport, hydrogen plays a growing role as a no longer indispensable energy carrier [28, 29]. The global sales market for hydrogen amounted to no less than 95 Mio. tons in 2022, with an annual growth rate of around 3% [30]. Nevertheless, the energy-intensive and carbon-dioxide-emitting technologies of steam reforming of natural gas and coal gasification are still largely used in its production today. *Fasihi, Weiss et al.* speak of circa 99% worldwide, which is attributable to this so called "brown" (or "grey") hydrogen production with CO_2 emissions of around 10 tons per ton of hydrogen generated [28, 31]. In order to make the production of hydrogen more climate-friendly and to meet the worldwide increasing demand for hydrogen, industry and nations are gradually turning to electrolysis technology connected with renewable energy sources instead of steam methane reforming or coal gasification [30]. In the recent past, so-called "green" hydrogen projects have been subsidized and hydrogen strategies have been developed by various nations (including Germany and Sweden) [28, 32]. From a German perspective, an electrolysis capacity of 10 GW by 2030 was set as the target, and from a Swedish perspective, a figure of 5 GW by 2030 [28, 32]. In Germany's case, this increase corresponds to covering around 30 to 50% of their national hydrogen demand [28]. For the purpose of completeness, blue, orange, turquoise and pink/yellow hydrogen production must also be mentioned here when classifying hydrogen. In this context, the term blue hydrogen is used when the carbon dioxide produced during the synthesis of brown hydrogen is processed and stored using CCS technologies. Orange hydrogen is claimed if the production is based on waste products (such as municipal waste). Turquoise describes the usage of methane pyrolysis for hydrogen generation. Last, but not least one is talking about pink/yellow hydrogen if nuclear power is utilized for running the electrolysis [33].

Table 2 breaks down once more the type and color of hydrogen production with a brief description [28, 30, 31, 33].

In this work, the main focus should lay on the green/orange hydrogen production as within the methanol production system, an electrolyzer is applied for the hydrogen and oxygen supply. A particular advantage of choosing an electrolyzer as a hydrogen source (for the later methanol production) is that the oxygen (which is usually treated as a by-product) is fed into the biomass combustion process, creating a kind of circular environment. Henceforth, the electricity to run the electrolyzer is provided by the CHP plant to reduce electrolyzer operating costs. As the electricity supply comes from a biomass fuel CHP plant, the hydrogen production can be either described as orange or green. For simplifying the nomenclature and eliminating confusion, the terms green hydrogen and green methanol are used in this project.

Table 2: Classification of hydrogen production. [28, 30, 31, 33, 34]

Hydrogen color	Description
Grey/brown	✓ Obtained from fossil fuels (mostly SMR) ✓ Alternatives: coal gasification, partial oxidation of crude oil ✓ The production of one ton of hydrogen produces around 10 tons of CO_2 ✓ **LCOH (2021): 1.0-2.9 USD/kg** ✓ **LCOH (2030): 0.5-4.0 USD/kg**
Green	✓ Produced mainly by water electrolysis ✓ Electricity from renewable sources ✓ H_2 production is therefore CO_2-free ✓ **LCOH (2021): 3.7-8.7 USD/kg** ✓ **LCOH (2030): 1.25-5.0 USD/kg**
Blue	✓ Grey hydrogen including CCS ✓ Advantage: No release of CO_2 into the atmosphere ✓ Disadvantages: Costs, location-related ✓ **LCOH (2021): 1.5-3.2 USD/kg** ✓ **LCOH (2030): 0.9-2.4 USD/kg**
Turquoise	✓ Thermal splitting of methane (methane pyrolysis) ✓ Does not produce CO_2, but solid carbon ✓ The prerequisite for CO_2 neutrality is the heat supply of the high-temperature reactor from renewable sources, as well as the permanent sequestration of the carbon
Orange	✓ Produced from waste and residual materials ✓ Advantage: CO_2-free ✓ Still in research status
Pink/yellow	✓ Electrolysis using nuclear power ✓ Advantage: CO_2-free ✓ Disadvantage: Radioactive waste, safety ✓ **LCOH (2021): 3.4-6.9 USD/kg** ✓ **LCOH (2030): 2.7-5.9 USD/kg**

Despite the significant characteristics and advantages of hydrogen as an energy carrier, the disadvantages such as significantly high and expensive pressure storage (200-950 bar) or liquid storage with cooling to 20 K (-253.15°C) must not be neglected [34, 35]. Literature sources estimate that the pressure storage process consumes around 10-15% of the calorific value of hydrogen which is a huge number compared to other energy storage technologies [36]. In addition, due to the high diffusion tendency of hydrogen, only austenitic steel and composite materials can be considered for safe storage [37]. Hydrogen storage also entails a number of safety-related problems, as in the event of a hydrogen leakage even a proportion of 18% in the air is sufficient to form an explosive mixture [38]. For these reasons, hydrogen is often used as an intermediate product for the synthesis of downstream products and is expected to play a greater role in the future. Some end products can be considered as Power-to-X energy carriers, such as ammonia, dimethyl ether, methane or methanol.

Figure 6 provides an overview of the various advantages and disadvantages of hydrogen downstream products such as scalability, efficiency and storage [39].

Figure 6: Qualitative study of main advantages and disadvantages of hydrogen transformation into different energy carriers. Illustration reproduced out of [39].

As the carbon dioxide from the CHP plant is to be used in the flue gas in this project, only hydrocarbons can be considered when selecting the final product. The focus in this master thesis is on methanol production due to the plant size in the MW range, a high overall efficiency of around 70%, simple storage in industrial tanks and the existing distribution infrastructure which leads us to the next subchapter. Nevertheless, the other hydrocarbons should be kept in mind as alternatives regarding as another power-to-X fuel.

2.5 Methanol

Methanol, the simplest form of alcohol (CH_3OH), is a fundamental component for various products such as paints, plastics, car parts and construction materials [40]. Additionally, it serves as a clean energy resource used to power cars, trucks, buses, ships, fuel cells, boilers and cook stoves [40].
In 2022, the global methanol market reached around 90 million tonnes and is projected to grow at a compound annual growth rate (CAGR) of 4.3% by 2032 [41].
However, methanol production and consumption contribute approximately 165 million tonnes of carbon emissions annually, accounting for about 0.3% of the global total, according to a report by the International Methanol Producers and Consumers Association (IMPCA) dated May 2022.
To address this issue, 'green methanol' (produced with minimal amount of greenhouse gas emissions), 'bio-methanol' (derived from sustainable biomass), and 'e-methanol' (synthesized from carbon dioxide and hydrogen produced from renewable electricity). The concept of 'renewable methanol' has also gained traction, with the latest projects utilizing renewable feedstocks and captured CO_2 [42].

Methanol Production

Methanol production can be achieved through various processes aimed at utilizing CO_2-comtaining exhaust gases to reduce CO_2 emissions in the atmosphere. The shift from conventional synthesis methods using syngas to CO_2 hydrogenation, though very popular, presents several challenges, including thermodynamic limitations, stability of catalyst and selectivity. This section explores the reactions, catalysts, reactor configurations, and most efficient boilers for methanol production.

REACTIONS INVOLVED IN METHANOL PRODUCTION

Methanol synthesis from CO_2 involves three primary reactions [42–44]:

1. **CO_2 hydrogenation:**

   $CO_2 + 3H_2 <-> CH_3OH + H_2O$; ΔH = -49.16 kJ/mol

2. **Reverse water-gas shift (RWGS)**

   $CO_2 + H_2 <-> CO + H_2O$; ΔH = 41.22 kJ/mol

3. **CO Hydrogenation**

   $CO + 3H_2 <-> CH_3OH$; ΔH = -90.8 kJ/mol

The synthesis involves a balance between these reactions to optimize methanol yield and minimize by-products.

CATALYSTS FOR METHANOL SYNTHESIS [43]

The catalyst plays a crucial role in methanol synthesis. The conventional $Cu/ZnO/Al_2O_3$ catalyst, although not optimized for pure CO_2 hydrogenation, remains the industry standard due to its high activity, stability and suitability for dynamic applications. It compensates for H_2 supply fluctuations from electrolyzer and facilitates methanol synthesis.

Challenges with Alternative Catalysts:
Alternative catalysts have been investigated, but none have outperformed the $Cu/ZnO/Al_2O_3$ catalyst under industrial conditions. Issues such as lower activity in the temperature range of interest and reduced stability under high water content hinder their commercial viability. Improvements in low-temperature activity and time-on-stream deactivation behavior are essential for future catalysts to be competitive.

REACTOR CONFIGURATIONS

Three reactor configurations are commonly used in methanol synthesis [44]:

- **Isothermal Reactor**: Generally operated at 250˚C, this reactor balances catalyst requirement and equilibrium conversion. It is favored for its consistent temperature profile, enhancing catalyst stability and performance.

- **Adiabatic Reactor**: This configuration reduces heat generation as the reaction progresses, necessitating higher operating pressures to maintain equilibrium conversion. It lacks heat transfer requiring additional power for compressors and larger heat exchangers due to lower LMTD (Log Mean Temperature Difference).

- **Reactor with Intercooling**: An intermediate option, this reactor allows partial cooling between reaction stages, increasing equilibrium conversion and recovering some heat as steam. However, it incurs higher investment costs due to complex design.

BOILER SYSTEMS

The three commercially used reactor designs each incorporate different heat transfer mechanisms:

- **Direct Cool via Feed Gas Injection (Quench)**: This system has the largest catalyst volume but is less efficient in heat distribution [42].

- **Counter-Current Gas Exchange (Tube-Cooled Converter, TCC)**: The TCC design is the most efficient, offering lower costs, higher efficiency, and simpler operation. It prevents catalyst sintering by improving heat distribution, thus extending catalyst life and minimizing process interruptions [42].

- **Isothermal Bed (Steam-Raising Converter, SRC)**: This design maintains consistent temperature profile, optimizing catalyst performance and stability [42].

In conclusion, while there are many pathways for methanol production, the hydrogenation of CO_2 over a $CU/ZnO/Al_2O_3$ catalyst remains the most viable. Reactor configurations and heat transfer mechanisms significantly impact the efficiency and feasibility of methanol synthesis, with the TCC design being the most advantageous.

3. Literature review

Due to the advantages mentioned in the previous chapters, BECCS technology is increasingly becoming the focus of modern science and industry. Nevertheless, only a few scientifically sound and detailed studies can be found in the media in which BECCS is coupled with methanol production and oxyfiring. Many journals and papers deal with individual specific technologies such as only CCS or only oxyfuel combustion in gas or coal-fired power plants. An investigation of the symbiosis of the individual applications and technologies mentioned such as CHP, CCS, methanol production unit (MPU), water electrolysis unit (WEU) on an overall system level could not be found and this is also the main motivation of this master thesis. In this study work, theoretical data and information from previous sources are combined with real-life data in order to be able to make a statement about the practical relevance and introduction of such a system constellation at the end of the day, both in terms of economy and ecology. For this reason, a few scientific papers were used to gain a solid database and starting point for this project. It is important to note at this point that only the most relevant studies have been summarized below so as not to prolong this section. In practice, further scientific studies were consulted and used as sources. It should also be noted that the literature research refers to the current time of writing this report. During the selection of the literature, emphasis was placed on both the coherence of the topic and the timeliness of the study, so that the data and results used correspond to the current state of scientific knowledge.

Beiron, Normann et al. provide in their research paper *"A techno-economic assessment of CO2 capture in biomass and waste-fired combined heat and power plants – A Swedish case study",* published in 2022, a techno-economic assessment of post-combustion absorption-based CO_2 capture in Swedish cogeneration plants [45]. Within that, they take their focus on relevant technical indicators such as carbon capture potentials, plant performance and utilization factors. Furthermore, they worked out an economic analysis. The main goal of the research is the quantification of the impact of CCS on biomass and waste-fired CHP plants and district heating system unit commitment in correlation to plant scales and utilization on the cost of capture.

The next research was done by *Stanger, Wall et al.* and deals with oxyfuel combustion for CO_2 capture in power plants [24]. Within this study, a comprehensive analysis of mass ratios, flue gas values, heat transfers, fluid dynamics, agglomeration and more was carried out. The authors investigated the behavior of oxyfuel technology combined with CO_2 storage in a pulverized coal (PC) boiler, circulating fluidized bed (CFB) boiler and a gas-fired boiler, including the required system components of the power plant. In addition, a variety of existing oxyfiring projects were presented. Potential safety risks and operational strategies for operation in oxyfuel mode were also noted and discussed. Connected to this Master thesis, having a close look at the emission treatment of the CFB boiler chapter and the control and operating strategies can be useful. Hence, the safety regulations of the whole power plant system could be interesting for the later discussion and validation of results. The main outcomes of the oxyfuel CFB chapter can be summarized like following [24]:

- Main energy consuming system parts are the ASU and the CPU
- Tests results are available with pilot projects for moderate (ca. 20-30 vol%) and high (ca. 40-55 vol%) oxygen content within the RFG-oxygen stream
- The same combustion parameters (heat flow, emissions, etc) as in the air-fired mode can be achieved quite easily by regulating the RFG mass flow in the oxyfuel mode; typically 22-24 vol% oxygen (and 76-78 vol% RFG) is used in the firing supply stream to match it

- Good emission handling can be achieved in OF mode, f.e. usage of limestone for in situ sulfur capture
- Around 10 % of sulfur and less than 5 % of nitrogen content in the fuel emits in the flue gas of oxyfuel CFB combustions
- Higher SO_2 and SO_3 can be expected in OF firing flue gas which could cause some corrosion issues in the boiler
- N to N_2O conversion rate is around 1-2 % (can be decreased by increasing the bed temperature)
- Combustion efficiency is slightly higher than in air-fuel firing

Within their research, *Sher, Pans et al.* worked on the question of the extent to which oxyfuel combustion in a 20 kW_{th} biomass fuel fluidized bed boiler makes sense [46]. For this purpose, extensive studies were carried out on technical parameters such as exhaust gas values or combustion temperatures with variation of the oxygen in the boiler fed stream. In more detail, three different oxygen concentrations (21 vol%, 25 vol% and 30 vol%) were investigated and compared with a standardized air-fuel combustion. Furthermore, different biomass fuels were used and investigated separately. In summary, the following key results were obtained [46]:

- A small amount of air was always added to the fuel hopper to avoid backfiring for safety aspects
- With 21 vol% O_2 in feed stream to combustor, the gas temperature drops significantly which leads to an extinction of the flame because of the larger specific heat of carbon dioxide compared to nitrogen. Consequently, to achieve same combustion profiles than air-fuel combustion, the concentration of oxygen has to be increased to 30% O_2/70% CO_2
- CO emissions can be reduced drastically for a mixture of 25% O_2/75% CO_2 or higher due to higher residence time of the gas inside of the combustor
- The CO_2 emissions are reduced for oxyfuel combustion with a ratio bigger than 25 vol% in the O_2/CO_2 mixture
- The same NO_x emissions can be achieved with the 30% O_2 in the O_2/CO_2 mixture. In general, NO_x decreases with the increase in oxygen content due to the increase of bed temperature and less dilution of the gases inside the dense bed zone
- NO_x and CO emissions depend strongly on the freeboard temperature

All in all, the paper is very useful, but attention should be paid to the fact that in this paper air is mixed with a specific concentration to the RFG-oxygen mixture. In this study, no air is preferably used for the power generation in the CHP plant.

A comprehensive overview of e-methanol production using an electrolyzer and a bagasse-biomass gas-fired power plant is provided in the study by *Safder, Loy-Benitez et al*. within they noted following techno-economic key results [47]:

- A methanol production rate of 430.25 kg/h
- A hydrogen production rate of 190 kg/h
- A total methanol production cost of 0.087 $/kg to 0.108 $/kg
- An overall energy efficiency of 78.13 %
- An overall exergy efficiency of 71.63 %
- A reduction to 78.5 % of total CO_2 emissions (0.61 $kgCO_2$/kg)

The paper provides a good basis for the master thesis about reference values and comparisons for power input, electrolyzer dimensioning and methanol production. Main differences to the topic of

this master thesis are the different power generation technologies (gas cycle here and steam cycle as a PGU in this work) and the lack of oxyfuel combustion. Nevertheless, the journal could be useful as it comes up with techno-economic data on the different system components which are also used in this thesis like the methanol production or the electrolyzer unit.

In their report published by Energiforsk, *Gustavsson, Särnbratt et al*. examine the question of whether and to what extent oxygen can be used as a byproduct from electrolysis today and, above all, in the future in Sweden [32]. The report provides quantitative data and facts on oxygen production and demand and based on this, develops various use cases for the use of oxygen in the energy and environmental sector. Specifically, the chapter on oxygen as an application in heat and power production can be particularly useful for this master's thesis. A disadvantage of this chapter is that, compared to other chapters, it unfortunately contains hardly any concrete facts and figures and is described in very qualitative terms. However, the following bullet points can mainly be used as knowledge input [32]:

- Swedish Energy Agency's goal was set to have 5 GW installed electrolyzers by 2030 and 15 GW by the year 2045
- 8 kg of oxygen is produced as a byproduct for every kilogram of hydrogen in an electrolyzer
- 6 GW electrolyzer power corresponds to 0.9 million tons of hydrogen (and 7.2 million tons of oxygen) per year
- Total oxygen production in 2020 was around 1.4 million tons and will be around 19 million tons in 2045
- Recent average oxygen price is between 0.8 and 1.0 SEK (0.08-0.1 EUR/kg)
- Oxyfuel combustion has two main benefits, namely a very low formation of nitrogen oxides and a high concentration of carbon dioxide in the flue gas which makes the capture easier
- Nowadays around 5 % of global GHG emissions have their origin in the grey hydrogen production mainly as a result of steam methane reforming
- Problems of an oxyfuel combustion are named as the "chemical reactions will occur faster and results in a larger heat flux and thereby increasing combustion temperature" [32]. Secondly, the "combustion air-, and thus flue gas flow will decrease slightly" [32]. Furthermore, the authors mention that the amount of added oxygen is limited by the boiler type used whereas CFB and BFB are very sensitive to the variation in combustion temperatures and gas volumes through the bed due to the usage of sand which might lead to local sintering.
- Heat control and combustion temperatures can relatively easily regulated by the change of flue gas recirculation which leads to the benefit that existing/commercial boilers and flue gas treatment systems can be used for oxyfuel combustion.

Summarized, the authors claim that oxyfuel combustion is highly competitive to conventional air-fuel combustion with a smaller footprint as combustion air volume flows (and corresponding flue gas volume flow) decreases which has a positive effect on the electrical power consumption of fans. Consequently, the overall energy efficiency of the system can be enhanced.

The next source is very similar to the master's thesis use case discussed here. Here, *Pratschner, Skopec et al.* investigated the generation of green methanol using an electrolyzer for hydrogen and oxygen production [21]. Further, carbon dioxide from the flue gas of an oxyfuel combustion is used in a 20 MW_{th} fluidized bed boiler for methanol production. Woodchips are used in the research as a fuel and the methanol production is done by CO_2 hydrogenation instead of syngas usage. Benefits of the hydrogenation are mainly the less impurities in the crude methanol, the lower chemical complexity and exothermic behavior, milder process conditions and higher methanol selectivity [21].

Henceforth, CO_2 hydrogenation can be advantageous regarding the economic feasibility due to the fact that boiling water reactors including an unconverted gas recirculation process can be easier installed than adiabatic reactors [21]. This can be explained with the lower reaction heat needed to get rid of the catalyst bed [21]. To continue, the authors compared the green methanol production with oxyfuel combustion if oxygen is provided by an ASU or an alkaline electrolyzer which was connected by a windpark with fluctuating power output. For the whole process, the article gives very detailed, almost step-by-step instruction for calculating the technical specifications of the subsystems as well as the overall process. Technical descriptions aside, Pratschner, Skopec et al. show different existing commercial oxyfuel projects and pilot systems such as Callide in Australia with a thermal power of 24-29 MW or Schwarze Pumpe in Germany with a power of 30 MW_{th}. Within the article, the authors arrive at the following results [21]:

- An oxygen concentration of around 30 vol% in the oxidant is necessary to sustain a comparable flame temperature as air-fuel combustion
- 80 % less volume flow in the emitted flue gas stream was identified as a consequence of the abstinent nitrogen
- A difference in the combustion regimes can be seen because of the change in gas stream properties (carbon dioxide and nitrogen), f.e. density or specific heat capacity
- For a 20 MW_{th} BFB boiler the fluidization velocity is kept in between 1-2.5 m/s to ensure a well heat transfer and prevent bed material segregation
- Flue gas of an oxyfuel combustion has to undergo a water removal and an excess oxygen removal (DeOxo reactor) process before entering the methanol production unit (inert nitrogen is not considered as a harmful trace for the methanol synthesis)
- For the carbon dioxide processing, a catalyst protection unit is required (f.e. fixed bed reactor with ZnO or CuO as adsorbent) to get rid of catalyst poisons such as H_2S or SO_2 in the CO_2 rich flue gas stream
- Methanol purity of 99.85 wt% (dry basis) with a CO_2 conversion rate of 98.11 % and a H_2:CO_2 ratio larger than 3 (to avoid the formation of elemental carbon)
- The methanol synthesis reaction is isothermal. Agglomeration of catalyst particles can occur when a critical temperature in the reactor is exceeded. For this reason, a catalyst bed cooling is necessary to this named agglomeration. Furthermore, one should be cautious of the occurrence of the reverse water gas shift reaction.
- When designing a methanol reactor, a trade-off between thermodynamics and kinetics has to be done with regards to temperature and pressure. Here, a pressure of 40 bar and a temperature of 513 K were taken.
- For a fuel input of 6133 kg/h of wood chips, an electrolyzer power of 17.14 MW and an air separation power of 4.73 MW, a methanol production rate of 1637 kg/h and a CHP heat output of 13 MW_{th} was achievable. More in detail, a H_2 flow of 342 kg/h for the methanol generation and an O_2 massflow of 6187 kg/h for the oxyfuel combustion is required for a CO_2 utilization rate of 0.3. A simplified global flow chart and a detailed flow chart of the system can be found in Appendix A and Appendix B, respectively.
- Oxyfuel applications can reach higher overall efficiencies compared to air combustion due to the fact that no additional heat is required for the MEA solution in the carbon dioxide processing unit

As a conclusion of this source, really extensive research and calculations were accomplished with a close connection to the discussed research questions within this thesis. Nevertheless, there are some differences, such as the fact that in *Pratschner, Skopec et al.* system an air separation unit was installed to provide oxygen for the oxyfuel process even if the wind speed was below a minimum value.

In addition, the use of a different type of boiler can be found. In the study by *Pratschner, Skopec at al.* a BFBC boiler was used, in our case a CFB boiler was examined. Despite the differences, the paper serves as a very good literature source for the use case discussed here due to the similarity in methanol production, oxyfuel combustion and the use of an electrolyzer for hydrogen and oxygen production.

In their paper '*Implementation of Oxyfuel Combustion in a Waste Incineration CHP Plant – A techno-economic Study*' [12], *Mostafa Saleh* and *Anton Heden Sandberg* have discussed the different carbon capture technologies and the available CO_2 separation methods. Considering *Mälarenergi's* refused-derived waste-fired CHP plant as the model for the thesis, an investigation on the viability of converting the existing CHP plants to oxyfuel combustion has been carried out. In addition to the existing CHP, an air separation unit (ASU), a cryogenic CO_2 purification unit (CPU) and a flue gas recirculation (FGR) have been modelled as a retrofit. Two scenarios: the FGR before flue gas condenser (FGC) and the FGR after FGC have been investigated. The findings of the work show that integrating waste incineration CHP plants with oxyfuel combustion for CO_2 capture, entails promising features under the condition of 97% oxygen purity and a flue gas recirculation system taking place after flue gas condensation. This is due to:

i. Energy penalty of approximately 8.7%
ii. High CO_2 recovery ratio of 92.4%
iii. Total investment cost of 554 M$ within a lifetime of 20 years.
iv. Cost of captured CO_2 of around 76 $/ ton.

To summarize the conclusions obtained in the study [12]:

- Approximately 37.5 m^2/MW of additional space is required to retrofit oxyfuel combustion into an existing plant.
- Fans are required for the FGR which must be sealed to avoid air leakage. The efficiency of the fans must be 69% for wet-FGR and 79% for dry-FGR. From a techno-economic viewpoint, the dry-FGR is preferred, owing to a relatively moderate energy penalty of 8.7%, a CO_2 recovery rate of 92.4%.
- The conversion of the CHP plant to oxy-waste combustion requires bare module costs for ASU and CPU of approximately 93 M$ for dry-FGR and 96 M$ for wet-FGR. The cost of CO_2 captured is highly affected by the total investment cost for the ASU, CPU, and boiler modification.
- The findings of the thesis show a total investment cost of 553.7 M$ for dry-FGR and 567 M$ for wet-FGR, over 20 years as a lifetime. The cost of carbon is advantageous during dry-FGR, 75.75 $/ton, compared with wet-FGR, 78.84 $/ton. Over 20 years, the total captured CO_2 is shown to be 9.6 million tons during dry-FGR and 9.5 million tons during wet-FGR, corresponding to EU-ETS savings of approximately 195.6 M$ and 193 M$.

The authors states that a detailed analysis of heat transfer in the furnace, investigating heavy metal formation for controlling pollutant emissions and preventing corrosion in the boiler and CO_2 separation units, and incorporating flue gas cleaning are some gaps in the work and should be the focus in future works.

Table 3 provides a quick summary of the literature which is described above.

Table 3: Overview on existing literature for different topics such as oxyfuel combustion, electrolysis, carbon capture and methanol production.

Authors [Ref no.]	**Year**	***Title* / Summary**
Beiron, Normann et al. [45]	2022	*"A techno-economic assessment of CO2 capture in biomass and waste-fired combined heat and power plants – A Swedish case study"* This work provides a techno-economic assessment of post-combustion absorption-based CO_2 capture in Swedish CHP plants, with respect to the carbon capture potential, plant performance and utilization, and costs. The aim of the study is to quantify the impact of CCS on biomass and waste-fired CHP plants and DH system unit commitment, as well as the effect of plant scale and utilization on the cost of capture.
Rufer [48]	2022	*"Quantitative Design of a New e-Methanol Production Process"* The work evaluates the feasibility of a new way of producing methanol using electricity from PVs. It provides detailed calculations/estimations of the utilities required in the process.
Vaquerizo, Kiss et al. [49]	2023	*"Thermally self-sufficient process for cleaner production of e-methanol by CO2 hydrogenation"* This work has presented an alternative process for the thermally self-sufficient production of e-methanol by CO_2 hydrogenation with the lowest power requirement per ton of produced methanol of all the works that have been published on this topic.
Safder, Loy-Benitez et al. [47]	2024	*"Techno-economic assessment of a novel integrated multigeneration system to synthesize e-methanol and green hydrogen in a carbon-neutral context"* The authors investigate a gas power plant combined with CC and e-methanol production with electrolysis from a techno-economic and ecological point of view.
Stanger, Wall et al. [24]	2015	*"Oxyfuel combustion for CO_2 capture in power plants"* The scientific paper provides a detailed overview on oxyfuel combustion technology and its use for coal fired power plants with CCS as well as gas fired power plants.
Sher, Pans et al. [46]	2018	*"Oxy-fuel combustion study of biomass fuels in a 20 kW_{th} fluidized bed combustor"* Detailed combustion and emission values for different oxygen shares in the supply stream of a fluidized bed boiler fired with biomass were worked out by the authors.
Hassan, Jalil et al [50]	2024	*"Recent review and evaluation of green hydrogen production via water electrolysis for a sustainable and clean energy society"* This paper deals with different ways and techniques of green hydrogen production and shows some countries' pathways and existing pilot projects.
Gustavsson, Särnbratt et al. [32]	2023	*"Potential use and market of Oxygen as a by-product from hydrogen production"*

		As the title already says, the report deals with the market potential and use of oxygen as a byproduct of hydrogen production. Therefore, five different use cases were worked out, one of them is the use of oxygen in oxygen enriched combustion in heat and power production units.
Pratschner, Skopec et al. [21]	2021	*"Power-to-Green Methanol via CO_2 Hydrogenation—A Concept Study including Oxyfuel Fluidized Bed Combustion of Biomass"* A very profound and detailed analysis on green methanol production with an electrolyzer and additional oxyfuel combustion within a 20 MW_{th} biomass fluidized bed boiler.
Raman Narayanan [42]	2023	*"Methanol from CO2: a technology and outlook overview"* The article provides information on the state-of-art methods to produce methanol. It digs into reactors, catalysts, and the different pathways to produce methanol. A technical study has also been conducted to produce green methanol.

In summary, it can be said that e-fuel production using BECCS is still in the early stages of scientific research and a great deal of research work still needs to be done in both theory and practice in order to advance this technology. Scientific studies are very rare, especially with regard to BECCS in combination with oxyfuel combustion. Pilot projects for e-fuel (and in particular e-methanol) production do exist, but most of these will only go into operation in the future and the implementation of the ambitious goals of Liquid Wind, for example, should be treated with caution. Any problems may only arise during operation and most projects are still in the development phase. Similarly, the use of the oxygen generated from the electrolysis process in biofuel combustion has not yet been implemented in practical projects and therefore offers a very interesting basis for further research.

3.1 Current projects

Carbon capture is playing an increasingly important role in slowing down climate change and reducing global CO_2 emissions. Mostly power plant operators with high carbon dioxide emissions are interested in solutions to minimize or even eliminate their emissions. One solution is the conversion of stored carbon dioxide into e-methanol. This can be referred to as green methanol if the methanol is produced from low-carbon sources. Some ongoing projects have already been launched in recent years or are in the development phase. For example, the Swedish company Liquid Wind with the headquarter in Gothenburg has been researching the in-situ production of e-methanol since 2017 and was able to implement the first project "FlagshipONE" in 2023. According to Liquid Wind, follow-up projects are to take place in the near future and concepts have already been developed. [51] Table 4 summarizes the claims and technical data of individual Liquid Wind projects to provide an overview of the dimensions. [52–55]

Table 4: Flagship projects by Liquid Wind for the production of e-fuels. [52–55]

Project	Key points
FlagshipONE [52, 55]	• Location: Örnsköldsvik • Acquired by Ørsted in 2022 • Construction start: 2023 • Production start: 2025 • Production capacity: 50.000 – 55.000 $t_{eMethanol}$ / year • CC rate: 70.000 $t_{biogenic\ CO2}$ / year • Avoided emissions: 100.000 t_{CO2} / year • 70 MW renewable power for electrolyzers • Financial support from Klimatklivet through the Swedish Environmental Protection Agency (funds) • eFuel facility is connected to biogenic fuel cogeneration plant Hörneborgsverket (operated by Övik Energi AB) where the CO_2 is captured • Hörneborgsverket provides steam and water for the process and excess heat is returned to Örnsköldsvik's DH system • Port availability to store and offload fuels for ships
FlagshipTWO [53]	• Location: Sundsvall • Construction start: 2024 • Production start: 2026 • Production capacity: up to 130.000 $t_{eMethanol}$ / year • Capture of: 140.000 $t_{biogenic\ CO2}$ / year • Avoided emissions: 283.000 t_{CO2} / year • Primarily replacing marine fossil fuels (ca. 199.000 t_{CO2} / year) • Permanent storage of 84.000 t_{CO2} / year • CCS permit is handled in Phoenix project by Sundsvall Energi • Next to CHP plant Korstaverket where biogenic CO_2 will be captured to produce e-fuel

FlagshipTHREE [54]	• Location: Umeå • Construction start: 2024 • Production start: 2027 • Production capacity: up to 130.000 t $_{eMethanol}$ / year • Capture of: 140.000 $t_{biogenic\ CO2}$ / year • Avoided emissions: 271.000 t_{CO2} / year • Supply of marine fossil fuels up to 130.000 t / year • Permanent storage of 84.000 t_{CO2} / year • CC long-term storage in bedrock • Goal: Climate neutrality of Umeå City by 2030 and Umeå Municipality by 2040 • Next to CHP plant Dåvaverket where biogenic CO_2 will be captured to produce e-Methanol

Besides the Swedish Liquid Wind projects, two German e-methanol projects can also be listed. One is the MefCO_2 project in Nierderaussem and the other one is the e-CO_2Met project in Leuna.

Starting with the MefCO_2 project, the structure can be seen in Figure 7. It consists of a 600 kW PEMEL electrolzyer for hydrogen production and a lignite fired power plant with a post-combustion carbon capture unit to synthesize methanol [56]. Hereby, a maximal methanol output of roughly 1 t/day with a CO_2 input of 1.5 t/day could be realized and documented [56]. Further information on the mass flows and the methanol unit reactor can be found in Appendix D. The project was funded by several companies including i-deals, Mitsubishi Hitachi Power Systems Europe, RWE, etc. as well as research institutes and educational facilities. Further, the European Commission contributed to the success of the project with a subvention of around 8.6 million Euros. The aim of the project was the analysis of the economic feasibility of green methanol production and the reduction of carbon emissions.

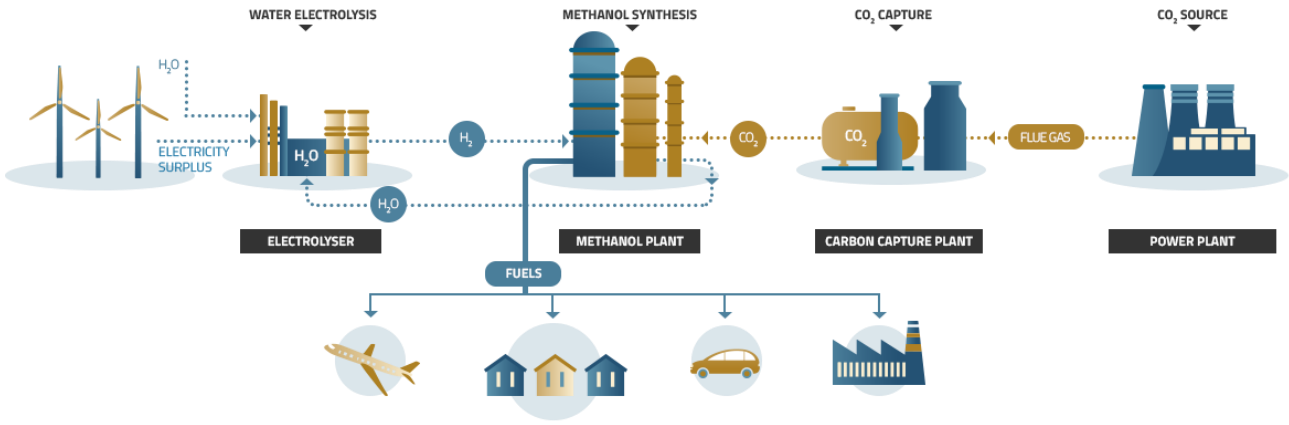


Figure 7: Illustration of the MefCO_2 project. [56]

Secondly, the German flagship project Leuna eCO2met can be cited as a good example of the production of green methanol. This project was worked out as a cooperation of the research institute Fraunhofer CBP and the energy company TotalEnergies. Within that, CO_2 from a partial waste gas

stream from Total Raffinerie Mitteldeutschland GmbH Leuna is taken to produce methanol with hydrogen provided by a 1 MW Sunfire solid oxide electrolyzer in two phases, starting in 2021 and 2022. Because the project is still in the construction phase, there is no specific data about yearly methanol production available, but probably in the near future there will be.

Another ongoing project is the Danish project "Kassø Power-to-X" which is located in Aabenraa and owned by European Energy A/S (share of 51%) and Mitsui (share of 49%) [57]. Its first drop will be in the second half of 2024 with a methanol production of 32,000 tons per year [57]. The shareholders claim to have the world largest Power-to-X facility with the help of 304 MW solar park nearby for operating electrolyzers to generate hydrogen for the methanol synthesis [57].

On closer inspection, the green e-methanol projects to date have focused almost exclusively on the use of carbon dioxide emissions from power plants with pure air combustion and the use of hydrogen from electrolysis processes. The oxygen generated from electrolysis is treated as a waste material and has not yet found any technical application. In this research work, however, precisely this oxygen is to be used as a source of oxygen in an oxyfuel combustion process of the CHP plant.

Two coal-fed oxyfiring projects can be stated here, respectively the "Callide" project in Australia and the "Schwarze Pumpe" project in Germany. Hence, the project of Spain's Fundación Ciudad de la Energía (CIUDEN) in Compostella can also be cited as an example of the large-scale use of oxyfuel technology. In the year 2008, the Swedish company Vattenfall developed the 30 MW oxyfuel and carbon capture and storage project "Schwarze Pumpe" in Germany. The power plant runs in the oxyfuel combustion for several years before it got shut down in 2014 due to economic insufficiencies. Figure 8 shows the scheme of the plant "Schwarze Pumpe" with the different components included in the system [22]. As can be detected, an ASU is responsible for supporting the boiler with the burned oxygen and CO_2 was processed to a liquid form for easier storage.

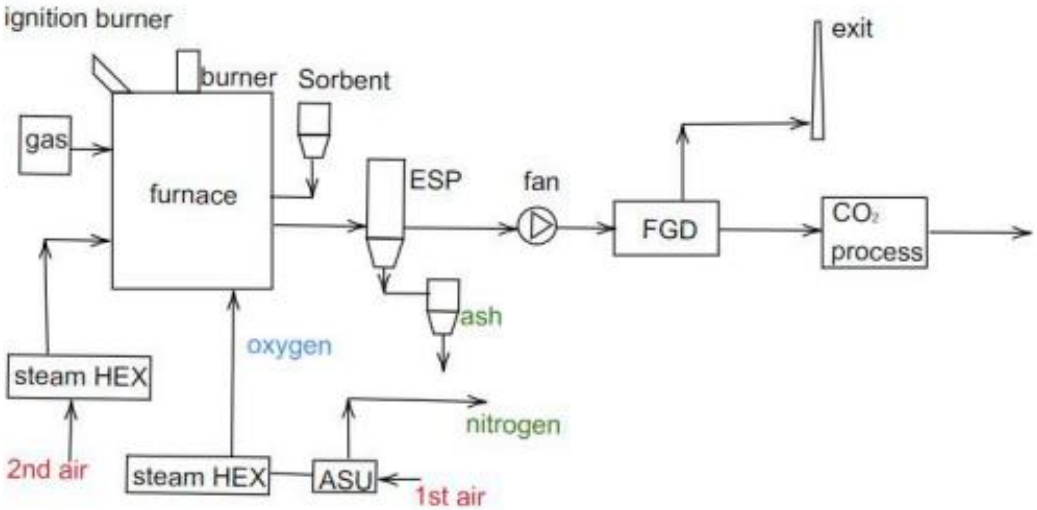


Figure 8: Schematic of the "Schwarze Pumpe" plant [22]

The second project which should be mentioned is the "Callide" project in Australia. Because it is the largest oxyfuel project until now, it received a lot of attention with an electric power output of 30 MW [22]. As well as in the "Schwarze Pumpe" project, the oxygen for the combustion is provided by an ASU which separates the oxygen from ambient air. The carbon capture rate is claimed to be

around 75 t/d with an operation of 10,000 hours of oxyfuel combustion and 5,000 hours of carbon capture.

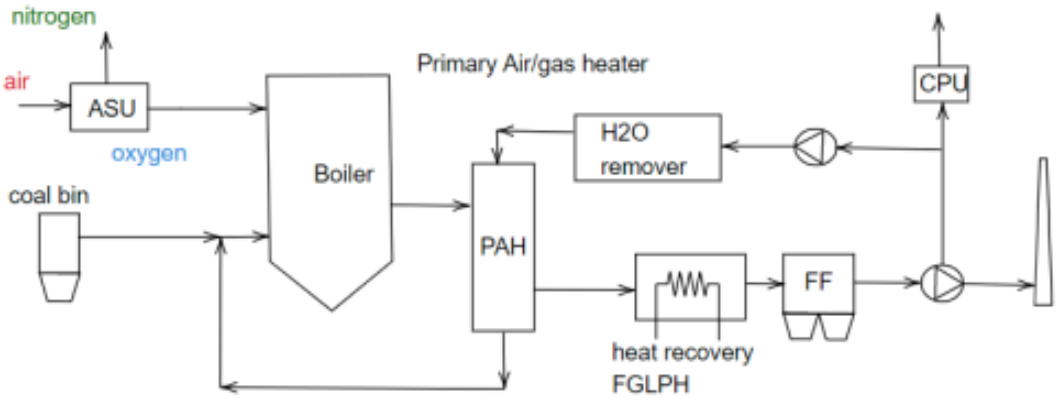


Figure 9: Schematic of the "Callide" oxyfuel plant [22]

As can be seen, both projects include an air separation unit to provide the needed oxygen for the oxyfuel combustion which differs from the present topic of the master thesis as oxygen is provided by electrolysis. Using oxygen from electrolysis can lead to energetic and economic benefits as the installing and running the ASU is a main cost factor in the whole system.

As a conclusion, it can be pointed out that most of the existing projects take their focus on green methanol production with the help of post-combustion carbon capture. The symbiosis of green methanol production by applying the oxyfuel combustion technology for carbon capture is not carried out yet and offers therefore a great opportunity for further investigations.

4. Process design

Despite a number of advantages such as easier storage of carbon dioxide in the exhaust gas, less impurities in the flue gas stream or improved combustion efficiency, the mentioned oxyfuel combustion technology has not yet been able to establish itself on the market. In order to understand the background to the lack of expansion of this technology, it is necessary to take a look at the elaborate oxyfuel designs of previous projects and research. As already mentioned in earlier chapters, most of the oxyfuel research and projects which were investigated are based on oxygen supply by an air separation unit (ASU). This is also the decisive factor for the niche consideration of oxyfuel combustion to date because of the incredibly high additional energy and technical costs of an ASU compared to conventional combustion, which overshadows the advantages of oxyfuel combustion.
However, an abrupt shift can happen due to the fact that nowadays electrolyzers are playing a growing role in the production chain of green e-methanol and, by splitting water, the susceptible oxygen is no longer considered a byproduct of the hydrogen generation. With this change in the system setup, high investment and operational expenditures of the ASU can be avoided. Instead, the electrolyzed oxygen could be actively used in the recirculation into the CHP plant to increase the overall efficiency of the process and further to lower the methanol production costs. Breaking it down, the chosen design of the overall system will consist of following applications which are leaned on the concept of [21]:

- Power Production Unit (PPU) – combustion of biomass & generation of heat and/or power
- Flue Gas Processing Unit (FGPU) – flue gas cleaning
- CO_2 Processing Unit (CO_2PU) – final purification of the CO_2 for methanol synthesis
- Water Electrolysis Unit (WEU) – oxygen supply for OF combustion and hydrogen supply for methanol synthesis
- Methanol Production Unit (MPU) – methanol synthesis

The final draft of the system design can be seen in Figure 10. For running electricity consuming applications such as the WEU or the MPU, primarily electricity from the CHP power plant is provided. If the electrical output of the CHP power plant is not sufficient, electricity will be purchased from the national grid. For the consideration and designation of green methanol, the assumption should be made that the purchased electricity is provided from renewable energies.

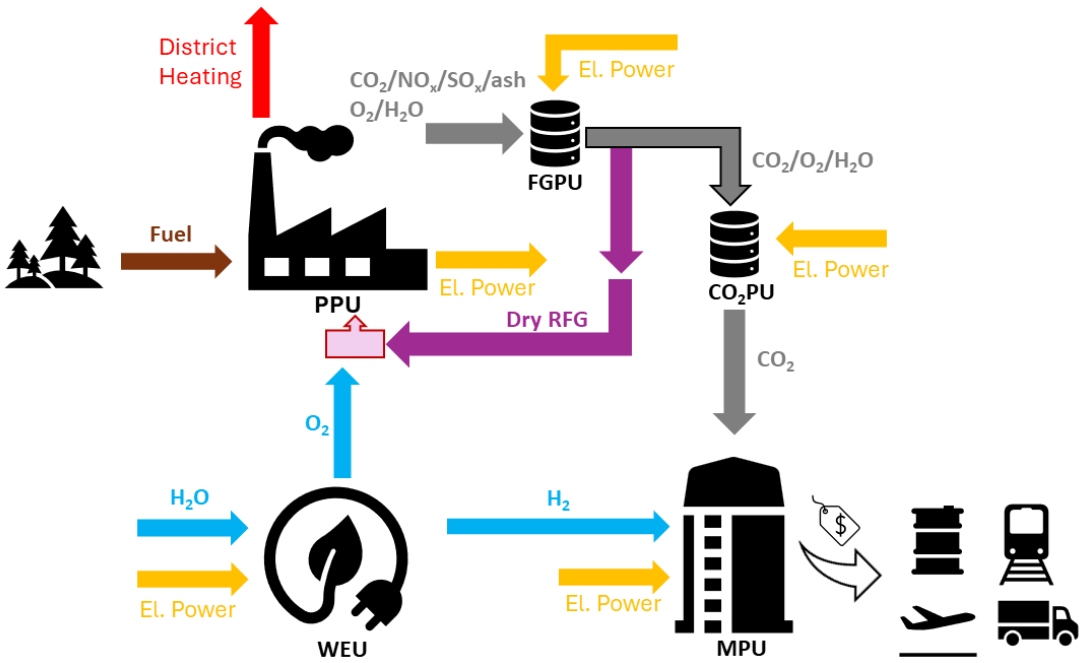


Figure 10: Illustration of the process design with the single applications and flows.

Because of high interconnectivity and a complex setup, a more detailed description of the individual subsystems (PPU, FGPU, CO_2PU, WEU, MPU) can be found in this chapter.

Power Production Unit (PPU)

Växjö Energi AB is an energy and communication company owned by Växjö municipality. The company produces district heating and electricity primarily at Sandviksverket, a biomass-fired plant. Växjö Energi serves 10,100 customers and manages a total grid of 46.000 km. The company utilizes 100% renewable biomass from forest residues, mainly constituting bark, woodchips and branches. The Sandviksverket facility houses three main boilers:

1. **Sandvik 1, Hot water boiler**: This boiler was originally built in 1974 as an oil-fired cogeneration plant, it was converted into biofuel in 1980 and decommissioned in 2014. A bio-heating plant remains operational for peak loads.
2. **Sandvik 2, Cogeneration**: This Ahlström/Foster Wheeler manufactured boiler is a CFB boiler which produces 65MW of heating and 35MW of electricity, with an additional 25MW of heating from flue gas condensation. It is fossil-free and operates entirely on biofuel.
3. **Sandvik 3, Cogeneration**: This boiler generates 65MW of heating and 39MW of electricity. It is fossil-free and operates entirely on biofuel. Like Sandvik 2, it also has a flue gas condenser which produces additional 25MW heating.

Växjö Energi is committed to decarbonizing its operations and is exploring carbon capture technologies, with oxyfuel combustion being an interesting option among others. In our thesis, we focus on implementing oxyfuel combustion at Sandvik 2, utilizing detailed plant data provided by Växjö Energi. Further details about this data and its application are described in the Methodology section of our report.

The main sections of the power production unit comprise combustion section (boiler), steam generation, electricity production /turbine and generator), district heating and flue gas.

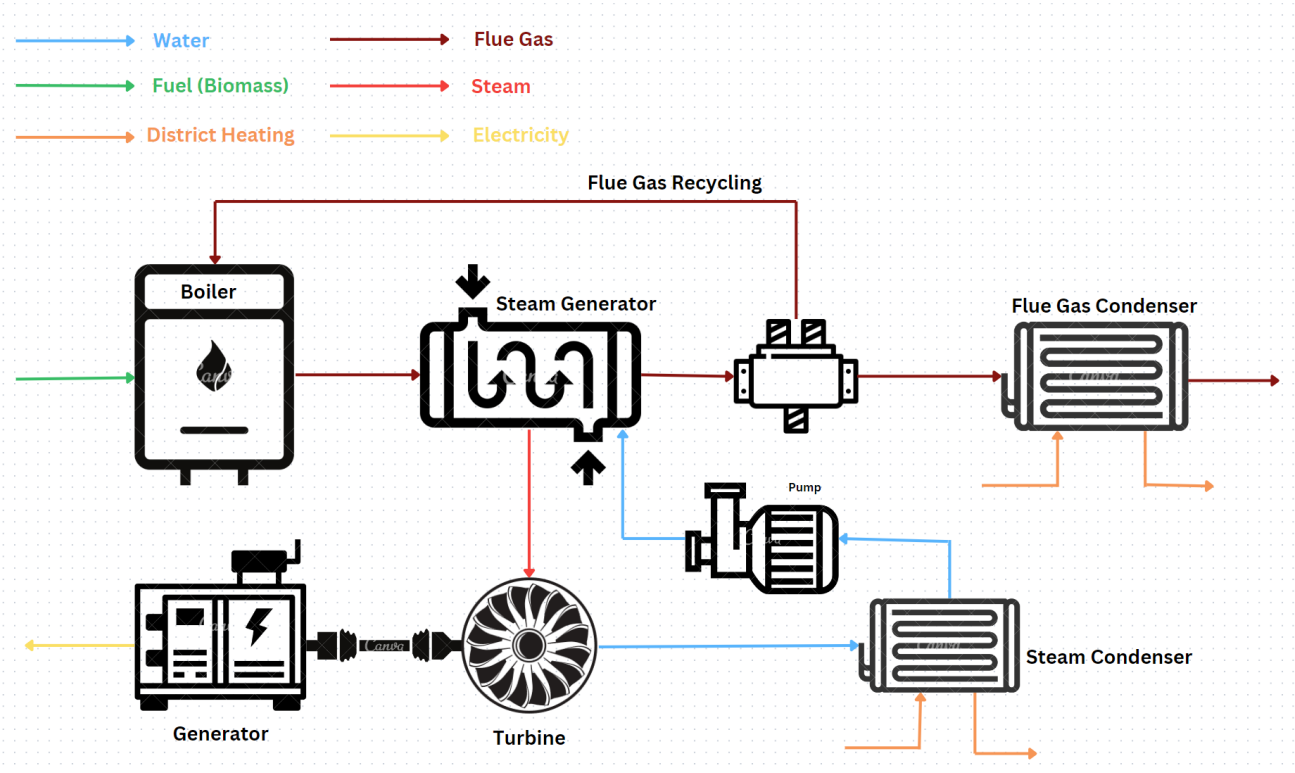


Figure 11: Steam cycle of the power production unit.

Biofuel comprises a mixture of forest residues, bark, saw dust, chipped wood and recycled wood is first crushed, shredded and filtered into fractions less than 63mm. The fuel, with the help of high purity oxygen and a small amount of flue gas is combusted in a CFB boiler to produce high pressure, high temperature flue gas. The newly resulted flue gas after combustion then goes to the steam generation unit which is mainly comprised of a stack of heat exchangers, here the flue gas exchanges heat with water to produce steam. This steam is used to power the turbine and form the exit stage, the steam is condensed and used for providing heat. The flue gas prior to the steam generation is lead through a flue gas condenser where more heat is extracted and used for in-plant and external steam demand applications.

Flue Gas Processing Unit (FGPU)

Likewise, as in a regular air-fuel combustion, flue gas treatment is inevitable to clean the flue gas from impurities, mainly ash, NO_x and SO_x. For reasons of heat conduction and mass balances, it is essential to keep in mind that the abstinence of nitrogen as the burning oxidant leads to a decrease in the overall flue gas volume flow of around 80% and a change in the heat capacity [21]. Compared to nitrogen, carbon dioxide has a greater molar mass which results in a higher density and heat capacity of the oxyfuel flue gas stream in contrast to air-fuel [21].

Ash and NO_x form the largest share in the flue gas in biomass-combustion and are for this reason investigated in more detail in this work. Although biomass generally contains low sulfur content, trace amounts of SOx may still be present. These can be partially removed by a flue gas condenser in

real-life operations. Other impurities and trace elements, such as heavy metals, must also be considered.
To ensure the removal of fly ash, a baghouse filter unit can be employed [21]. The chemical reactions involved in the flue gas treatment process are described in equation (1) [21]. The efficiency of desulfurization in the presence of a flue gas condenser can be expected to contribute to the removal of SOx, albeit to a lesser extent given the low sulfur content in biomass [21].

Secondly, the NO_x is removed from the flue gas stream with a selective catalytic reduction (SCR-DeNO$_x$) unit in which aqueous ammonia (NH_4OH) with a respective concentration of 19-29 wt% is inserted in front of a ceramic honeycomb catalyst at high temperatures (around 453-703 K) [21]. As a result, NO_x is reduced to nitrogen (N_2) and water (H_2O) as can be seen in equation (*1*) [21, 58].

$$4NO + 4NH_3 + O_2 \rightarrow 4N_2 + 6H_2O \quad (1)$$

Summing it up, flue gas treatment, even for oxyfuel combustion, is crucial. Advantageous is the fact that the flue gas processing unit of a conventional air-fuel combustion can be used resulting in a cheap and easy purchase and installation of existing FGPUs. Even more beneficial is the implementation of oxyfuel combustion, if the power plant is retrofitted and the existing FGPU can be utilized which saves capital expenditures.

CO_2 Processing Unit (CO_2PU)

Before the CO_2 rich flue gas stream is led into the methanol reactor, it has to be concentrated and processed. This means that excess oxygen has to be removed after getting rid of water in a condenser [21]. Excess nitrogen does not act as a risk for the methanol reactor [21].Specific requirements for the CO_2PU is a catalyst protection unit (f.e. a fixed bed reactor with ZnO or CuO as adsorbent) as it eliminates dangerous catalyst poisons such as H2S and SO_2 [21]. Further, a DeOxo reactor is applied to remove the already mentioned excess oxygen in the flue gas stream (calculations on that later). The stated reactor operates at a pressure of 10 bar and a temperature of 323 K. Particular care must be taken as the chemical reaction in the DeOxo reactor is strictly exothermic and cooling is therefore essential. The required energy input and the chemical reaction can be found in equation (*2*).

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O \qquad \Delta H_r^0 = -285.8\frac{kJ}{mol} \quad (2)$$

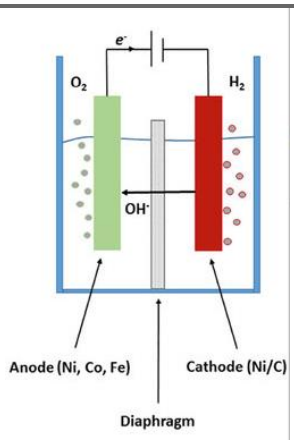
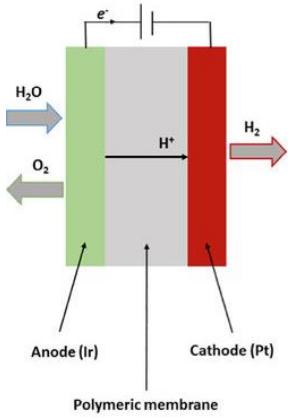
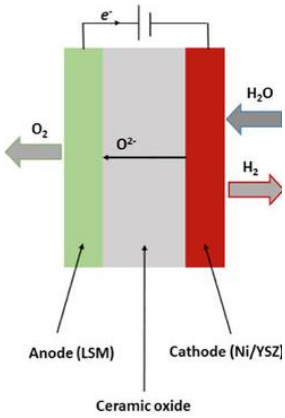
After the CO_2 processing, the flue gas stream is ready to be converted into methanol.

Water Electrolysis Unit (WEU)

To get more insight into the hydrogen and oxygen supply, it is essential to briefly familiarize yourself with the thermodynamics and functioning of electrolysis. There are currently three commercial types of electrolysis with different properties. Firstly, the alkaline electrolysis (AEL), secondly the proton exchange membrane electrolysis (PEMEL) and lastly the solid oxide electrolysis (SOE), which all have the same basic function, namely the splitting of water into its components oxygen and hydrogen while consuming electric energy. The latter technology involves a high-temperature electrolysis process, which mainly distinguishes it from AEL and PEMEL. The chemical principle, the electrolyte material, the degree of efficiency or the energy requirement are just a few indicators which distinguish the variant electrolysis technologies from each other. For a better overview, the

most important parameters and facts can be found in Table 5. Depending on the application and system parameters, the choice of a suitable electrolyzer may vary and must therefore be considered on a project-specific basis. A market analysis of existing companies and their availability must also be scrutinized when selecting the electrolyzer. Therefore, the selection of an optimal electrolyzer for this project is later discussed.

Table 5: Electrolysis technologies. [29, 59–61]

	AEL	**PEMEL**	**SOE**
Scheme (out of [60])			
Anode reaction (out of [60])	$4OH^- \rightarrow 2H_2O + 4e^- + O_2$	$2H_2O \rightarrow 4H^+ + 4e^- + O_2$	$O^{2-} \rightarrow 0.5*O_2 + 2e^-$
Cathode reaction (out of [60])	$4H_2O + 4e^- \rightarrow 4OH^- + 2H_2$	$4H^+ + 4e^- \rightarrow 2H_2$	$H_2O + 2e^- \rightarrow H_2 + O^{2-}$
Electrolyte	20-40 wt.% KOH [59]	Nafion [59]	YSZ/SSZ [59]
Temperature [°C]	60-95 [61]	50-80 [61]	700-1000 [61]
Pressure [bar]	1-32 [61]	1-40 (demonstration up to 700) [61]	1-3 [61]
Hydrogen purity [vol. %]	>99.5 [59]	99.99 [59]	99.9 [59]
Load range [%]	10-110 [59]	0-160 [59]	20-100 [59]
Efficiency [%]	Up to 65 [61]	Up to 65 [61]	Up to 82 [61]
Stack lifetime [*1000 h]	60-90 (2020) [59] 90-100 (2030) [59]	30-90 (2020) [59] 60-90 (2030) [59]	10-30 (2020) [59] 40-60 (2030) [59]
TRL	9 [59]	8-9 [59]	5-6 [59]
System size [MW]	up to 100 [61]	up to 100 [61]	up to 0.15 [61]

Because PEMEL electrolysis often uses expensive and rare catalyst materials (platinum or iridium) [61], it is mainly used for mobile solutions and not for stationary applications as in our case. For this reason, this technology will not be considered further in the later system design. Especially in stationary applications, SOE can play an increasingly important role due to its high efficiency and consequently a reduction in hydrogen production costs compared to the AEL. Nevertheless, there are also drawbacks with SOE, namely the high technical complexity at extremely high temperatures or slow adaptation to load changes due to the thermal inertia of the system. AEL on the other hand is a commonly installed electrolysis technology within the past decades because of cheap catalysts and long stack lifetimes [61]. Furthermore, big sized AEL systems which were designed in the past reach an electric power up to 100 MW [61]. After taking the pros and cons into account, the AEL and SOE will be looked in more into detail in this work and builds the basis for later system calculations.

Methanol Production Unit (MPU)

Considering how factors such as reactor configurations, heat transfer mechanisms and the characteristics of the catalyst used significantly impact the efficiency and feasibility of methanol synthesis, Pratschner, Skopec et al chose the single multi-tubular fixed-bed BWR with closed loop configuration for the methanol synthesis. $Cu/ZnO/Al_2O_3$ is the catalyst used, and to avoid agglomeration of catalyst particles when the critical temperature is exceeded in the reactor. The input to the reactor are the CO_2 stream from the DeOxo reactor, hydrogen from the electrolyzer and the unconverted gases which is filtered from a flash drum and fed back. The main output to the reactor is methanol which is separated from water (the other output from the reactor) in a distillation column. IMPCA claim that the methanol purity of 99.85 wt% is obtained at the head of the distillation column [62].

Pratschner, Skopec et al also found the checkboxes the process has to tick in order for efficient working of the process:

- Low temperature and high-pressure levels favour the conversion of CO_2 following the principle of Le Chatelier.
- Preventing the occurrence of the reverse water-gas shift reaction is a key factor for reactor design.
- Minimum H_2:CO_2 ratio of 3 must be maintained to avoid the formation of elemental C

The operation condition for the reactor are as follows:

- Reactor temperature, T_{MeOH} = 513K
- Reactor pressure, P_{MeOH} = 40 bar

5. Methodology

In order to achieve valid results later, the methodology must first be examined more closely. This serves to give the reader an understanding of the calculation method so that the individual calculation steps and dimensioning can be shown in a comprehensible manner. Again, in this chapter, based on the process design, the individual components were considered separately at the beginning and then linked. For the implementation of input data and equations to get to the final results, the worldwide used and well-known software program Microsoft Excel was used. The reason for this choice lays in the easier handling of data in table format as well as the better visualization of calculation steps and results. Henceforth, Microsoft Office products are one of the most spread programs around the globe with a huge amount of end users able to access and possibly adjust the worked-out program.

5.1 Data processing and subsystem design

As mentioned earlier, the data for the power production unit is provided by Växjö Energi. A physical meeting with the head engineer of the plant followed by a visit around the plant helped gain knowledge of the working in the plant. The hourly and weekly average load profile, typical operating conditions of Sandvik 2 and the fuel specification are the major data provided by Växjö Energi. More information on how the data provided is filtered and processed is discussed in the sections below. In this study, the weekly data is used to design the discussed system components.

PPU

On having a discussion with the plant engineer, it was decided to work using the weekly average data as it would provide simplicity to the program. The weekly data displays the average heating demand for each week of the year 2023 fulfilled by Växjö Energi. The heat is divided by operating both Sandvik 2 and Sandvik 3 mainly and Sandvik 1 only in case of peak load. To maximize the methanol production, the boiler is run at maximum capacity (94 MW) throughout the year primarily to fulfil heat demand and the rest to produce electricity. In this thesis, the heat demand was assumed to be for an industry that needs high-quality, high-pressure steam. A flue-gas condenser additionally provides heat by extracting the heat from the flue gases. This is considered a constant value of 20 MW heat based on the experience of the plant engineer. With a constant boiler efficiency of 92% as per the data provided, the energy required in the fuel before combustion is calculated.

$$Q_{in,B}(MW_f) = \frac{Q_{out,B}(MW_{th})}{\eta_B} \tag{3}$$

where,

$Q_{out,B}$ is the heat output after combustion in MW
$Q_{in,B}$ is the fuel input in MW

This results in a constant fuel input throughout the year. From the records, the full load hours (FLH) of the plant in 2023 is 8743 hours/year. With this known the energy required from the fuel is calculated:

$$Q_{in,B}\ (MWh_f/year)\ =\ Q_{in,B}(MW_f)\ *\ FLH\ (hours/year) \tag{4}$$

Växjö Energi also provided an estimate composition of feedstock which is following:

- Forestry residues / GROT (45-65%) – Branches and tops left after final cutting and to a smaller extent thinning.
- Bark (10-20%)
- Saw dust (10-20%)
- Chipped wood (5-25%)
- Recycled wood / RT (2-5%) – Only untreated wood is used.

In this work, we assume a constant composition of the feedstock, given the abundant biomass resource available in Sweden. Next, the energy required from each feedstock is identified.

$$Q_{in,x}\ (MWh_f/year) = Fuel.Composition_x * Q_{in,B}(MWh_f/year) \tag{5}$$

Where, x is any feedstock for fuel.

With the lower heating values as received ($LHV_{(AR)}$) provided by Växjö Energi the amount/quantity of each feedstock in the fuel is calculated.

$$Q_{in,x}\left(\frac{kg}{year}\right) = \frac{Q_{in,x}\left(\frac{MWh_f}{year}\right)}{LHV_x\left(\frac{kJ_f}{kg}\right)} * 3.6 * 10^6; \tag{6}$$

$$[1\ MWh = 3.6 * 10^6\ kJ]$$

As mentioned earlier, the primary purpose of the CHP is to provide high-quality, high-pressure gas to an industry, with Sandvik 2 and Sandvik 3 sharing the demand equally. Using the average weekly demand, the steam demand supplied from Sandvik 2 is calculated.

$$Q_{DH,Sandvik\ 2}\ (MW_{th}) = \frac{Q_{DH,overall}(MW_{th})}{2} \tag{7}$$

Where, $Q_{DH,Sandvik\ 2}$ is the heat demand in the industry provided by Sandvik 2

A constant efficiency of 95% is implemented for the steam transmission system, i.e., 5% of the heat is lost due to transmission loss or thermal losses at heat exchangers.

$$Q_{DH,Sandvik\ 2}\ (MW_{th}) =\ \eta_{DH}[Q_{SC} + Q_{FGC}] \tag{8}$$

Where,

Q_{SC} is the heat recovered from steam condenser

Q_{FGC} is the heat recovered from flue gas condenser

Also, the turbine efficiency of 40% and generator efficiency of 98% have been used in the calculations. The efficiencies used for the calculations are based on the historical performance recorded by Växjö Energi. The design capacity of the turbine at Sandvik 2 is 37MW and is operated in one stage. With the following data the electricity produced is calculated.

$$P_{el}(MW_{el}) = Q_{out,B} * \eta_T * \eta_G \quad (9)$$

Oxyfuel combustion

One of the primary design parameters in our system is the amount of oxygen which should be provided by the elctrolyzer to keep a stable combustion with comparable conditions as the regular air combustion. For this purpose, the oxygen by the electrolyzer is mixed with parts of the flue gas stream to get a sufficient heat carrier and (for fluidized bed boilers) to achieve a sufficient fluidization medium volume [63]. The calculations for the amount of needed O_2 is based on research done by Skopec and Hrdlička [63] and Pratschner, Skopec at al. [21]. An assumption which was made at this point is that the oxygen purity of the electrolyzer will be set to 100 % [63]. This assumption had to be stated because electrolyzer manufacturer often provide stats about hydrogen purity, but not regarding oxygen purity. The oxygen stream of the electrolyzer is mixed with the recycled flue gas stream in an O_2/CO_2 ratio (dry) of 30/70. An illustration of the described process is shown in Figure 12 [63].

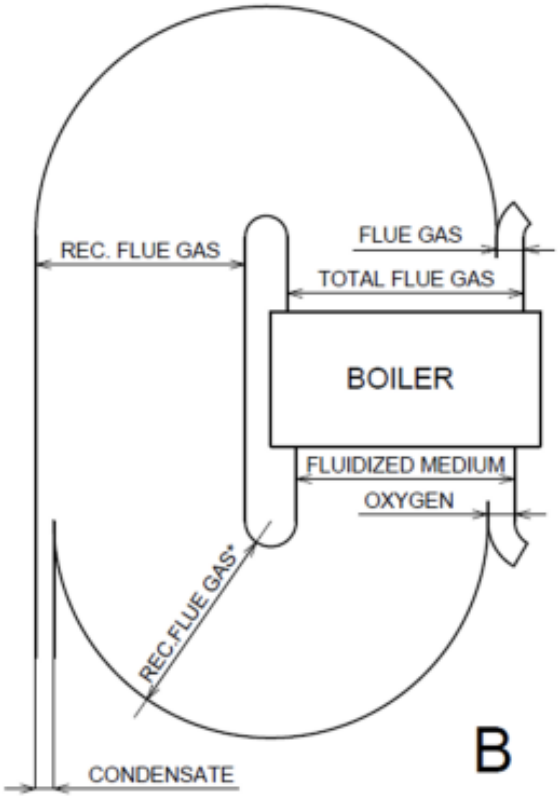


Figure 12: Illustration of oxyfuel combustion process. [63]

First of all, the ratio of excess oxygen in the oxidant needs to be discussed which is defined as the actual oxygen volume flow divided by the needed O_2 volume flow for the stoichiometric combustion. Mathematically, the ratio is described as following (eq. (*10*)) [21, 63]. Skopec and Hrdlička determined an excess of oxygen for oxyfuel combustion of 1.06 [63] whereas Pratschner, Skopec et al. uses a value of 1.08. This value is verified by two real BFB boiler experiments and is therefore used in the subsequent sections [63].

$$\alpha = \frac{\dot{V}_{Ox,O2,real}}{\dot{V}_{O2,stochiometric}} \tag{10}$$

As previously mentioned, flue gas recycling is crucial in the oxyfuel combustion. Because of this, the amount of oxygen is enhanced by the recirculation loop. As a conclusion, the new parameter β has to be defined which considers also this additional oxygen share. This parameter can be seen in equation (*11*) [21]. Pratschner, Skopec at al. mention a value for β of 1.4 [21].

$$\beta = \frac{\dot{V}_{Ox,O2,real} + \dot{V}_{RFG,O2,real}}{\dot{V}_{O2,stochiometric}} \tag{11}$$

Further, the share of recycled flue gas in relation to the volume flow which leaves the combustor is an important parameter and can be defined as shown in equation (*12*) [21, 63].

$$r = \frac{\dot{V}_{RFG}}{\dot{V}_{FG,W}} \tag{12}$$

Approved value by [63] for the recycled flue gas ratio is claimed to be 3.24, the authors in [21] speak about a number of 4 to ensure a boiler fluidization velocity of 1-2 m/s [21]. As stated in the literature sector, a share of 70:30 vol% of CO_2:O_2 in the fluidization medium lead to similar combustion properties as a conventional air fuel combustion. For this reason, a CO_2:O_2 ratio of 70:30 was chosen which leads to a recycled flue gas ratio of around 3.04.

Additionally, with the Boie equation found in [21] and the ultimate (and proximate) analysis, the lower heating value (LHV) of the fuel can be calculated with equation (*13*). For this purpose, the data from Växjö Energi AB about the used fuel input was used. A restriction here is that a nominal fuel was used. In reality, the content of the biofuel is a mixture of different kinds of biomass (such as bark, saw dust, woodchips, etc) and varies transiently which has an effect on the share of species in the feedstock and on the LHV.

$$LHV = 34.8 * c + 93.9 * h + 6.3 * n + 10.5 * s - 10.8 * o - 2.5 * w \quad \left[\frac{MJ}{kg}\right] \tag{13}$$

After considering the above parameters α, β and r, the volume flows of the boiler can now be calculated step by step. All of the formulas are extracted from [63] and [21]. To start with determining the stoichiometric volume flow, the oxygen demand for burning the different kind of fuel species is needed. Those values were set by [21] and can be found in Table 6.

Table 6: Specific O_2 demand of the combustion reaction per species i. [21]

Species i	$V_{O_2,i}$ [Nm³/kg of species i]
C	1.8659
H	5.5608
O	−0.7003
S	0.6988

With those values, the calculated mass flows based on the boiler output and the share of the species i in the fuel input, the volume of needed oxygen is the sum of the individual oxygen volumes to burn the species (equation (*14*)).

$$\dot{V}_{O_2,Stoichiometric} = \sum V_{O_2,i} * \dot{m}_i \quad (14)$$

After multiplying the stoichiometric oxygen flow rate with the oxygen excess value α of 1.08, one get the real oxygen demand which is supplied external by an electrolyzer and/or and ASU. Further, with the set β value of 1.40, the total oxygen volume flow of the fluidization medium can be determined which consists of the oxygen content of the external source and the oxygen in the recycled flue gas stream. As we declared a CO_2:O_2 ratio of 70:30, the carbon dioxide volume flow of the fluidization medium (which is the same as in the RFG stream) can be calculated. Assuming there is no significant slip in the system, the total flue gas after the boiler is the same as the volume flow of the fluidization medium due to the conservation of mass. The flue gas is cleaned in the flue gas processing unit (FGPU) which contains a SO_x elimination with $Ca(OH)_2$, an ash removal system (such as a baghouse filter), a SCR for NO_x removal and a condenser to cool down the flue gas before splitting up [21]. Again, the flue gas is split up in a ratio of 70:30 which means that 70 vol% of the volume flow is recirculated and 30 vol% is sent for further processing before entering the methanol synthesis reactor. The volume flow after the FGPU is made up of 89.8 vol% CO_2, 2.48 vol% H_2O, 7.41 vol% O_2 and 0.31 vol% N_2. Hence, the SO_2 content is around 69.7 ppm. Those values are based on researches and results from [21].
To make the oxyfuel combustion process more visible, all the previously mentioned equations and assumptions are shown in Figure 13.

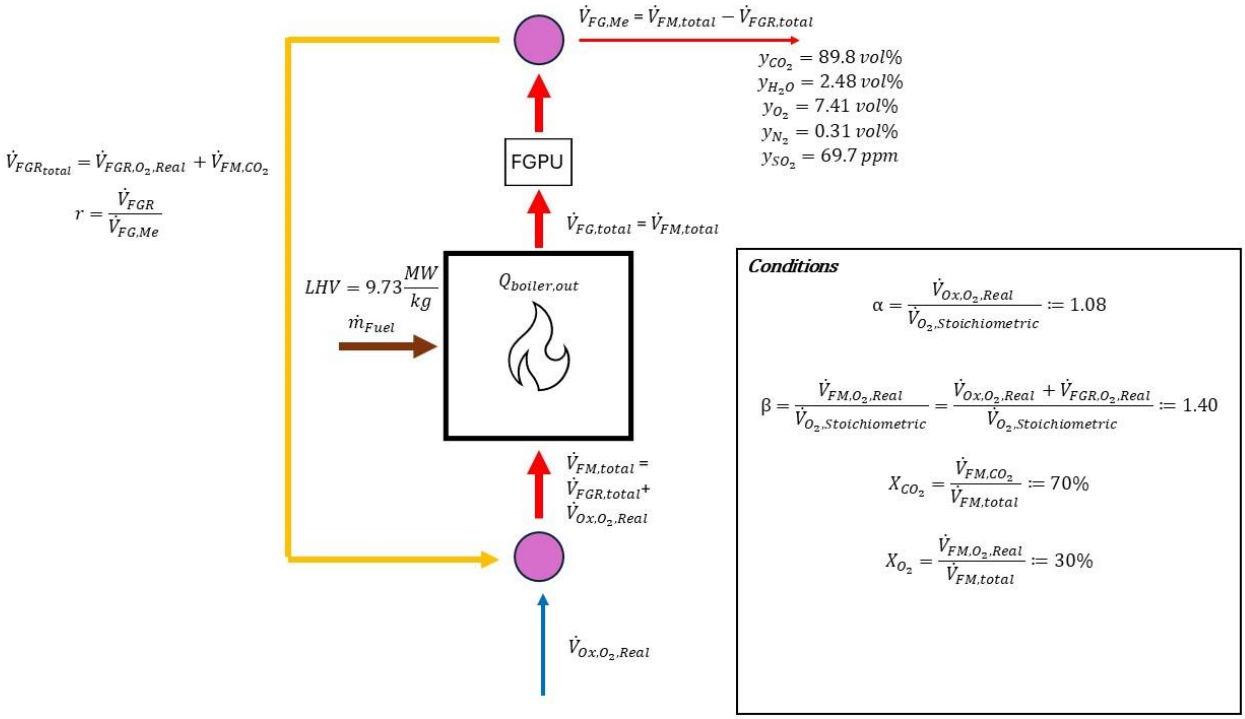


Figure 13: Scheme and calculations of the oxyfuel combustion process. Own illustration based on [21].

Because the flue gas going to the methanol production unit still has a relatively high share of water and oxygen, a water removal (with another condenser) and a DeOxo component are necessary [21]. After that, the purity of the flue gas entering the MPU can be claimed to be around 99.85 vol% [21].

WEU

For the production of methanol via CO_2 hydrogenation, not only CO_2 is needed, but also hydrogen, which in our case is to be provided with the help of an electrolyzer (and possibly an additional ASU). The dimensioning of the electrolyzer can be done in different ways, depending on the desired design parameters. Three different approaches are pursued in this master's thesis. Firstly, the design can be based on the required volume flow of oxygen to ensure safe oxyfuel combustion in the boiler. The second design method will be based on the amount of hydrogen required to convert the total flue gas flow from the boiler into green methanol. This method will ensure the CO_2 neutrality of the power plant. The last alternative of the electrolyzer design is to consider it from an economic point of view in order to ensure the lowest price for methanol production. In other words, this method is aimed at using the electricity produced by the CHP plant to produce methanol. More on this later in the chapter on the results.

Based on the explanations of the process design chapter, the AEL and SOE technology was taken into account in this work. For the implemetation, research on commercially available solutions were done which lead to the choice of electrolyzers by the German manufacturer Sunfire located in Dresden. Those chosen electrolyzers are namely the “Sunfire-Hylink Alkaline” and the “Sunfire-Hylink SOEC”.

Firstly, the most important values and parameters of the datasheet of the ”Sunfire-Hylink Alkaline” datsheet were added in the software which are a hydrogen net production rate of 2174 Nm^3/h (195 kg/h) with a module power of 10 MW, a production range of 25-100%, a delivery pressure of 30 bar(g) and a hydrogen purity of 99.8% [64]. Furthermore, two ranges are given for the specific energy

consumption, one in DC at stack level and the second in AC at system level. The first range in DC is 4.18...4.54 kWh/Nm^3, the second range in AC is 4.29...4.67 kWh/Nm^3 [64]. As the power supply for the electrolyzer is to be covered by the CHP power plant (and possibly with additional purchases from the power grid), it makes more sense to look at the system level in AC. In addition, the upper limit for the specific energy consumption in AC was chosen for the calculations in the Excel program, as this represents the worst-case scenario. If the actual energy input is lower than the taken maximal value, this has a positive effect on the hydrogen production costs (and therefore also on the methanol production costs). Using the maximum value of 4.67 kWh/Nm^3 therefore provides certainty in the system design. As an input, water has to be delivered to the system which is stated to be 1.85 m^3/h [64].

Alternatively, the use of an SOE is taken into account in the Excel tool, also by Sunfire. Sunfire claims that its high-temperature SOEC is the optimal electrolysis solution for industrial applications, provided that steam is available for the process [65]. The outstanding advantage that distinguishes the SOEC from other electrolyzers is the significantly higher system efficiency of 84% thanks to the use of industrial waste heat [65]. The manufacturer declares a hydrogen production of approximately 750 Nm³/h hydrogen with a specific power consumption of 3.6 kWh/Nm³ and a hydrogen purity of maximal 99.99% [65]. The hydrogen delivery pressure is stated to be 0 bar(g) and the SOE can vary the load between 5 and 100 % [65]. For the hydrogen production, around 860 kg/h of steam is used as input with a temperature between 150°C and 200°C and a pressure of 3.5 bar(g) to 5.5 bar(g) [65]. 2680 kW is the rated system power in AC, but Sunfire stated that the system size can be scaled up individually through modular designs [65].

FGPU

As previously mentioned the FGPU sums up a fly ash removal process by an baghouse filter, the addition of $Ca(OH)_2$ for SO_x reduction, a SCR for NO_x removal and a condenser to cool down the hot flue gas [21]. The needed streams for the single components were calculated stoichiometrically. For the spray desulfurization process after the ash removal, an excess of 50% $Ca(OH)_2$ with an efficiency of maximal 95% were stated by [66]. The amount of needed $Ca(OH)_2$ was determined by upscaling linearly the value of 7.23 kg/h which can be found in [21]. Putting all together leads to equation (*15)*.

$$\dot{m}_{Ca(OH)_2} = 7.23\ \frac{kg}{h} * \frac{\dot{V}_{FG,total}}{21664\ \frac{Nm^3}{h}} \tag{15}$$

The same steps were taken for the nitrogen oxide filtration by an SCR unit. Here, NH_4OH with a concentration of 19-29 wt% and a temperature range of 453-703 K is utilized to reduce NO_x to N_2 and water [21]. Once again the required amount of NH_4OH was set to be 50 % bigger than stoichiometrically needed [58] and the value of 2.45 kg/h of NH_4OH from [21] was extrapolated which results in equation (*16)*.

$$\dot{m}_{NH_4OH} = 2.45\ \frac{kg}{h} * \frac{\dot{V}_{FG,total}}{21664\ \frac{Nm^3}{h}} \tag{16}$$

CO_2PU

Before the flue gas stream can be converted into methanol in the synthesis reactor, it has to be processed by reducing the excess oxygen and water. Pratschner, Skopec et al assume therefore a DeOxo reactor with a pressure of 10 bar and a reactor temperature of 323 K [21]. Further a catalyst protection unit to remove catalyst poisons (such as H_2S and SO_2) has to be installed previously to the DeOxo reactor [21]. Since the separation process is strongly exothermic (ΔH = -285.8 kJ/mol) it must be cooled (this cooling is not taken into account in this work). As a result of the oxygen removal, water is formed and afterwards separated by two adsorbent beds with activated alumina [21]. The required volume flow of hydrogen for this formation of water is given by equation (*17)*.

$$\dot{V}_{H_2,DeOxo} = \frac{\dot{V}_{FG,Me,DeOxo} * y_{O_2} * \rho_{O_2}}{M_{O_2}} * 2 * \frac{M_{H_2}}{\rho_{H_2}} = \dot{V}_{H_2,total,i} - \dot{V}_{H_2,Me,i} \quad (17)$$

As can be seen the required amount of hydrogen for the DeOxo reactor depends on the volume flow of flue gas to be washed and the composition. As an assumption based on result of [21], an oxygen share of 7.41 vol% is utilized in the flue gas. In case the produced hydrogen by electrolysis is not sufficient for converting all of the flue gas stream, a splitter will be installed in front of the DeOxo reactor. This will save energy as well as hydrogen for the DeOxo process and more hydrogen is available for methanol production. The volume flow of the emitted flue gas stream and the stream going into the DeOxo reactor can be defined as following, whereas γ describes the share of non-emitted flue gas. In other words, if γ equals 0.7, that means that 70 % of the generated flue gas stream is going into the DeOxo reactor and 30 % will be emitted into the environment. With this share, the resulting volume flows can be described with equation (*18)* and (*19)*.

$$\dot{V}_{FG,Me,DeOxo} = \gamma * \dot{V}_{FG,Me} \quad (18)$$

$$\dot{V}_{FG,Me,emitted} = (1 - \gamma) * \dot{V}_{FG,Me} \quad (19)$$

After the DeOxo process, the flue gas stream which reaches the methanol production unit has a purity of 99.66 vol% CO_2. The volume flow of this stream can be calculated using equation (*20)*.

$$\dot{V}_{FG,Me,processed} = y_{CO_2} * \dot{V}_{FG,Me,DeOxo} \quad (20)$$

With all of the upper equations, a mass flow scheme was drawn for a better visualization of the DeOxo process in which the red paths represent the flue gas and light blue the hydrogen from electrolysis.

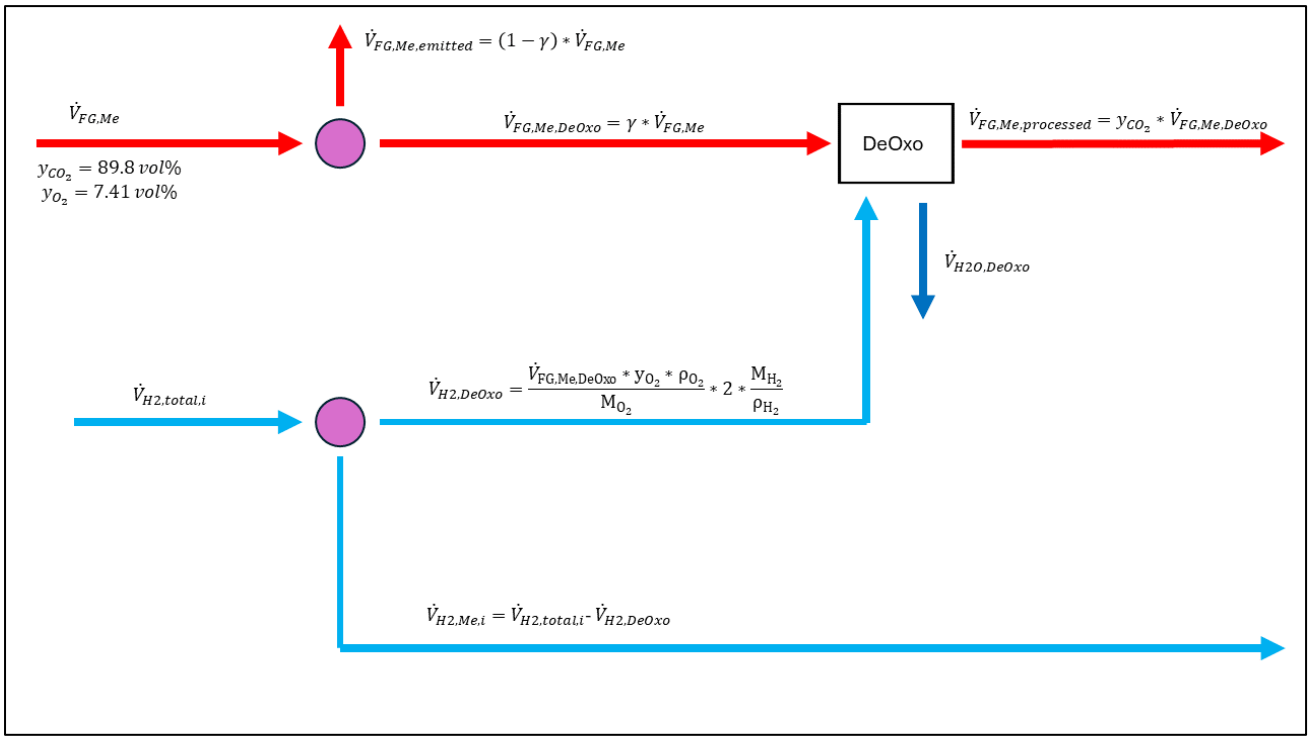


Figure 14: Volume flows and equations used for the DeOxo process.

MPU

The calculations performed to quantify the methanol production are as follows:

In the base case, the methanol production was designed to use up all the hydrogen produced from the electrolyzer, by hypothetically assuming the electrolyzer has the maximum operation costs due to high electricity demand. The mass flow of hydrogen was the input for the calculations. Using molar masses of hydrogen and other components involved in the CO_2 hydrogenation reaction, the stoichiometric mass flow rate was calculated. The formula used for the calculation is given below (eq. (*21*)).

$$\dot{m}_x = \dot{m}_H * \left(\frac{M_x}{M_H}\right) \tag{21}$$

where,

ṁ is the mass flow in kg/h
M is the molar mass
Subscript 'H' is with reference to hydrogen
Subscript 'x' is with reference to any elements in the hydrogenation reaction [CO_2, CH_3OH, H_2O]

The volume flow rate of all the elements involved in hydrogenation reaction were also calculated using density of the respective elements as shown in FGPU calculations.

Further, the actual mass and volume flows were calculated by subtracting excess/ non-reacting CO_2 and H_2 during the reaction. Pratschner, Skopec et al used the equations to calculate excess CO_2 and H_2 in the reactor. This was made use of in our work as well.

$$\dot{n}_{CO_2,Unc.} = (1 - \Psi).\dot{n}_{CO_2.} \tag{22}$$

where,

Ψ is the CO_2 conversion rate which based on experience is estimated to be 98.11%
ṅ is the number of moles
Subscript 'Unc' refers to unreacted [here $\dot{n}_{CO2,\,Unc}$ is the number unreacted moles of CO_2].

Similarly, excess volume flow of H_2 is calculated using equation *(23)*

$$\dot{V}_{H_2,excess} = \dot{V}_{H_2,MeOH} - 3.\dot{V}_{CO_2,MeOH} \tag{23}$$

where,

$\dot{V}$ is the volume flow in m^3/h
Subscript 'excess' refers to the excess volume flow [for hydrogen in the equation]
Subscript 'MeOH' refers to the elements in the methanol synthesis

The excess moles and excess volume flows from equation *(22)* and *(23)* respectively is then converted to excess mass flow using molar mass and density as the conversion factors respectively.
Subtracting these excess mass flows of CO_2 and H_2 from their respective stoichiometric mass flows, gives the actual mass flows.

Finally, using the actual mass flows of CO_2 and H_2, the amount of methanol and water is calculated with reference to the balanced hydrogenation chemical equation.

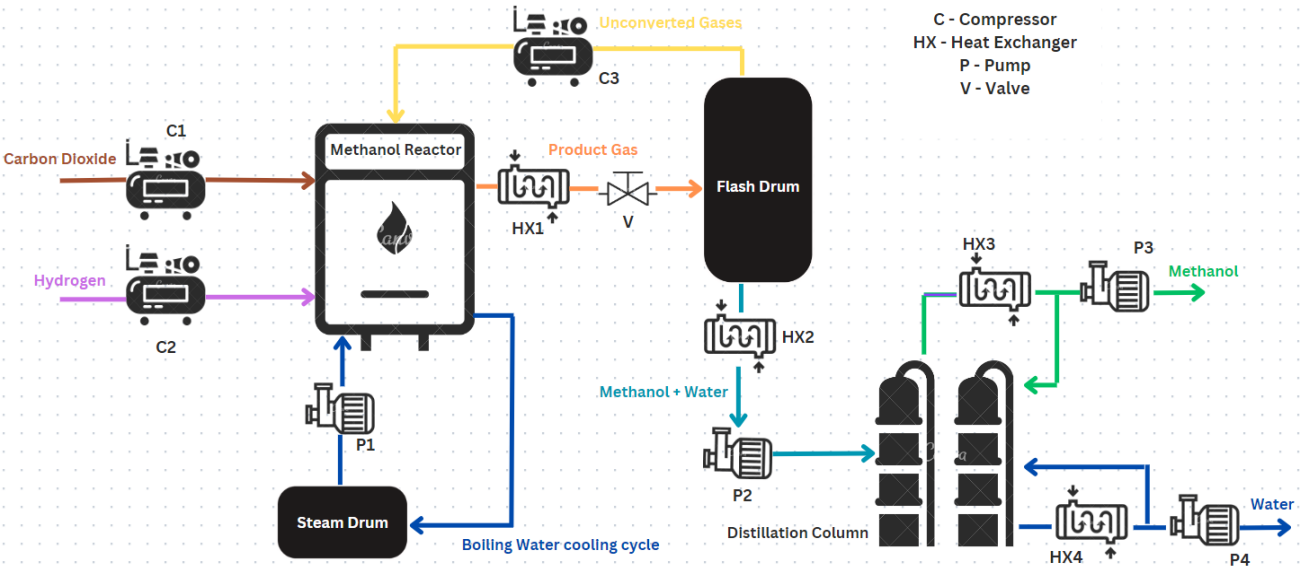


Figure 15: Scheme of flows for the methanol production unit (MPU). [21]

5.2 Cost calculations

After having a look at the technical design of the system, economic analysis is inevitable to conceive a market competitive advantage compared to other conventional carbon capture technologies like pre- or post-combustion carbon capture and storage. Therefore, operational expenditures (OPEX) as well as capital expenditures (CAPEX) are taken into account in the following cost calculation to provide an all-encompassing overview of the economies.

5.2.1 Operational expenditures

First, the running costs and revenues of the systems were investigated. More detailed, electricity costs (and/or revenues) and water costs of the elctrolyzer were considered whereas steam costs for the SOEC can be neglected as the steam is assumed to be generated by using waste heat of the power plant. Furthermore, the system design focuses on the retrofit of an existing CHP plant which means that fuel costs as well as income from heat supply are set to zero. In a later sensitivity analysis, the impact of fuel cost, carbon taxation and heating revenues on the total annualized costs were investigated.

Analyzing the running costs of the system, one has to take a look at the electricity production of the power production unit and the electricity consumption of the whole system which consists of methanol production unit, the water electrolysis unit, the air separation unit (if necessary) and the CO_2 processing unit. All those values are on a weekly basis and can be calculated with equation (*24*).

$$W_{total,weekly} = W_{MPU,weekly} + W_{WEU,weekly} + W_{ASU,weekly} + W_{CO2PU,weekly} \tag{24}$$

Now, two cases can occur in the system. In the first scenario the power production unit cannot provide enough electricity to cover the total weekly electricity demand. If this is the case, additional electricity from the grid has to be purchased which can be calculated with equation (*25*). In this thesis it is assumed that the additional electricity comes from renewable sources. On the other hand, if the PPU electricity outcome is greater than the required electric energy to run the system, no additional electricity has to be purchased and is therefore zero.

$$W_{additional,weekly} = W_{total,weekly} - W_{PPU,weekly} \tag{25}$$

In the second scenario, the PPU can provide enough electricity to cover the electricity need and the resulting overproduction of electricity is based on equation (*26*) otherwise the overproduced electric energy equals zero.

$$W_{overproduction,weekly} = W_{PPU,weekly} - W_{total,weekly} \tag{26}$$

Those mentioned scenarios are useful later, if the purchasing electricity price differs from the selling price of electricity from own production. In this thesis for simplicity, both prices have no price difference. Because the electricity market price varies a lot throughout the year, an hourly dataset of Swedish electricity prices was broken down to average weekly prices. This dataset was provided internally by Norconsult Svergie AB. Finished with that, weekly electricity costs and revenues were calculated with equations (*27*) and (*28*) and the weekly electricity saldo can be formed with equation (*29*).

$$El.costs_{weekly} = W_{additional} * p_{el,weekly} \quad (27)$$

$$El.revenues_{weekly} = W_{overproduction} * p_{el,weekly} \quad (28)$$

$$El.saldo_{weekly} = El.revenues_{weekly} - El.costs_{weekly} \quad (29)$$

Generating hydrogen and oxygen with electrolysis, demineralized water is required. The costs for the water consumption can be determined as following (equation (*30*)) with a price of 0.12 EUR/m³ [67].

$$Costs_{Dem.water,weekly} = \dot{V}_{Dem.water,weekly} * p_{Dem.water} \quad (30)$$

After this step, the total weekly costs can be calculated with equation (*31*).

$$Costs_{\text{Total},weekly} = El.saldo_{weekly} - Costs_{Dem.water,weekly} \quad (31)$$

All the mentioned results in this chapter are on a weekly basis. To transfer the results into yearly data, the weekly numbers are summed up over the year what equation (*32*) illustrates.

$$Yearly\ data = \sum_{1}^{52} Weekly\ data \quad (32)$$

5.2.2 Capital expenditures

The major capital investments made to modify the CHP plant to Oxyfuel combustion-CHP with methanol production are:

- Oxyfuel retrofit
- Electrolyzer
- CO_2 purification unit
- Methanol production unit
- Air separation unit (in case of downsized system)

The 'six-tenths rule' as shown in equation (*33*) has been used to estimate the costs of most components and equipment. With this rule the capital costs of the required component are scaled using the costs and size of the component used in references [15]. The costs for the boiler modification and retrofitting costs are calculated as 30 % of the total plant cost. The installation and labor costs are included in the capital costs for all the components except the electrolyzer, here the installation costs are an additional which is estimated as 9 % of the electrolyzer CAPEX [68].

$$C_{capital} = C_{capital,ref} * \left(\frac{S}{S_{ref}}\right)^{sf} \quad (33)$$

Where,

$C_{capital}$ is the capital cost
S is the size of the component
sf is the scaling factor
sf = 0.6 [15]
Subscript 'ref' is reference

Table 7: The size and costs of components for the reference plants.

Component	Reference	Reference size	Reference costs
Alkaline Electrolyzer	[69]	-	800-1300 EUR/kW_{el}
SOEC	[69]	-	3000-5000 EUR/kW_{el}
Methanol Production Unit	[70]	0.08 Mt/year	27.8 Mio. EUR
CO_2 Processing Unit	[15]	54.81 MW_{el}	120.093 Mio $
Air Seperation Unit	[15]	68.6 MW_{el}	78.845 Mio $

Further annualized capital costs (ACC) are calculated for the simplification of results. The formula to calculate the ACC is given in equation (*34*) out of [71].

$$ACC = CRF * C_{capital} \tag{34}$$

Where,

ACC is the annualized capital costs
CRF is the capital recovery factor
$C_{capital}$ is the capital cost

The CRF is calculated using equation (*35*) found in [71].

$$CRF = \frac{k(1+k)^t}{(1+k)^t + 1} \tag{35}$$

Where,

k is the interest rate in %
t is the component lifetime

5.2.3 Total annualized costs

To get the total annualized costs, the operational and capital expenditures are combined with the help of equation (*36*).

$$TAC = OPEX_{yearly} + ACC \tag{36}$$

In order to compare final results of the different systems with a various TAC and methanol production rate, the break-even price of green methanol was calculated by dividing the TAC of the system by the yearly methanol production outcome of the system which is shown in equation (*37*).

$$BEP_{green\ methanol} = \frac{TAC}{\dot{m}_{methanol,yearly}} \tag{37}$$

Furthermore, a factor is introduced which describes the relationship between the conventional methanol price and the break-even price of green methanol (see equation (*38*)). The conventional methanol market price is fluctuating throughout time, but for simplicity it was assumed to be constant at a level of 327 EUR/t (2515 CNY/t, accessed on 05.07.2024) [72].

$$Green\ methanol\ price\ factor = \frac{BEP_{green\ methanol}}{327\ \frac{EUR}{t}} \tag{38}$$

6. Results

Once the input data and formulas discussed in the methodology chapter have been implemented in Excel, the results of the study are summarized and presented in this chapter. Further, it was divided into four cases. The first use case is the design of the electrolyzer according to the required oxygen demand, so that a reliable oxygen supply for oxyfuel combustion can be guaranteed. The next use case is aimed at CO_2 neutrality of the CHP power plant, i.e. the CO_2 emissions from combustion should be eliminated and all CO_2 should be converted into green methanol. In the third case, the focus should be on maximizing the profitability of the overall system. This should be done by minimizing the electricity costs for mainly the electrolyzer and the MPU and covering these components with high electricity demand mainly by the produced electricity of the CHP power plant. The fourth and final case is based on the first case, but additionally carbon emission taxes, subsidies as well as fuel costs and heating revenues were considered.

Important to mention is that for all four use cases the technical data of the CHP power plant remains the same as the boiler output is kept at a constant value of 94 MW throughout the year. What changes during seasonally is the distribution of generated heat and power as can be seen in Figure 16. The plot is based on data which can be found in Table 16 (Appendix E). Due to this non abstinence of change, the mass flow of the fuel input does not vary over time. For this reason, the hourly amount of oxygen for the oxyfuel combustion is constant as well. Within that, the amount of oxygen to burn an ash and water free nominal fuel flow of 19.8 t/h (alias 37.8 t/h fuel including ash and water) can be clarified as roundabout 38.4 t_{O2}/h. Based on this value, around 29.6 t_{O2}/h of oxygen must be supplied externally. Around 8.78 t_{O2}/h of oxygen need for the combustion is coming from flue gas recycling. The flue gas volume flow before splitting with the γ rate is 20,735 Nm^3/h with a share of 18,620 Nm^3/h CO_2. The recirculation ratio is determined as 3.04. For the desulfurization, a mass flow of 30.0 kg/h $Ca(OH)_2$ is required. Furthermore, a mass flow of 10.2 kg/h NH_4OH is needed for the $DeNO_x$ process.

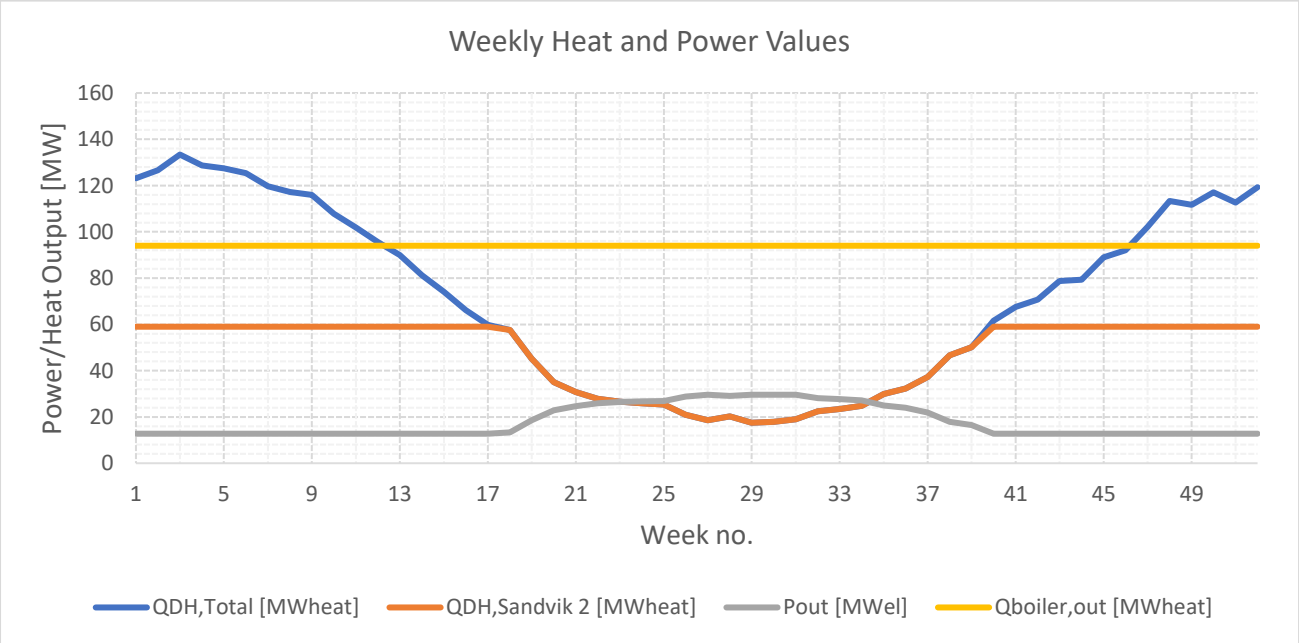


Figure 16: Weekly heat and power output from Sandvik 2 out of data provided by Växjö Energi AB.

The main results considered in the four use cases are technical parameters such as component sizes, energy consumption, CO_2 utilization rates, etc. as well as cost-related aspects such as capital expenditures (CAPEX), operational expenditures (OPEX) and total costs. From this, a conclusion will be drawn about the green methanol break-even price which will be later compared with the price from conventional methanol production. This is an essential step in order to draw conclusions about the technical implementation as well as the economic feasibility and competitiveness of green methanol production with this system setting.

In the base case, the electrolyzer was designed to match the maximum needed oxygen for the oxyfuel combustion. As previously mentioned, the fuel input flow in this case does not change over time which results in a constant hourly oxygen demand of around 29.6 t_{O2}. This value combined with the given data of Sunfire leads to a maximum required alkaline electroyzer size of circa 191 MW or a maximum SOEC electrolyzer size of about 158 MW.
Because of the modular design of the alkaline electrolyzer, a decimal number is not achievable which means that in the following results, an oversized system and an undersized system was introduced for the alkaline systems. One alkaline module is declared to be 10 MW which means that in the undersized system, 19 modules are used to get a value of 190 MW. On the other hand, in the oversized system, 20 modules are introduced to achieve a total electrolyzer power of 200 MW. Obviously, the oversized system can cover the needed amount of oxygen whereas in the undersized system, a small amount of oxygen must be provided by an additional ASU. This approach of rounding up and down the module numbers is redundant if an SOEC is used because the manufacturer Sunfire claims a feasible match of the system power to the required size according to the customer. An important point to keep in mind is that the electrolyzer is designed to match the maximum amount of oxygen which means in weeks with less oxygen need, the system can fulfill the requirements to provide a specific amount of oxygen. Due to the fact that in our use case the oxygen demand remains constant, the maximum amount of oxygen is the same as the needed oxygen per single week. With another boiler output (and therefore also fuel input) this pattern can change.

To continue with the electrolyzer power values, the matching amounts of hydrogen for the produced oxygen can be calculated which is 3.85 t_{H2}/h for the oversized alkaline system and 3.94 t_{H2}/h for the SOEC system. The amount of hydrogen for the undersized system can be stated as 3.66 t_{H2}/h with an oxygen production rate of 29.0 t_{O2}/h. The difference between the required amount of oxygen for the oxyfuel combustion and the oxygen production rate of the downsized alkaline system is the oxygen flow rate which comes from the ASU. This figure amounts to 0.601 t_{O2}/h.

For the upsized alkaline electrolysis, a demineralized water supply of 35.3 t/h must be guaranteed, whereas this is 34.6 t/h for the downsized system. As steam is needed for the SOEC electrolysis, a steam flow rate of around 47.6 t/h can be stated.

After getting the above results, the CO_2PU could be parametrized. To achieve this, the perfect share of used volume for the methanol production (namely γ) was determined for the three different electrolysis systems by matching the produced hydrogen, the hydrogen demand for DeOxo and the hydrogen needed for the stoichiometric transformation into methanol by linear regression. As a result, the optimal ratio γ for the downsized alkaline system is 0.699, for the upsized alkaline system 0.740 and for the SOEC system 0.753. As some hydrogen is demanded for the DeOxo reaction, the total amount of hydrogen for the methanol production unit is decreased in the alkaline system settings. The total amount of hydrogen produced by the electrolyzer has now covered the hydrogen

demand of the DeOxo reactor and the hydrogen which is used for methanol production. As shown in Table 8, the available hydrogen mass flows for methanol production are as follows: 3.46 t/h for the downsized alkaline system, 3.64 t/h for the upsized alkaline system, and 3.73 t/h for the SOEC system. Correspondingly, the required CO_2 inputs for the reactor are 25.2 t/h for the downsized system, 26.5 t/h for the upsized system, and 27.2 t/h for the SOEC system. From these inputs, 476 kg/h of CO_2 in the downsized system, 501 kg/h in the upsized system, and 713 kg/h in the SOEC system remain unreacted. This unreacted CO_2, along with excess hydrogen—66 kg/h for the downsized system, 70 kg/h for the upsized system, and 71 kg/h for the SOEC system—is recirculated into the reactor. Table 8 provides a summary of the results based on the choice of electrolyzer.

Table 8: Results of technical design after oxygen demand.

		Sunfire – Hylink Alkaline (Downsized system)	**Sunfire – Hylink Alkaline (Upsized system)**	**Sunfire – Hylink SOEC**
Electrolysis				
P_{El}	$[MW]$	190	200	158
N_{El}	$[-]$	19	20	-
$\dot{m}_{H_2,Methanol}$	$[t_{H_2}/h]$	3.46	3.64	3.73
$\dot{m}_{H_2,DeOxo}$	$[t_{H_2}/h]$	0.193	0.205	0.208
$\dot{m}_{H_2,total}$	$[t_{H_2}/h]$	3.66	3.85	3.94
$\dot{m}_{O_2,oxyfuel}$	$[t_{O_2}/h]$	29.6	29.6	29.6
$\dot{m}_{O_2,El}$	$[t_{O_2}/h]$	29.0	29.6	29.6
$\dot{m}_{ASU,O_2}$	$[t_{O_2}/h]$	0.601	-	-
$\dot{m}_{El,H_2O}$	$[t_{H_2O}/h]$	34.6	35.3	-
$\dot{m}_{El,steam}$	$[t/h]$	-	-	47.6
Methanol production				
$\dot{m}_{FG,Me,CO_2}$	$[t_{CO_2}/h]$	36.0	36.0	36.0
$\dot{m}_{FG,CO_2,reactor}$	$[t_{CO_2}/h]$	25.2	26.5	27.2
$\dot{m}_{H_2,reactor}$	$[t_{H_2}/h]$	3.46	3.64	3.73
$\dot{m}_{CO_2,used}$	$[t_{CO_2}/h]$	24.72	26.0	26.64
$\dot{m}_{H_2,used}$	$[t_{H_2}/h]$	3.4	3.57	3.66
$\dot{m}_{Methanol}$	$[t_{CH_3OH}/h]$	18.1	19.0	19.5

$\dot{m}_{Water}$	$[t_{H_2O}/h]$	10.11	10.64	10.9
$\dot{m}_{FG,CO_2,emitted}$	$[t_{CO_2}/h]$	10.8	9.5	8.85
CO_2 *utilization rate*	[%]	68.6	72.2	73.9
γ	$[-]$	0.699	0.740	0.753

Having an overall view on the economics of the three different systems, it can be cleared out that in total the break-even price (BEP) for green methanol is the lowest when utilizing the Sunfire-Hylink Alkaline electrolyzers. Both the downsized and upsized system achieve almost the same methanol BEP with a value of 1485-1553 EUR/t whereas the system with the SOEC has a BEP of 1979-2483 EUR/t. The main difference in the BEP of the alkaline and the SOEC system lies in the around 7-8 times higher investment costs of the electrolyzer. On the other hand, it can be seen that the SOEC system has the lowest running costs, which stem mainly from the reduced electrolyzer electricity costs compared to the electric energy consumption of the alkaline electrolyzer systems. Running costs for the systems are around 210 Mio. EUR/a for the 190 MW alkaline system, 222 Mio. EUR/a for the 200 MW alkaline system and around 201 Mio. EUR/a for the 158 MW SOEC system respectively. Those high electricity prices have their roots in the low own electricity usage of 135.3 GWh/a in relation to an electricity demand of around 3215 GWh/a (for the SOEC system) up to 3540 GWh/a (for the upsized alkaline system) to run all the components for methanol production and oxyfuel combustion. The highest amount of electricity is consumed by the methanol production unit followed by the electrolyzer. The electricity demand of the ASU and CO_2 processing unit is neglectable. This is shown in Figure 17.

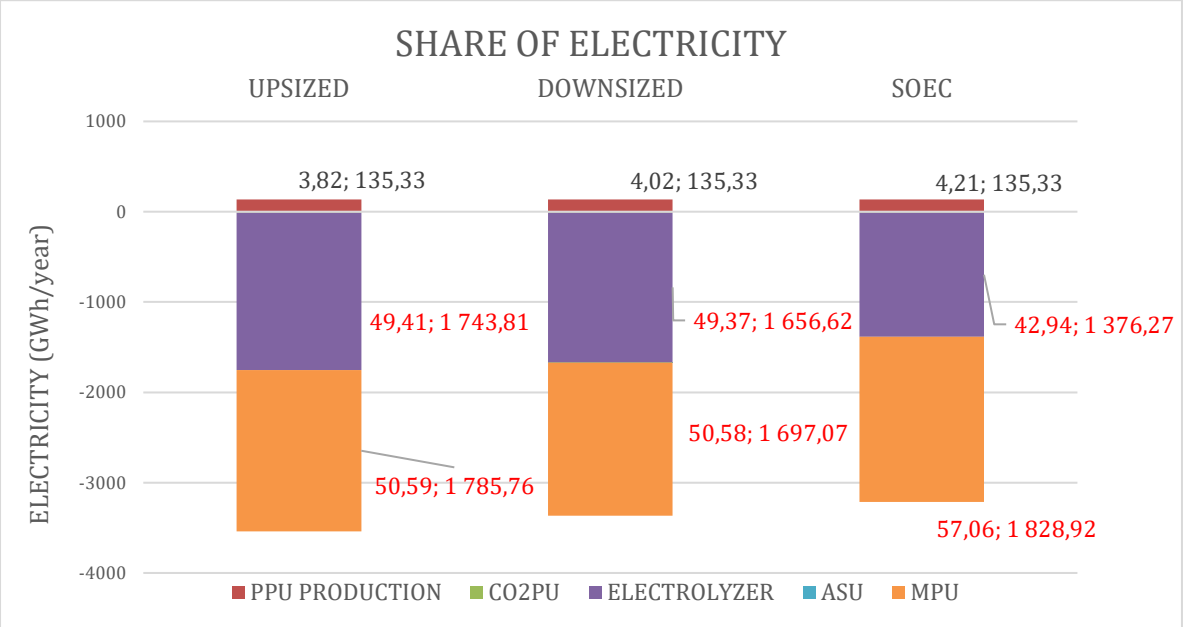


Figure 17: Share of annual electricity production and consumption. The values connected to the bars indicate the percentage of share of annual electricity consumption followed by the electricity consumption in GWh/year. Percentage share for PPU is the total annual electricity production by the annual electricity consumption.

Even though the SOEC system has the greatest methanol production rate of circa 170,400 t/a, the costs for the production are significantly higher than the production with the alkaline electrolyzer. Methanol production rates of the 190 MW alkaline system were determined as around 158,200 t/a and for the 200 MW alkaline system a value of 166,400 t/a can be stated. In comparison to the conventional methanol price of 327 EUR/t, this leads to a green methanol price factor of 4.5-4.7 for the alkaline systems and 6.1-7.6 for the SOEC system.

The total annualized costs can be declared as 235-246 Mio. EUR/a for the downsized alkaline system, 247-258 Mio. EUR/a for the upsized alkaline system and 337-423 Mio. EUR/a for the SOEC system. Looking at the OPEX and total annualized CAPEX of each system, it is essential to show the shares of both costs on the TAC. For the alkaline systems around 10-14 % of the TACs are made up of annualized investment costs. This value is immensely higher for the SOEC system, namely 41-53 % depending on whether the upper or lower electrolyzer investment costs are considered. This means that the distribution between annualized CAPEX and OPEX of the SOEC system is split up around half-half whereas 86-90 % of the TAC for the alkaline systems are running costs.

A summary of the single costs, OPEX as well as CAPEX and total costs, is given in Table 9.

Table 9: Economic results of technical design after oxygen demand.

		Sunfire – Hylink Alkaline (Down-sized system)	Sunfire – Hylink Alka-line (Up-sized sys-tem)	Sunfire – Hylink SOEC
Annualized OPEX				
$PPU - Electricity\ generation$	$[GWh/a]$	135.3	135.3	135.3
$MPU - Electricity\ consumption$	$[GWh/a]$	1697	1786	1829
$WEU - Electricity\ consumption$	$[GWh/a]$	1657	1744	1376
$ASU - Electricity\ consumption$	$[GWh/a]$	1.651	0	0
$CO_2PU - Electricity\ consumption$	$[GWh/a]$	9.259	9.807	9.978
$Electricity\ purchase$	$[GWh/a]$	3229	3404	3080
$Electricity\ overproduction$	$[GWh/a]$	0	0	0
$Electricity\ costs$	$[Mio.EUR/a]$	210.2	221.6	200.5
$Electricity\ sellings$	$[Mio.EUR/a]$	0	0	0
$Demineralized\ water\ costs\ for\ WEU$	$[Mio.EUR/a]$	0.0015	0.0016	-
$Steam\ costs\ for\ WEU$	$[Mio.EUR/a]$	-	-	0
$Total$	$[Mio.EUR/a]$	210.2	221.6	200.5
Annualized CAPEX				
MPU	$[Mio.EUR/a]$	2.72	2.81	2.85
WEU	$[Mio.EUR/a]$	17.0-27.6	17.9-29.0	129-215
ASU	$[Mio.EUR/a]$	0.21	0	0
CO_2PU	$[Mio.EUR/a]$	0.45	0.46	0.47
$Oxyfuel\ retrofit$	$[Mio.EUR/a]$	4.40	4.40	4.40
$Total$	$[Mio.EUR/a]$	24.7-35.4	25.5-36.7	137-223
$Total\ annualized\ costs$	$[Mio.EUR/a]$	235-246	247-258	337-423
$Yearly\ methanol\ production\ rate$	$[t/a]$	158150	166420	170440
$Break - even\ price\ green\ methanol$	$[EUR/t]$	1486-1553	1485-1552	1979-2483
$Green\ methanol\ factor$	$[-]$	4.5-4.7	4.5-4-7	6.1-7.6

For an enhanced visualization of the costs, the shares of capital expenditures are shown for the 190 MW electrolyzer choice in Figure 18 and for the 158 MW SOEC electrolyzer system in Figure 19. Important to mention is that the total annual CAPEX in Figure 18 is 24.7 Mio. EUR whereas the SOEC system has total annual investment costs of 136.7 Mio. EUR. Furthermore for both cases, the minimal electrolyzer investment costs were used which is 800 EUR/kW_{el} for the alkaline electrolyzer and 3000 EUR/ kW_{el} for the SOEC. The plots show that the electrolyzer investment costs make up the biggest part of the total annualized investment costs with a share of 69 % for the alkaline system and even 94 % for the SOEC system respectively. The second biggest part in both systems build the oxyfuel retrofit with a share of 18 % for the alkaline and just 3 % for the SOEC design followed by the methanol production unit with a share of 11 % and 2 % respectively. The remaining 3 % for the alkaline system form the CO_2PU and the ASU whereas those values together approach zero in the SOEC system. If the upper electrolyzer investment costs of 1300 EUR/kW_{el} for alkaline and 5000 EUR/kW_{el} for SOEC is used, the share of electrolyzer CAPEX is even increasing.

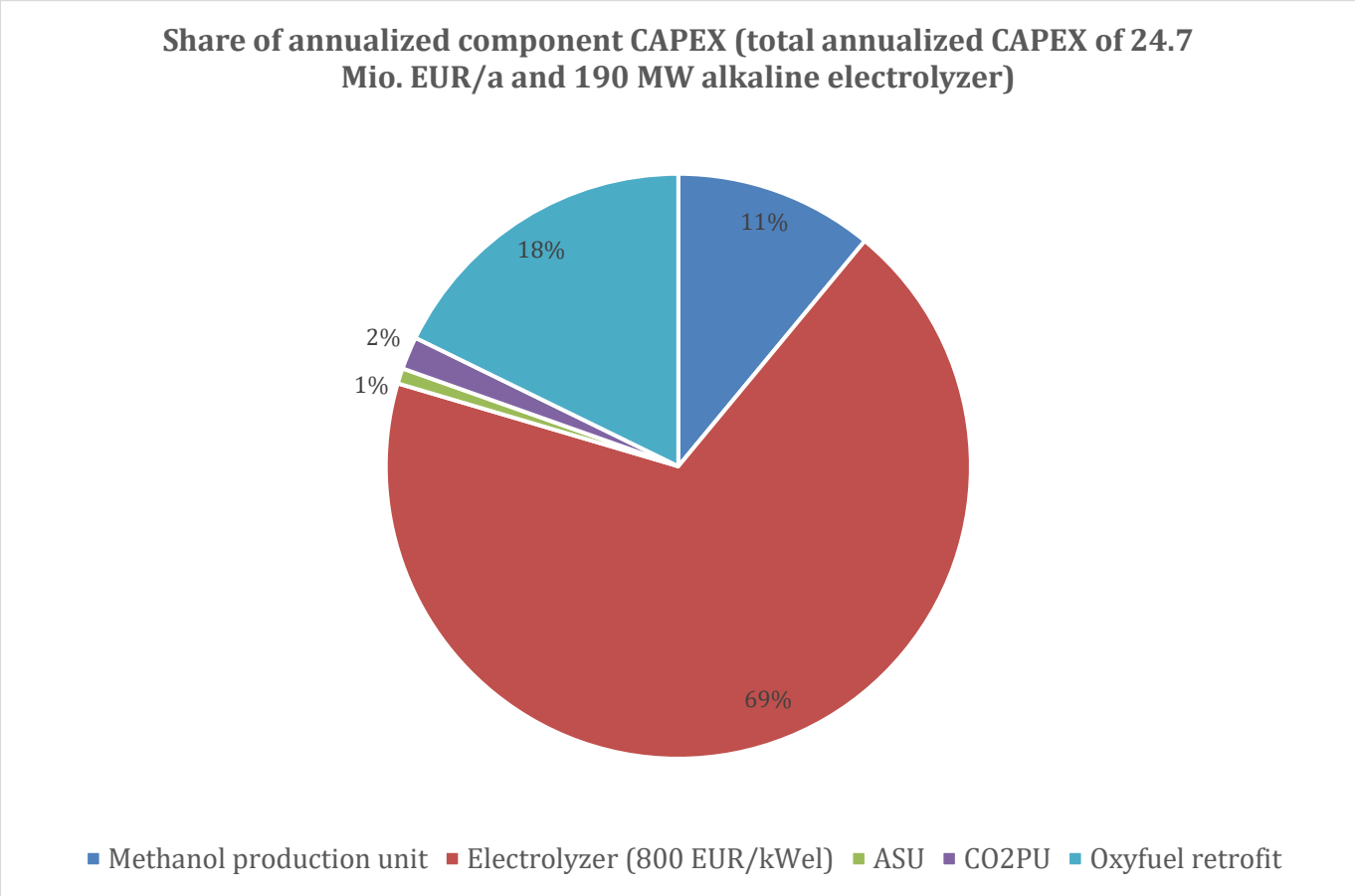


Figure 18: Share of annualized CAPEX of different components. The total annual investment costs are 24.7 Mio. EUR/a with the usage of the 190 MW alkaline electrolyzer. Further, an electrolyzer price of 800 EUR/kW_{el} was taken.

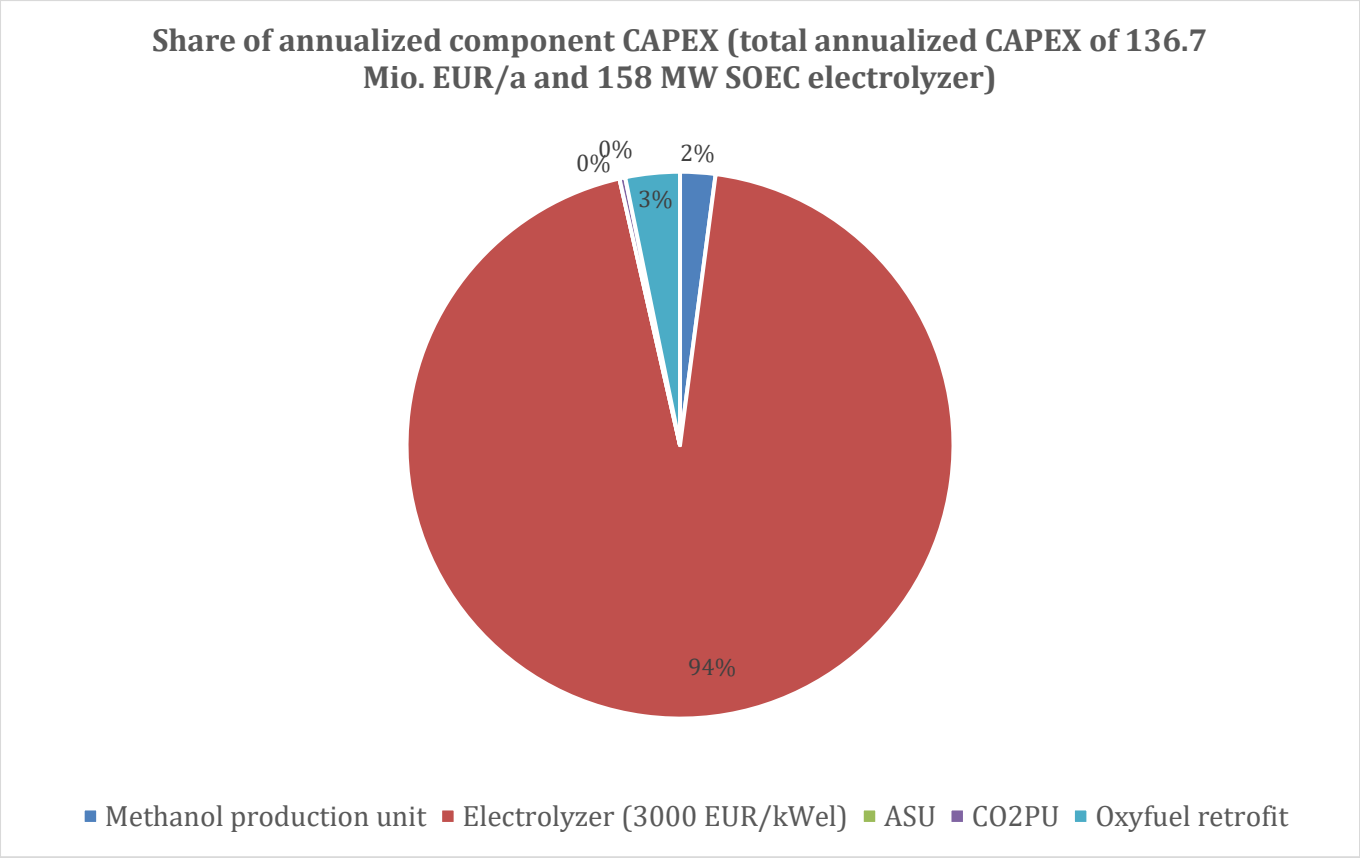


Figure 19: Share of annualized CAPEX of different components. The total annual investment costs are 136.7 Mio. EUR/a with the usage of the 158 MW SOEC electrolyzer. Further, an electrolyzer price of 3000 EUR/kWel was taken.

As previously mentioned, two of the main economic relevant parameters which were examined in this study are the green methanol break-even prices and the green methanol price factor for the different choice of electrolyzers in the whole system. More in detail, the break-even price describes the turning point of the system where the revenues are zero and the expenditures equals the income. In other words, the break-even price is the lowest price the system operator can sell the green methanol without generating profit. Due to the fact that the electrolyzer capital costs vary a lot depending on the source and manufacturer, the lower limit and upper limit of electrolyzer CAPEX was taken into account for calculating the above stated parameters which resulted in price spans. Figure 20 illustrates the green methanol break-even price spans for the 190 MW alkaline, the 200 MW alkaline and 158 MW SOEC system whereas Figure 21 shows the price factor for green methanol production referenced to a conventional synthesis price of 327 EUR/t. In the plots, it can be detected that the two alkaline system have lower BEP (1485-1553 EUR/t) than the SOEC system (1979-2483 EUR/t). The same pattern is also visible in the price factor of green methanol where the methanol production with use of the alkaline electrolyzers is around 4.5-4.7 times more expensive than the conventional production. Is the methanol production based on hydrogen from a SOEC electrolyzer, the price is even 6.1-7.6 times bigger than the conventional one.

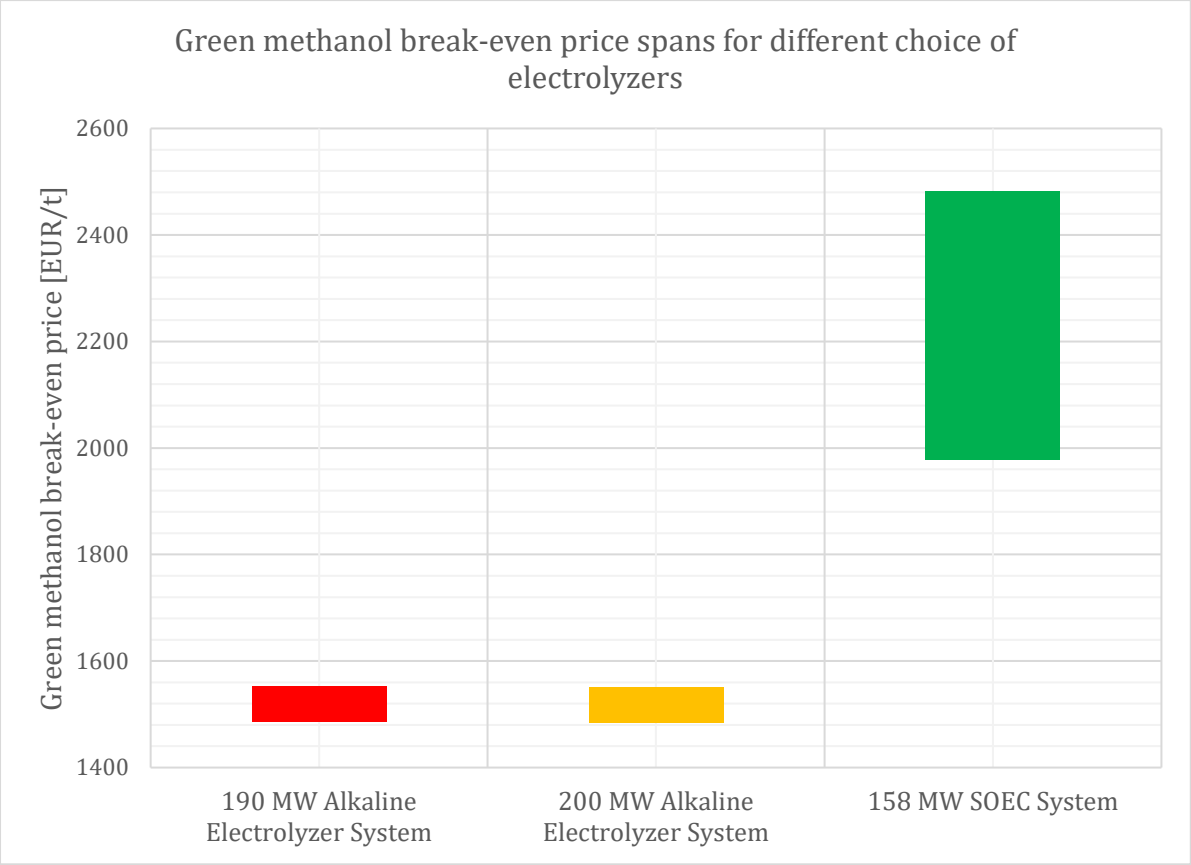


Figure 20: Break-even price of green methanol depending on the electrolyzer choice.

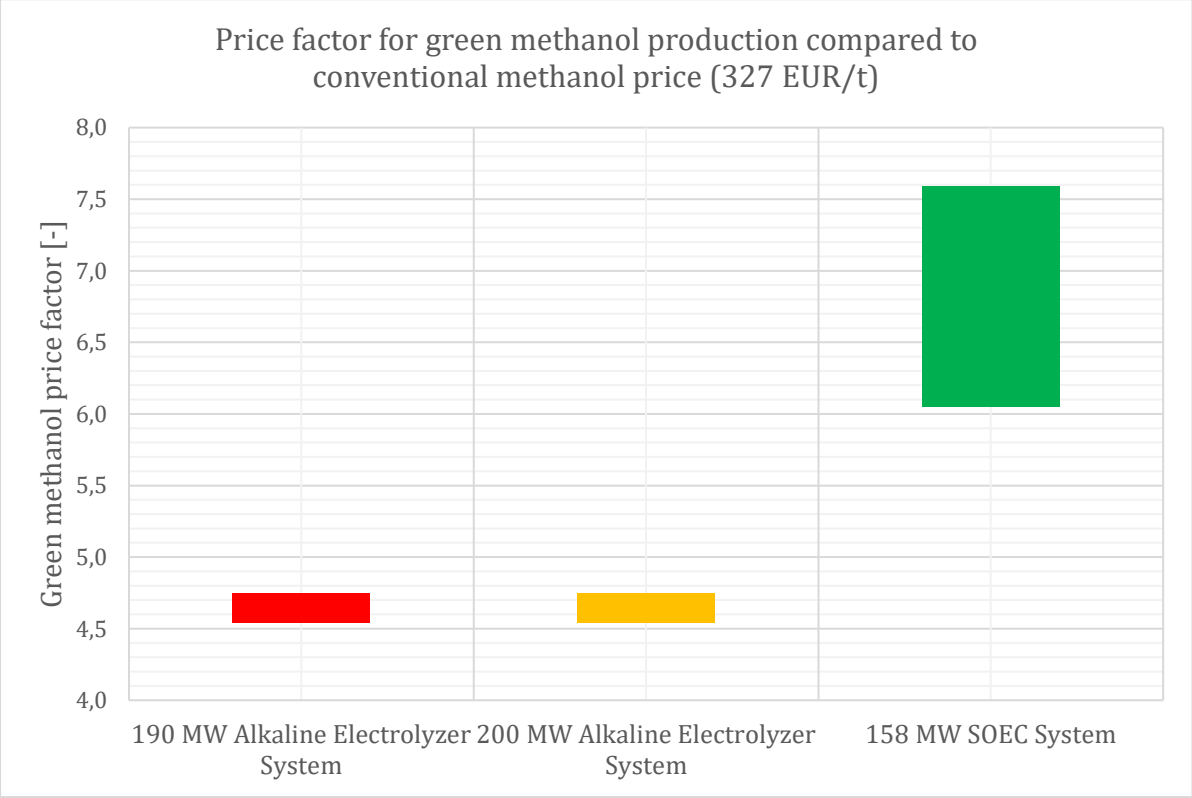


Figure 21: Green methanol price factor referenced to a price of 327 EUR/t for conventional methanol production.

7. Sensitivity analysis

Keeping the previous model as the base of our project, three additional cases are modelled to serve different purposes. Doing this also helps understand the strength of certain variables and determines the robustness of our model. The first case is an ecological design to minimize the CO_2 emissions. This model is designed to provide a pathway to carbon neutrality. The second case is an economical model to reduce overall system cost. The third and last analysis will consider fuel costs, heating revenues as well as CO_2 taxation according to the EU Emissions Trading System (ETS).

7.1 Ecological design to achieve CO_2 neutrality

Unlike the base model, where the electrolyzer is dimensioned to fulfill the oxygen requirement in the oxyfuel combustion, this model's electrolyzer is dimensioned to produce hydrogen in order to utilize all the CO_2 in the flue gas stream and produce methanol. In the base case, there is excess CO_2 which is emitted to match the H_2 produced from the electrolyzer. Whereas, in this model there is excess O_2, because large quantities of H_2 is required to convert all the CO_2 into methanol. To do this the order of quantifying the inputs and outputs changes from the base case.

In this case, the inputs and outputs of the oxyfuel combustion remain the same as the base case. The amount of CO_2 after the CO2PU is taken as the input to the methanol production unit which is 36t/h. Based on this, the amount of H_2 required in the CO2PU and the stoichiometric amount of H_2 required to use all the CO_2 to produce CH_3OH is calculated to be 277kg/h and 4954kg/h. Therefore, the total amount of H_2 needed, which is 5231kg/h of H_2 is set as the parameter to decide the size of the electrolyzer needed. The Y factor in this case will be 1.00, since all the CO_2 and the required amount of H_2 is used for the methanol production. The technical and economic results of this case are shown in Table 10 and Table 11 respectively.

Table 10: Results of technical design to achieve CO_2 neutrality (Case 2).

$\boldsymbol{Methanol\ Production}$		
$\dot{m}_{FG,Me,CO_2}$	$[t_{CO_2}/h]$	36.046
$\dot{m}_{FG,CO_2,reactor,i}$	$[t_{CO_2}/h]$	36.038
$\dot{m}_{H_2,reactor,i}$	$[t_{H_2}/h]$	4.95
$\dot{m}_{CO_2,used}$	$[t_{CO_2}/h]$	35.35
$\dot{m}_{H_2,used}$	$[t_{H_2}/h]$	4.86
$\dot{m}_{Methanol,i}$	$[t_{CH_3OH}/h]$	25.87
$\dot{m}_{Water,i}$	$[t_{H_2O}/h]$	14.47
$\dot{m}_{FG,CO_2,emitted}$	$[t_{CO_2}/h]$	0.0084
$CO_2\ utilization\ rate$	[%]	98.09
γ	$[-]$	1

$\boldsymbol{Electrolysis}$		Sunfire – Hylink Alkaline (Downsized system)	Sunfire – Hylink Alkaline (Upsized system)	Sunfire – Hylink SOEC
$\boldsymbol{P_{El}}$	$[\boldsymbol{MW}]$	270	280	212
$\boldsymbol{N_{El}}$	$[-]$	27	28	-
$\boldsymbol{\dot{m}_{H_2,Methanol}}$	$[\boldsymbol{t_{H_2}/h}]$	4.95	4.95	4.95
$\boldsymbol{\dot{m}_{H_2,DeOxo}}$	$[\boldsymbol{t_{H_2}/h}]$	0.27	0.27	0.27
$\boldsymbol{\dot{m}_{H_2,total}}$	$[\boldsymbol{t_{H_2}/h}]$	5.28	5.29	5.29
$\boldsymbol{\dot{m}_{O_2,oxyfuel}}$	$[\boldsymbol{t_{O_2}/h}]$	29.6	29.6	29.6
$\boldsymbol{\dot{m}_{O_2,El}}$	$[\boldsymbol{t_{O_2}/h}]$	41.87	42	41.5
$\boldsymbol{\dot{m}_{O_2,excess}}$	$[\boldsymbol{t_{O_2}/h}]$	12.27	12.4	11.9
$\boldsymbol{\dot{m}_{ASU,O_2}}$	$[\boldsymbol{t_{O_2}/h}]$	-	-	-
$\boldsymbol{\dot{m}_{El,H_2O}}$	$[\boldsymbol{t_{H_2O}/h}]$	49.95	50.14	-
$\boldsymbol{\dot{m}_{El,steam}}$	$[\boldsymbol{t/h}]$	-	-	67.75

Table 11: Economic results of technical design to achieve CO_2 neutrality (Case 2).

		Sunfire – Hylink Alkaline (Downsized system)	Sunfire – Hylink Alkaline (Upsized system)	Sunfire – Hylink SOEC
$\boldsymbol{Annualized\ OPEX}$				
$\boldsymbol{PPU - Electricity\ generation}$	$[\boldsymbol{GWh/a}]$	135.3	135.3	135.3
$\boldsymbol{MPU - Electricity\ consumption}$	$[\boldsymbol{GWh/a}]$	2427	2427	2427
$\boldsymbol{WEU - Electricity\ consumption}$	$[\boldsymbol{GWh/a}]$	2390	2399	1850
$\boldsymbol{ASU - Electricity\ consumption}$	$[\boldsymbol{GWh/a}]$	1.651	0	0
$\boldsymbol{CO_2PU - Electricity\ consumption}$	$[\boldsymbol{GWh/a}]$	9.2	13.25	13.25
$\boldsymbol{Electricity\ purchase}$	$[\boldsymbol{GWh/a}]$	3074	4704	4155
$\boldsymbol{Electricity\ overproduction}$	$[\boldsymbol{GWh/a}]$	0	0	0
$\boldsymbol{Electricity\ costs}$	$[\boldsymbol{Mio.EUR/a}]$	199.7	306	270
$\boldsymbol{Electricity\ sellings}$	$[\boldsymbol{Mio.EUR/a}]$	0	0	0

$\boldsymbol{Demineralized\ water\ costs\ for\ WEU}$	$[\boldsymbol{Mio.EUR/a}]$	0.0022	0.0022	-
$\boldsymbol{Steam\ costs\ for\ WEU}$	$[\boldsymbol{Mio.EUR/a}]$	-	-	0
$\boldsymbol{Total}$	$[\boldsymbol{Mio.EUR/a}]$	305.4	306	270
$\boldsymbol{Annualized\ CAPEX}$				
$\boldsymbol{MPU}$	$[\boldsymbol{Mio.EUR/a}]$	3.37	3.37	3.37
$\boldsymbol{WEU}$	$[\boldsymbol{Mio.EUR/a}]$	24.49-39.79	24.58-39.94	129-215
$\boldsymbol{ASU}$	$[\boldsymbol{Mio.EUR/a}]$	0	0	0
$\boldsymbol{CO_2PU}$	$[\boldsymbol{Mio.EUR/a}]$	0.6	0.6	0.6
$\boldsymbol{Oxyfuel\ retrofit}$	$[\boldsymbol{Mio.EUR/a}]$	4.40	4.40	4.40
$\boldsymbol{Total}$	$[\boldsymbol{Mio.EUR/a}]$	32.8-48.1	32.9-48.3	181.7-297.3
$\boldsymbol{Total\ annualized\ costs}$	$[\boldsymbol{Mio.EUR/a}]$	338-354	339-354	337-423
$\boldsymbol{Yearly\ methanol\ production\ rate}$	$[\boldsymbol{t/a}]$	226201	226201	226201
$\boldsymbol{Break-even\ price\ green\ methanol}$	$[\boldsymbol{EUR/t}]$	1495-1563	1498-1556	1998-2509
$\boldsymbol{Green\ methanol\ factor}$	$[-]$	4.6-4.8	4.6-4.8	6.1-7.7

Since the electrolyzer is dimensioned after finding out the hydrogen requirement in the entire system, all the units except for the electrolyzer have only one system. This can be seen in Table 10 and the repeated values in Table 11 for the three electrolyzer systems. The CO_2 utilization rate of the system comes up to 98.09%. The methanol production in this case has increased significantly compared to the base case which explains the high total annualized costs in Table 11. The OPEX and CAPEX per unit in this case follows the same pattern as the base case with MPU having highest electricity demand, hence increasing OPEX and the electrolyzers responsible for the high CAPEX. There is no significant difference in the overall costs between the alkaline electrolyzer systems and the SOEC system (especially the lower limit values), unlike the base case where the difference is huge. Due to proportional increase of methanol production with the total expenses, the BEP and green methanol factor hardly changes when compared to the base case.

7.2 Economical design to improve the profitability

In this case of sensitivity analysis, a hypothesis is written and later analyzed: 'Saving on electricity costs results in a significant deduction of overall costs, hence producing a comparatively more profitable model '.

To validate the hypothesis, the CHP load profile is altered. The CHP in this case produces the maximum electrical output which is 35 MW. Unlike the base case where high-quality, high-pressure steam was produced to fulfil demand from an industry, in this case the heat produced is of lower quality and low pressure to fulfil district heating demand. In the base case required steam for industry demand is separated from the overall steam from boiler, hence the electricity is produced

with the resulting steam. In this case, all the steam produced in the boiler goes through the turbine which results in maximum electricity production and then the required amount of steam is extracted for heating purposes.

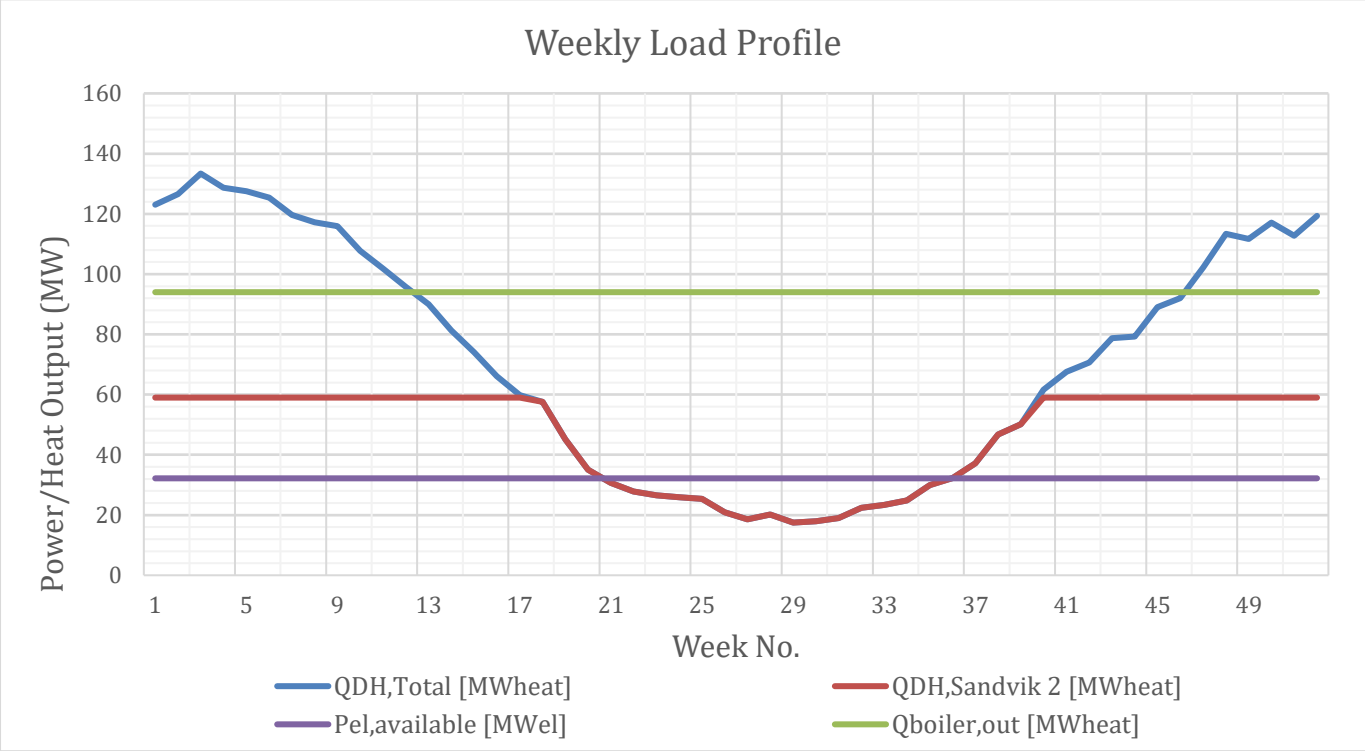


Figure 22: Weekly heat and power output from Sandvik 2 out of data provided by Växjö Energi AB. (Case 3)

The technical results for the Oxyfuel combustion, CO_2PU, WEU and the MPU remain the same as the base case, because the amount of flue gas leaving the power production unit remains the same. But in the economic results, the OPEX and hence the overall costs decrease when compared to the base case. So has the BEP and the green methanol factor. The economic result for this case is displayed in Table 12.

Table 12: Economic results of technical design to improve profitability. (Case 3)

		Sunfire – Hylink Alkaline (Downsized system)	**Sunfire – Hylink Alkaline (Upsized system)**	**Sunfire – Hylink SOEC**
Annualized OPEX				
$\boldsymbol{PPU - Electricity\ generation}$	$[GWh/a]$	280.67	280.67	280.67
$\boldsymbol{MPU - Electricity\ consumption}$	$[GWh/a]$	1697	1786	1829
$\boldsymbol{WEU - Electricity\ consumption}$	$[GWh/a]$	1657	1744	1376
$\boldsymbol{ASU - Electricity\ consumption}$	$[GWh/a]$	1.651	0	0

$CO_2PU - Electricity\ consumption$	$[GWh/a]$	9.259	9.807	9.977
$Electricity\ purchase$	$[GWh/a]$	3084	3259	2935
$Electricity\ overproduction$	$[GWh/a]$	0	0	0
$Electricity\ costs$	$[Mio.EUR/a]$	200.3	211.7	190.6
$Electricity\ sellings$	$[Mio.EUR/a]$	0	0	0
$Demineralized\ water\ costs\ for\ WEU$	$[Mio.EUR/a]$	0.0015	0.0016	-
$Steam\ costs\ for\ WEU$	$[Mio.EUR/a]$	-	-	0
$Total$	$[Mio.EUR/a]$	200.3	211.7	190.6
$Annualized\ CAPEX$				
MPU	$[Mio.EUR/a]$	2.72	2.81	2.85
WEU	$[Mio.EUR/a]$	17-27.6	17.9-29.0	129-215
ASU	$[Mio.EUR/a]$	0.21	0	0
CO_2PU	$[Mio.EUR/a]$	0.45	0.46	0.47
$Oxyfuel\ retrofit$	$[Mio.EUR/a]$	4.40	4.40	4.40
$Total$	$[Mio.EUR/a]$	25-35	26-37	137-223
$Total\ annualized\ costs$	$[Mio.EUR/a]$	225-236	237-248	327-413
$Yearly\ methanol\ production\ rate$	$[t/a]$	158154	166419	170441
$Break-even\ price\ green\ methanol$	$[EUR/t]$	1423-1490	1425-1492	1920-2425
$Green\ methanol\ factor$	$[-]$	4.4-4.6	4.4-4-6	5.9-7.4

7.3 Addition of fuel costs, heating revenues and EU CO_2 tax

In the last and final sensitivity analysis, the fuel costs, heating revenues as well as CO_2 taxation by the EU ETS (EU Emissions Trading System) was added to the cost calculation of the base case with following the oxygen demand of the oxyfuel combustion. Within that, the technical results remain the same as in Table 8. In the economical point of view, following additions can be detected as summed up in Table 13. According to [73], the prices for wooden fuel such as sawdust, pellets, etc vary a lot throughout the location in Europe or Sweden. To keep it simple, a nominal fuel price of 150 SEK/MWh fuel input was considered which is around 13.2 EUR/MWh (actual currency factor of 0.088 EUR/SEK was used). As a result, the fuel costs for the CHP plant could be determined as 11.8 Mio. EUR. Hence, a district heating selling price of 85.7 öre/kWh (75.4 EUR/MWh) was found on the web-site of Växjö Energi AB [74]. Keep in mind that this is just the energy price per sold kWh of heating.

The total revenues are way higher because the heating contract between the plant operator and the demanding facility contains a monthly fixed price too. This means that the green methanol BEP and the price factor for green methanol in this case is overestimated and can be dropped if the fixed price for the district heating is taken into account in real life. Furthermore, a CO_2 tax of 70 EUR/t_{CO2} was assumed based on data from [75]. In addition, governmental subsidies were considered as well. Herefore, the same number of subsidies as the FlagshipOne project received was assumed which is namely 151 Mio. SEK (around 13.3 Mio. EUR) provided by Klimaklivet [76]. Annualizing this value with a lifetime of 20 years leads to a subsidy of 1.07 Mio. EUR/a. After all of the changes are done in the Excel, the updated costs can be found in Table 13.

If all the costs and revenues listed are taken into account, it can be seen that the green methanol BEP and the green methanol price factor have been significantly reduced. For example, the price using an alkaline electrolyzer is now between 1306 and 1373 EUR/t and using the 158 MW SOEC electrolyzer between 1800 and 2304 EUR/t. This has also led to a reduction in the price factor to values of 4.0-4.2 for the alkaline solutions and 5.5-7.0 for the SOEC variant.

Table 13: Updated costs of each system including fuel costs, CO_2 taxation, heating revenues and governmental subsidies.

		Sunfire – Hylink Alkaline (Downsized system)	**Sunfire – Hylink Alkaline (Upsized system)**	**Sunfire – Hylink SOEC**
Annualized OPEX				
Value without additional costs	$[Mio.EUR/a]$	210.2	221.6	200.5
Avoided CO_2 emissions costs	$[Mio.EUR/a]$	15.1	15.9	16.3
CO_2 emissions costs	$[Mio.EUR/a]$	6.91	6.12	5.7
Fuel costs	$[Mio.EUR/a]$	11.8	11.8	11.8
District heating revenues	$[Mio.EUR/a]$	30.7	30.7	30.7
Total	$[Mio.EUR/a]$	183.1	192.9	171.1
Annualized CAPEX				
Value without additional costs	$[Mio.EUR/a]$	24.7-35.4	25.5-36.7	137-223
Annualized subsidies	$[Mio.EUR/a]$	1.1	1.1	1.1
Total	$[Mio.EUR/a]$	23.6-34.3	24.4-35.6	136-222
Total annualized costs	$[Mio.EUR/a]$	207-217	217-229	307-393
Yearly methanol production rate	$[t/a]$	158154	166419	170441
Break − even price green methanol	$[EUR/t]$	1308-1375	1306-1373	1800-2304

$\boldsymbol{Green\ methanol\ factor}$	[−]	4.0-4.2	4.0-4.2	5.5-7.0

8. Discussion

The analysis and discussion of the presented result is a crucial point of understanding relationships and dependencies of singe parameters. In order to make a comprehensive statement about this, it is necessary to revisit the purpose of this master's thesis. The aim of this thesis was to investigate the techno-economic feasibility of the application of oxyfuel combustion and subsequent green methanol synthesis. Some papers and scientific journals already dealt with similar topics of oxyfuel combustion and corresponding carbon capture, but the system design including an electrolyzer and the conversion of CO_2 into a power-to-X fuel was newly designed in this thesis.
As can be seen from the results, the system design can vary depending on the objective being pursued. Defined goals can be either the design according to the oxygen demand, the maximum achievable reduction of carbon dioxide emissions or an economic optimization. The results vary slightly from use case to use case. Nevertheless, the main conclusions that can be drawn are as follows.

With the implementation of oxyfuel combustion, the flue gas stream can be transferred into methanol easily with the help of commercially available flue gas treatment systems. This means that a retrofit from conventional combustion to oxyfuel combustion can be achieved simply with the use of already installed technical applications which makes the switch cost effective. If the required oxygen is provided by means of electrolysis, the selection of a suitable electrolyzer is crucial. Three different methods were introduced in this work, two systems based on alkaline electrolysis and one system based on solid oxide electrolysis. The following points can be noted:

- Oxyfuel combustion and power-to-methanol represents an adequate solution to reduce the carbon footprint compared to conventional pre- or post-combustion carbon capture and storage technologies especially if the CO_2 rich flue gas is turned into high value carbon containing fuels such as methanol. A very big advantage of the presented system setup is that the electrolysis splits up water to supply oxygen for the oxyfuel combustion and simultaneously hydrogen for the methanol synthesis. This benefit differs from previous studies on oxyfuel combustion where mostly the high oxygen demand was fulfilled by running an energy intensive air separation unit.

- As a result of the analysis, a green methanol price factor for the best solution (upsized alkaline electrolyzer system) is in a range of 4-5 compared to the current conventional methanol price, for the worst option a factor of 6-8 (SOEC system) was determined. Those values seem significantly larger than the conventional one, but one has to keep in mind that the conventional methanol price will most likely increase as the synthesis is based on steam reforming of natural gas. On the other side, a reversed trend in the investment costs of electrolyzers (which is a main cost factor) is remarkable which means that electrolysis CAPEX will decrease and resulting in the break-even price for green methanol will decrease as well. An explicit rate of the cost decrease of electrolyzers is hard to state as it is strongly dependant on location, demand and scaling. Another advantage of the methanol synthesis with help of electrolysis is that the methanol production price can be decoupled from the natural gas price and scarcity

as Europe experienced as a consequence of the Russian-Ukrainian war. With a production in one's own border (f.e. producing methanol in Sweden with the presented system), political pressure and dependency on rich natural gas states could be avoided.

- The component sizes such as the size of the electrolysis, methanol production unit etc are dependent on the amount of oxygen which is needed for the oxyfuel combustion or the share of captured carbon dioxide from the power plant. In the first use case, a carbon capture ratio of around 70% in all system setups can be achieved (with small advantages of the SOEC).

- The alkaline systems (downsized and upsized) are preferred due to a lower break-even price of green methanol and a corresponding green methanol price factor. Even though the SOEC system has advantages in the running costs and CO_2 capture ratio, the significantly higher investment costs and the lower stack lifetime turns the SOEC system into the most expensive alternative and is not competitive with the alkaline solutions.

- In the investigated system, the downsized and upsized variants do not differ a lot from each other due to the fact that the needed electrolyzer power is in a range of 190 MW to 200 MW. Relatively one electrolyzer module of 10 MW more or less does not have a big impact on the final results. Nonetheless, one should keep in mind that in a smaller system setting this difference can become important.

- Main cost driver for all system setups are the electricity costs for running the electrolysis and the methanol production unit. Because of the small own electricity output of the CHP plant, a huge amount of electricity has to be purchased from the grid which has a big negative influence on the green methanol break-even price. An approach to reduce those costs could be the connection of the system to a renewable energy system with low levelized costs of energy such as a wind or solar park. This approach is already suited by exemplary the FlagshipOne project with the electricity provided by a nearby windfarm or the Kassø project in Denmark with a connection to a 304 MW solar park. Another solution for reducing the running costs could be to change the load profile of the power plant. In our case, the cogeneration plant Sandviksverket in Växjö must provide heat at all times. The system setting as we presented could be beneficial for a sole power production plant to increase the amount of own used electricity.

- A nearly 100% carbon-free operation of the cogeneration plant can be achieved when aiming for that goal. The disadvantage in this case is that the electrolyzer has to be designed even bigger than in the base case which results in slightly higher break-even prices for green methanol. Further, the electrolysis has now an excess production of oxygen which is no usage for it.

- Introducing carbon emission penalties such as carbon taxes can enhance the profitability of the system enormously. In this study, a CO_2 tax of 70 EUR/t was taken into account in the last sensitivity analysis which is based on current levels. If this price even increases in the future it will have a positive effect on the green methanol break-even price presented in this study as the cost savings for emitting less carbon dioxide raises.

- If the calculated break-even prices are compared to other sources, it can be seen that for instance, a methanol price of 823 EUR/t for the alkaline system and 605 EUR/t for the SOEC system was calculated in accordance with [29]. Those costs are around 2-4 times lower than the results presented in this work. The difference between the results in the literature and our results could be the deviation in cost assumptions and which costs are considered in detail, including the variance in the system setup and load profiles. Nonetheless, the results are in the same order of magnitude and therefore can be seen as valid.

Overall, it can be said that this work contains many technical and economic aspects and provides a solid basis for future research. As is so often the case, some limitations had to be made in this work in order not to go beyond the scope of the research work and to simplify connections in some areas. Limitations and restrictions are, for example, the consideration of a constant boiler output or the limited number of implemented electrolyzer types and manufacturers. The linear extrapolation of results and values from other journals also offers scope for interpretation and should be considered in a more detailed analysis. In addition, all calculations were performed in Microsoft Excel. More precise analyses and the behavior of various chemical reactions, volume gas flows, etc. were therefore difficult to depict. It would be advantageous to transfer these systems to a chemical process simulator such as Aspen Plus or Aspen HYSIS.

9. Conclusion

This master's thesis demonstrates the feasibility and profitability of integrating oxyfuel combustion technology into a Bioenergy Combined Heat and Power plant (BioCHP), complemented by Power-to-Methanol technology. Conducted for Norconsult and using real-life data from Växjö Energi, the study confirms the system's capability to significantly reduce CO_2 emissions and efficiently produce e-methanol.

Key findings include:

- The integrated system can produce 0.15-0.16 or 0.17 megatons of e-methanol annually, depending on whether an alkaline or an SOEC electrolyser is used. It also meets the majority of the municipality's heating demand of 407 GWh annually. The total annual costs range from 235-258 million Euros for the alkaline variant and 337-423 million Euros for the SOEC variant. These costs can be recovered by selling the e-methanol at 1486-1553 EUR/ton for the alkaline variant and 1979-2483 EUR/ton for the SOEC variant (break-even pricing), which are 4.5-4.7 and 6.1-7.6 times the average methanol price for the respective variants. The system utilizes 68.6-72.2% of CO_2 with the alkaline variant and 73.9% with the SOEC variant, which would otherwise be emitted.

- The system can be further upgraded to utilize 98.09% of CO_2 emissions to produce 0.22 megatons of methanol annually while fulfilling the same heat demand. This upgrade aligns with energy targets. The annual costs for this scenario are 338-354 million Euros for the alkaline variant and 337-423 million Euros for the SOEC variant. The break-even price for methanol is 1495-1550 EUR/ton for the alkaline variant and 1998-2509 EUR/ton for the SOEC variant.

- To lower overall costs, the CHP can maximize electricity production to 281 GWh by delivering lower quality steam. This approach results in reduced overall costs of 225-248 million Euros annually for the alkaline variant and 327-413 million Euros for the SOEC variant, with a break-even price of 1423-1492 Euros/ton for the alkaline and 1920-2425 Euros/ton for the SOEC variant, while utilizing 68.6-72.2% of CO_2 for the alkaline and 73.9% for the SOEC variant from the flue gas to produce 0.15-0.16 megatons with the alkaline and 0.17 megatons with the SOEC variant.

- Considering supportive economic factors such as heating revenues with a DH price of 75.4 EUR/MWh, subsidies estimated at 13.3 million Euros, a CO_2 tax of 70 EUR/MWh, and fuel purchase costs of 11.8 million Euros, the overall costs reduce to 207-229 million Euros for the alkaline variant and 307-393 million Euros for the SOEC variant. The break-even price for methanol drops to 1306-1375 EUR/ton for the alkaline variant and 1800-2304 EUR/ton for the SOEC variant.

The study identifies several technical risks and limitations, including the components' lifespan and the inclusiveness of all costs. These challenges necessitate further research and development to optimize system performance and cost-effectiveness. Additionally, further research is needed on the scope of e-methanol in Sweden, permits and licenses required for oxyfuel combustion, and the area required for the setup.
In conclusion, the findings underscore the potential of the integrated system to contribute to Sweden's transition towards carbon neutrality, providing a viable solution to the global climate crisis. This thesis offers a valuable pathway for integrating advanced carbon capture and synthetic fuel production technologies into existing energy infrastructures, supporting global efforts to combat climate change and transition to a low-carbon economy.

10. References

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11. Appendix

Appendix A

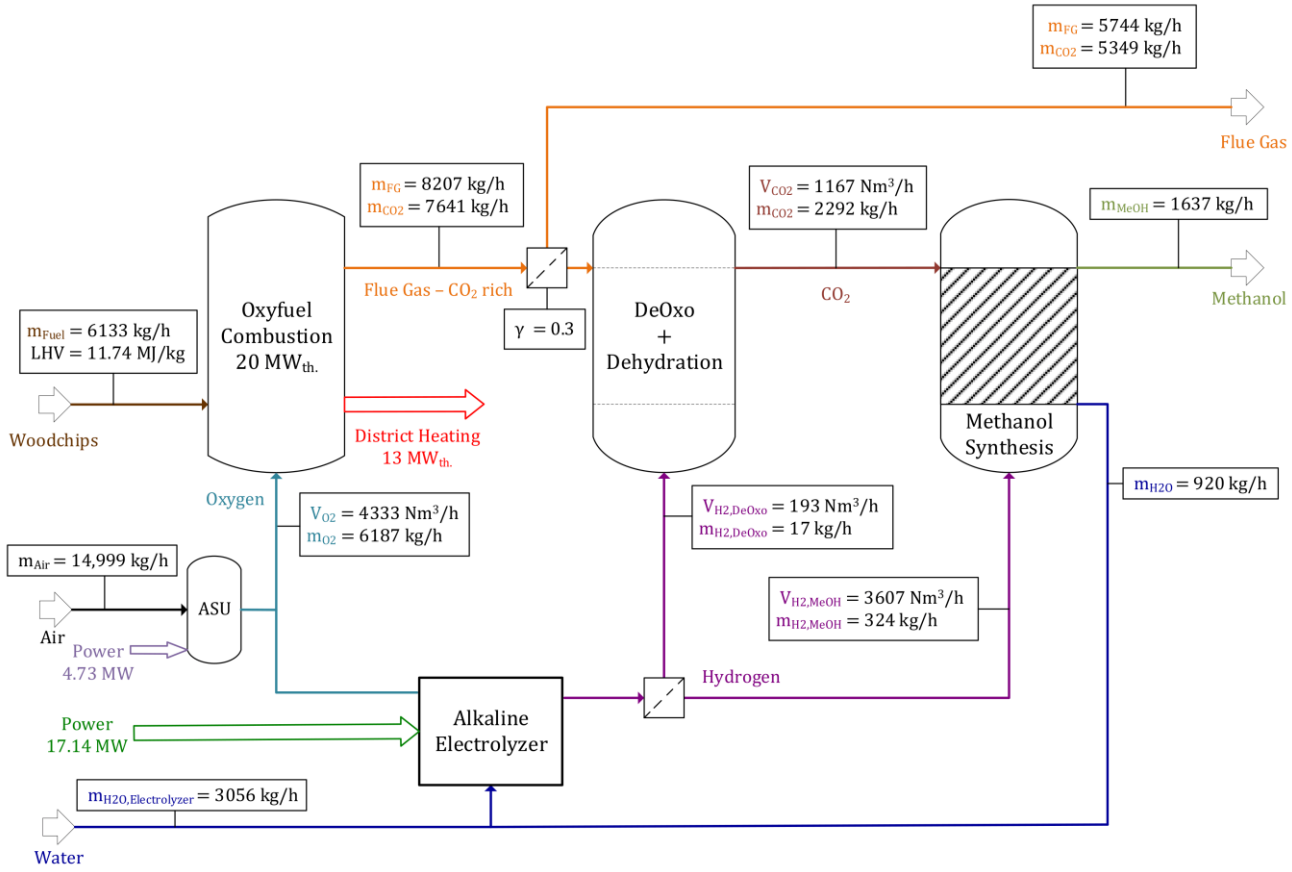

Figure 23: Simplified flow chart of oxyfuel combustion and green methanol production [21]

Appendix B

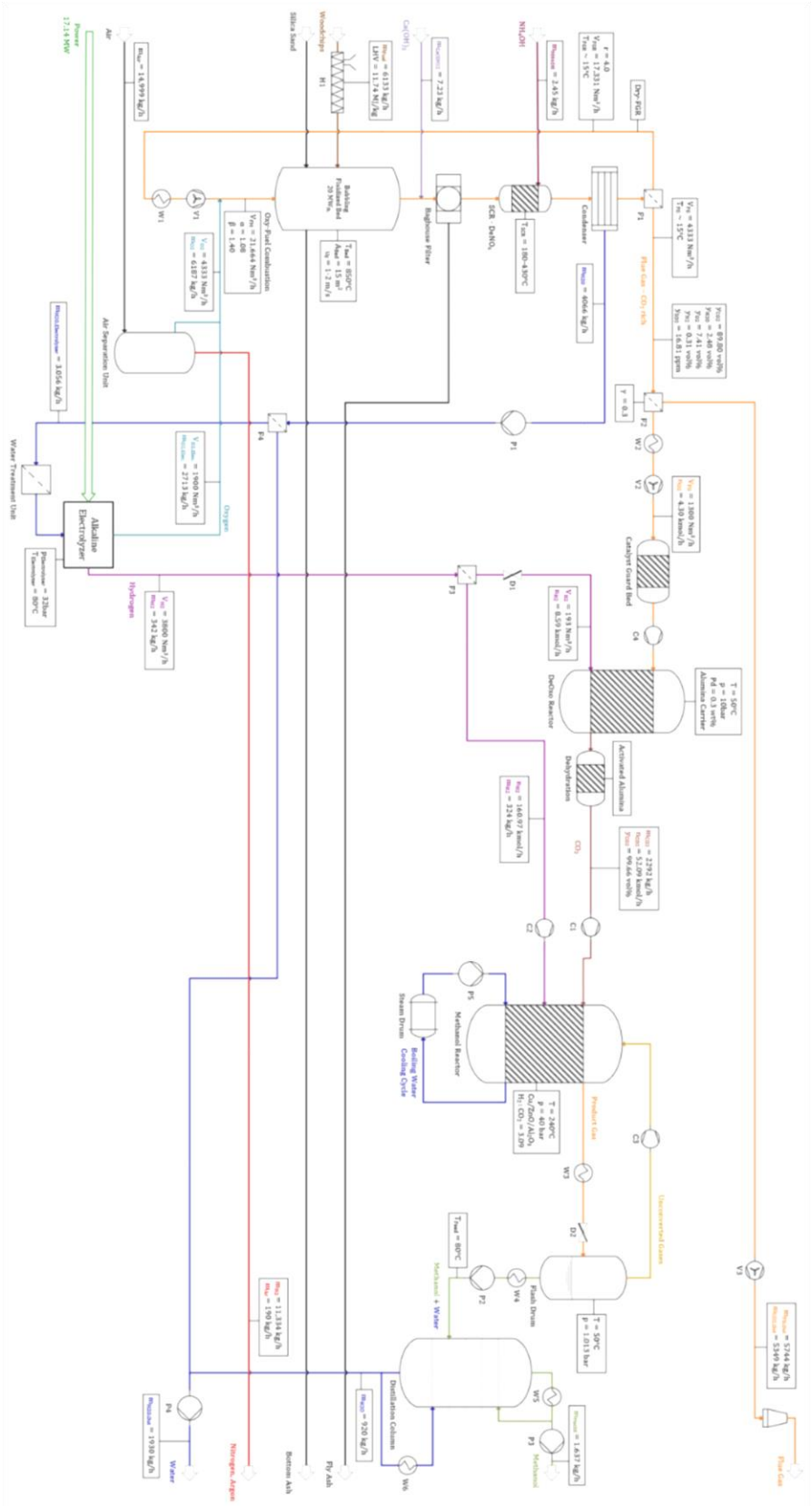

Figure 24: Detailed flow chart of oxyfuel combustion and green methanol production [21]

Appendix C

Table 14: Methanol properties. [77]

	Methanol
Formula	CH_3OH
Molecular weight [g/mol]	32.0
Carbon/Hydrogen/Oxygen [wt-%]	37.5/12.5 /49.9
Methanol purity [wt-%]	>99.7
Water [wt-%]	<0.1
Chlorides as CL ion [ppm]	<0.5
Sulfur [ppm]	<0.5
Density at 15 °C [kg/dm^3]	0.796
Boiling point [°C]	64.6
Freezing point [°C]	-97.6
LHV [MJ/kg]	20.0
LHV [MJ/l]	15.9

Appendix D

Table 15: Main process streams and their composition for the MefCO2 pilot plant producing 1000 kg methanol per day at Niederaussem. [78]

	H_2 (gas)	**CO_2 (gas)**	**Methanol (liq)**
Total molar flow (kmol/h)	4.3	1.5	2.8
Mass flow (kg/h)	10.2	66.1	68.7
Phase	gas	gas	liquid

Within the report, the author describes following process for the methanol unit reactor showed in Figure 25: Scheme of methanol unit reactor at Niederaussem. [78] [78]:

> *In the fresh feedstock compression unit, the mixture of the hydrogen stream from the electrolyzer and the carbon dioxide stream from the CO2 Conditioning unit is compressed to the reaction pressure, up to 80 bar. The streams are mixed with a molar H2:CO2 ratio of around 3:1. The synthesis gas stream is premixed by fresh feedstock and the gaseous recycle stream before it is fed into the methanol reactor […]. This combined stream is preheated, before entering the bottom of the methanol reactor. The methanol reactor is filled with solid catalysts, which enable the reaction of hydrogen and carbon dioxide to methanol and water. As in all chemical processes, not all reactants are converted to methanol and thus there are also unreacted species. The gas from the reactor is cooled, and then the methanol and water are condensed before entering the catchpot, where the unreacted synthesis gas is separated from the condensed liquid. The unreacted synthesis gas is divided into the recycle stream and the purge stream, and the condensed methanol and water (crude methanol). The purge stream is required to prevent an accumulation of inert gases within the loop of the recycling stream [78, p. 27].*

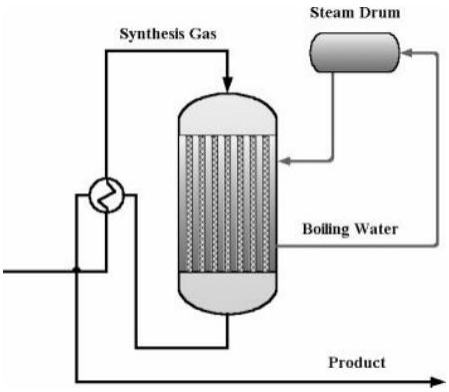

Figure 25: Scheme of methanol unit reactor at Niederaussem. [78]

Appendix E

Table 16: Weekly data for heat and power for base case.

Week no.	$Q_{DH,Total}$ [MW_{th}]	$Q_{DH,Sandvik\ 2}$ [MW_{th}]	P_{out} [MW_{el}]	$Q_{boiler,out}$ [MW_{th}]
1	123,1	59,00	12,76	94,00
2	126,6	59,00	12,76	94,00
3	133,4	59,00	12,76	94,00
4	128,7	59,00	12,76	94,00
5	127,5	59,00	12,76	94,00
6	125,4	59,00	12,76	94,00
7	119,7	59,00	12,76	94,00
8	117,2	59,00	12,76	94,00
9	115,9	59,00	12,76	94,00
10	107,8	59,00	12,76	94,00
11	101,8	59,00	12,76	94,00
12	95,7	59,00	12,76	94,00
13	90	59,00	12,76	94,00
14	81,3	59,00	12,76	94,00
15	74,1	59,00	12,76	94,00
16	66,1	59,00	12,76	94,00
17	59,8	59,00	12,76	94,00
18	57,6	57,60	13,35	94,00
19	45,1	45,10	18,61	94,00
20	35,1	35,10	22,82	94,00
21	30,7	30,70	24,67	94,00
22	27,8	27,80	25,89	94,00
23	26,6	26,60	26,40	94,00
24	25,9	25,90	26,69	94,00
25	25,4	25,40	26,91	94,00
26	20,9	20,90	28,80	94,00
27	18,6	18,60	29,60	94,00
28	20,2	20,20	29,09	94,00
29	17,5	17,50	29,60	94,00
30	17,9	17,90	29,60	94,00
31	19	19,00	29,60	94,00
32	22,4	22,40	28,17	94,00
33	23,4	23,40	27,75	94,00
34	24,8	24,80	27,16	94,00
35	29,9	29,90	25,01	94,00
36	32,3	32,30	24,00	94,00
37	37,2	37,20	21,94	94,00
38	46,7	46,70	17,94	94,00
39	50,1	50,10	16,51	94,00
40	61,6	59,00	12,76	94,00

41	67,6	59,00	12,76	94,00
42	70,7	59,00	12,76	94,00
43	78,7	59,00	12,76	94,00
44	79,3	59,00	12,76	94,00
45	89	59,00	12,76	94,00
46	92	59,00	12,76	94,00
47	102,2	59,00	12,76	94,00
48	113,4	59,00	12,76	94,00
49	111,7	59,00	12,76	94,00
50	117,1	59,00	12,76	94,00
51	112,7	59,00	12,76	94,00
52	119,3	59,00	12,76	94,00

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