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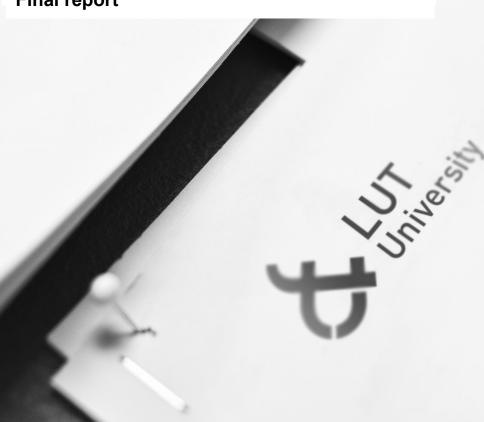
Tutkimusraportit - Research Reports

123

Petteri Laaksonen, Hannu Karjunen, Jenna Ruokonen, Arto Laari, Mariia Zhaurova, Sini-Kaisu Kinnunen, Antti Kosonen, Timo Kärri, Tiina Sinkkonen, Tommi Rissanen, Antero Tervonen, Juha Varis

Feasibility Study for Industrial Pilot of Carbon-Neutral Fuel Production – P2X

Final report











Lappeenranta-Lahti University of Technology LUT LUT School of Energy Systems LUT School of Engineering Science LUT School of Business and Management

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Feasibility Study for Industrial Pilot of Carbon-Neutral Fuel Production – P2X

Final report

Petteri Laaksonen, Hannu Karjunen, Jenna Ruokonen, Arto Laari, Mariia Zhaurova, Sini-Kaisu Kinnunen, Antti Kosonen, Timo Kärri, Tiina Sinkkonen, Tommi Rissanen, Antero Tervonen, Juha Varis

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Foreword

This project is one of the results following research work initiated already in 2014 in Neo Carbon Energy by LUT and VTT, and subsequent multiple LUT research projects and studies in utilization of hydrogen both in CO₂ (methanol) and N₂ (ammonia) routes. In LUT, the huge societal transition, which impacts not only energy production but the whole society, is called transition to *sustainable* energy-economy.

We want to thank all the companies, and especially the individuals in firms with enough foresight, who made this possible. Less than two years ago, when the decision was made, P2X was quite unknown area, and electrification and hydrogen economy subject to interest to only a small group of strategists. Today the results of the project have been to great interest globally.

We would like to express our special thanks to main financing organization, Regional Council of South Karelia, for its visionary finance decision. The project was financed by European Regional Development Fund ¹, LUT University ² as lead partner, and partner firms. The other partners in project were St1, Wärtsilä, Kemira, Finnsementti, Shell, Neste, Finnair, Refinec, Premekon, Jotex works, Terästorni, and City of Lappeenranta.

Project execution took place between 1.1.2020 and 30.4.2021.

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¹ Euroopan aluekehitysrahasto (EAKR) in Finnish

² https://www.lut.fi/web/en/

Executive Summary

Transition towards *sustainable energy-economy* will be led by renewable electricity. Electricity and hydrogen produced out of it are the building blocks of the new system. Sectors and applications which can be easily electrified, such as passenger vehicles and heating, will be electrified. The drivers of electrification in transport and heating/cooling are very low CO₂ emissions, low operational expenses and demand for better air quality especially in large cities. Transition to complete *sustainable energy-economy*, however, requires clear direction and right investments in global scale in coming decades due to size and diffusion speed of the transition.

Electricity will be used wherever it is possible to use. Most obviously the demand of liquid fuels will continue in the coming decades especially in aviation, shipping, and heavy-duty transport. Carbonneutral synthetic fuels will replace fossil fuels simultaneously with electrification of the society. Electric fuels will be used in the transport sector, as well as an energy carrier and storage. Synthetic raw materials, like methanol and ammonia, will also be needed to replace the fossil feedstocks of chemical industries.

The target of the P2X Joutseno project was to make a thorough feasibility study, both technical and economical, for industrial-size pilot of carbon-neutral fuel production through methanol route from excess hydrogen produced in water electrolysis for chlorate production at Kemira³ at Joutseno and captured CO₂ from Finnsementti cement plant at Lappeenranta (**Figure 0.1**).

-

 $^{^3}$ Annual amount of excess hydrogen was estimated to be 5 000 tons. The chemical reaction in the process is NaCl + $3H_2O$ + $6e^- \rightarrow NaClO_3$ + $3H_2$. The total energy consumption for one ton of NaClO $_3$ is in the range of 5–6 MWh

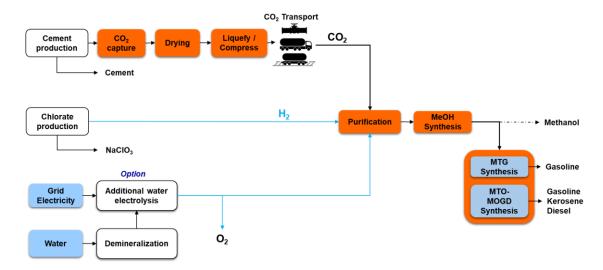


Figure 0.1. Schematic overview of the studied pathways. MTG refers to methanol-gasoline and MTO-MOGD to methanol to olefins, Mobil's olefins to gasolines and distillates.

Project was financed by European Regional Development Fund⁴, LUT University⁵ as lead partner and partner firms. The other partners in project were St1, Wärtsilä, Kemira, Finnsementti, Shell, Neste, Finnair, Refinec, Premekon, Jotex works, Terästorni, and City of Lappeenranta.

Project execution took place between 1.1.2020 and 30.4.2021.

The technical part of the research was made using Aspen Plus modelling of the process elements through methanol route to gasoline, kerosene, and diesel. As an alternative, production of hydrogen by water electrolysis was also studied. The capital expenditures (CAPEX) and operational expenses (OPEX) of the process were evaluated by modelling the process. In order to confirm the results of the economic modelling, both CAPEX and OPEX were also gathered and analyzed from budgetary offers⁶ together with LUT, Wärtsilä and St1.

The economic analysis was based on 20-year discounted cash flow calculation model (**Figure 0.2**), which was used to analyze different scenarios and sensitivities in the scenarios. A base case was set to be a process starting from hydrogen and CO₂ to produce methanol as an intermediate which is then upgraded to gasoline. The base case was selected because all the technology for the

⁴ Euroopan Alueellinen Kehitys Rahasto (EAKR) in Finnish

⁵ https://www.lut.fi/web/en/

⁶ Budgetary offers were received from many major global manufacturers

process is on Technology Readiness Level (TRL) 9, meaning that all the whole process is commercially available.

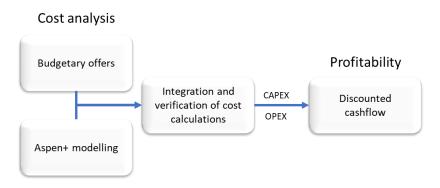


Figure 0.2. Profitability analysis concept.

Main findings of the project were:

- The cost of hydrogen is essential for the economic feasibility. In large scale production it
 means that electricity needed for hydrogen production must be affordable (below 20
 €/MWh).
- The demand for new, green electricity production, will be vast. In order to enable the investments, all hindering factors in regulation and legal framework should be cleared.
- Technology is available for the most part on TRL 9. The conversion process of methanol to gasoline and distillates (i.e. gasoline, kerosene, and diesel in a combined process) requires further development. Regulatory approval of the produced fuels will also need to be considered, especially for aviation.
- Alkaline electrolysers are technologically sound, but manufacturing and demonstration of operation has so far been done in relatively small scales in comparison to potential future demand⁷.
- EU regulation concerning renewable energy (e.g. RED II⁸) is causing delays and possible showstoppers in e-fuels production. Essential for speeding up the e-fuels production would be the approval of the guarantees of origins (GO) for electricity, regulatory

⁷ Total European electrolyser capacity estimated to be 1 GW, which represents only about 1.4 % of *current* hydrogen production capacity [61]. Hydrogen demand could increase significantly if large-scale transitions are made to shift towards hydrogen economy or P2X.

⁸ Renewable Energy – Recast to 2030 (RED II)

acknowledgement of hydrogen obtained as a by-product⁹ for utilization purposes, and approval of the blending of e-fuels with fossil fuels. The demand in RED II directive to have green electricity production tied up with e-fuels synthesis on an hourly basis as well as the demand to use only new green electricity production should be reconsidered because they delay the investment processes by tying up closely two separate investments.

- Methanol provides also multiple other routes than fuel, such as olefins to plastics, or methanol to solvents and adhesives.
- The location of the electricity production, hydrogen production, and CO₂ source has an impact on profitability, which can manifest itself through transportation and storage costs as well as location-related production costs.
- P2X fuels can achieve a lower greenhouse gas emission level compared to fossil fuel alternatives. The origin of the hydrogen is critical, and renewable electricity is necessary to achieve significant emission reductions when electrolysis is used to produce the hydrogen.

-

⁹ When obtained from renewable sources

The LUT's research group was formed from a multi-disciplinary research team comprising all the departments of the University.

LUT School of Energy Sys-	LUT School of Engineering	LUT School of Business and	
tems (LES)	Science (LENS)	Management (LBM)	
Petteri Laaksonen	Jenna Ruokonen	Tommi Rissanen	
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Esa Vakkilainen			
Olli Pyrhönen			
Jarmo Partanen			

During the project, LUT also had close co-operation with Veikko Kortela from Wärtsilä and Jukka Hietanen from St1, who have also provided vital input and comments into this report and project. Julia Ranta, who at that time was a student at Turku University (Faculty of law, environmental law) has also provided valuable input into the project by performing an extensive outlook on the regulatory framework related to synthetic electric fuels [1].

Keywords: P2X, e-fuels, methanol, gasoline, kerosene, sustainable energy-economy,

Tiivistelmä

Kokonaisvaltainen energiajärjestelmän murros pohjautuu vahvasti nykyisen sähköntuotantojärjestelmän uusiutumiseen ja kestävään kehitykseen, joka on vahvasti kytköksissä aina yhteiskunnan perusrakenteisiin asti työllisyysvaikutusten ja talouden kautta. Tulevaisuudessa sähkön käyttö tulee lisääntymään kohteissa, joissa se on helppo toteuttaa, kuten henkilöliikenteessä ja lämmityksessä. Nestemäisiä polttoaineita tarvitaan kuitenkin myös jatkossa tietyissä käyttötarkoituksissa, kuten esimerkiksi lentoliikenteessä, laivaliikenteessä ja raskaan tavarankuljetuksen saralla. Hiilineutraalit polttoaineet voivat näissä kohteissa korvata nykyisiä fossiilisia polttoaineita – samanaikaisesti kun sähköjärjestelmä uudistuu ja vähentää omia päästöjään. Sähköpohjaiset polttoaineet soveltuvat niin energian käyttöön kuin sen varastointiin, ja niitä voidaan lisäksi käyttää kemianteollisuuden raaka-aineina.

Tämän projektin tavoitteena oli toteuttaa kattava kannattavuusselvitys sekä taloudellisessa että teknillisessä mielessä teollisen kokoluokan pilot-laitokselle, joka tuottaisi hiilineutraaleja polttoaineita hyödyntämällä Finnsementin sementtitehtaan savukaasuista kaapattavaa hiilidioksidia ja Kemiran kloraattitehtaan ylijäämävetyä. Prosessissa tuotettaisiin ensin metanolia, joka sitten jalostettaisiin valitusta reitistä riippuen joko pelkästään bensiiniksi, tai yhdistelmäksi eri hiilivetyjakeita (bensiini, kerosiini ja diesel).

Projektin pääasiallinen rahoitus on peräisin Euroopan aluekehitysrahastosta Etelä-Karjalan liiton ohjauksessa. Muu täydentävä rahoitus saatu LUT-yliopistosta sekä projektin osakkailta, joita ovat St1, Wärtsilä, Kemira, Finnsementti, Shell, Neste, Finnair, Refinec, Premekon, Jotex works, Terästorni ja Lappenrannan kaupunki. Projekti toteutettiin aikavälillä 1.1.2020 ja 30.4.2021.

Tutkimuksen tekninen osuus pohjautuu Aspen Plus -ohjelmalla toteutettuun yksityiskohtaiseen mallinnukseen metanolisynteesistä ja kahdesta vaihtoehtoisesta jatkosynteesistä. Vedyn lähteenä tutkittiin ylijäämävedyn lisäksi elektrolyysitekniikalla tapahtuvaa vedyntuotantoa erillisenä vaihtoehtona. Mallinnuksen perusteella saatavia investointi- ja käyttökustannuksia verrattiin laitevalmistajilta saatuihin alustaviin tarjouksiin. Kannattavuutta arvioitiin suorittamalla eri prosessivaihtoehdoille kassavirtalaskelmat, sekä haastattelemalla alalla toimivia henkilöitä markkinanäkemysten kartoitusta varten.

Avainsanat: P2X, sähköpolttoaineet, metanoli, diesel, kerosiini, kestävä energiatalous

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Abbreviations

APEA Aspen Process Economic Analyzer

B/C Benefit-Cost ratio

BMC Business model canvas
CAPEX Capital expenditure
DME Dimethyl ether

DSCR Debt-service coverage ratio

EDI Electrodeionization

EU ETS European Emissions Trading System

FH Fired heat

FT Fischer-Tropsch

GAC Granular activated carbon

GHG Greenhouse gas
GO Guarantee of origin

GWP Global warming potential

HP High-pressure

IRR Internal rate of return
ISBL Inside battery limits
LCA Life-cycle assessment

LP Low-pressure

LPG Liquefied petroleum gas

LUC Land-use change MEA Monoethanolamine

MeOH Methanol

MOGD Mobil's olefins to gasoline and distillate

MTG Methanol-to-gasoline MTO Methanol-to-olefins

NDA Non-disclosure agreement

NPV Net present value

O&M Operation and maintenance

OPEX Operating expense

P2X Power-to-X

RCF Recycled carbon fuel

RED II Recast renewable energy directive 2018/2001/EU

RFNBO Renewable liquid and gaseous transport fuel of non-biological origin

RO Reverse osmosis
ROE Return on equity

SMR Steam methane reforming

TEM Ministry of Economic Affairs and Employment of Finland (Suomen työ- ja elinkeino-

ministeriö)

TOC Total organic carbon

TRL Technology readiness level WACC Weighted average cost of capital

1 Introduction

The production of power-to-x products, i.e. products made of electricity, came to LUT's research agenda already during Neo Carbon Energy project (2014-2017). The matter realized into further studies with Wärtsilä [1] and St1¹⁰.

First initiative to study the utilization of waste hydrogen from Kemira was made by LUT already early 2017. Eventually study was carried out by Gasum, Kemira and City of Lappeenranta with a focus of synthetic methane. The production of synthetic methane turned up to be unprofitable according to the study.

The new initiative for production of synthetic fuels waste hydrogen from Kemira, as a solution to decarbonizing the traffic emissions, was made by LUT in end 2019. Methanol route was selected in research plan due to two reasons: synthesis can be made directly from H₂ and CO₂, and methanol is a universal raw material for chemical industry¹¹.

Paris Climate Change Agreement came to force in 2016. The public awareness of climate issues and impact of emissions into climate had risen and need for new solutions had become evident.

The proposal for the project for a "Feasibility Study for Industrial Pilot of Carbon-Neutral Fuel Production – P2X" at Joutseno was approved and financed by Regional Council of South Karelia and large group of leading fuel, manufacturing and end-user companies.¹² The project was approved in December 2019 and begun in January 2020. The research was carried out by LUT University and all LUT Schools¹³ participated the work.

Project was split into task packages (**Figure 1.1**). Work begun from defining the process and technology providers for the process as well as the raw material qualities. The acceptable level of impurities in the feedstock was determined by the requirement of the synthesis process.

¹⁰ Study on recycling of carbon dioxide emissions at the St1 Gothenburg refinery, 2019

¹¹ E.g. fuels, plastics, adhesives, and solvents.

¹² St1, Wärtsilä, Kemira, Finnsementti, Shell, Neste, Finnair, Refinec, Premekon, Jotex works, Terästorni, and City of Lappeenranta

¹³ School of Energy Systems, School of Engineering Science, and School of Business and Management

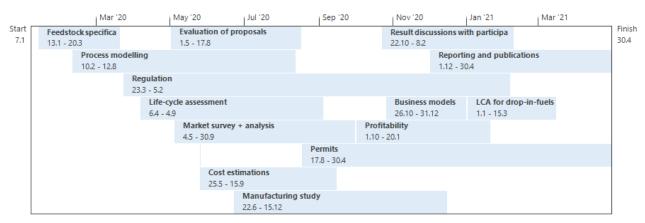


Figure 1.1. Project work packages and timetable.

From the very beginning St1 was heavily involved in the project. Wärtsilä joined also at the time of costs and profitability analysis. The work in the core team, together LUT, St1 and Wärtsilä, was seamless and continuous. Regulation study on RED II was carried out by Julia Ranta in her M.Sc study financed and supported by one of the leading Finnish law firms, Hannes Snellman. As a result of deep business and academic co-operation, the outcomes of the project are both academically and businesswise trustworthy.

The progress of the project was reported and discussed in strategic management meetings¹⁴, where all the parties attended.

¹⁴ As a matter of fact, it can be argued that the COVID-19 improved the communications due to digital Teams meetings allowing multiple people sharing the time compared to time before.

2 Technical process description

The process studied in the project starts from the acquisition of the raw material feedstock, which are hydrogen (H₂) and carbon dioxide (CO₂). After capturing CO₂ from the flue gases of the cement plant, it is dried and compressed prior to transportation. Hydrogen is obtained either as a by-product from chlorate production using electrolysers, or alternatively from a separate water electrolysis unit. Both feedstocks are purified to prevent catalyst poisoning and then delivered to methanol synthesis.

Two alternative drop-in fuel synthesis processes are studied, which are termed in this work as methanol-to-gasoline (MTG) and methanol-to-olefins (MTO) coupled with Mobil's olefins to gasoline and distillates (MOGD). Modelling of the MTG process was based on the work published by Yurchak [2] and Grimmer et al. [3]. Studies of Avidan [4] and Tabak and Yurchak [5] were used as references in MTO-MOGD modelling.

Overview of the process is given in **Figure 2.1**. In the figure, inputs are marked with a gold color, main outputs with green and by-products with light pink. Main processes are indicated with light blue background color and sub-process with light green. Apart from the water electrolysis, process simulation models were created using Aspen Plus V11 simulation software. Each main process block is explained further in the following sections.

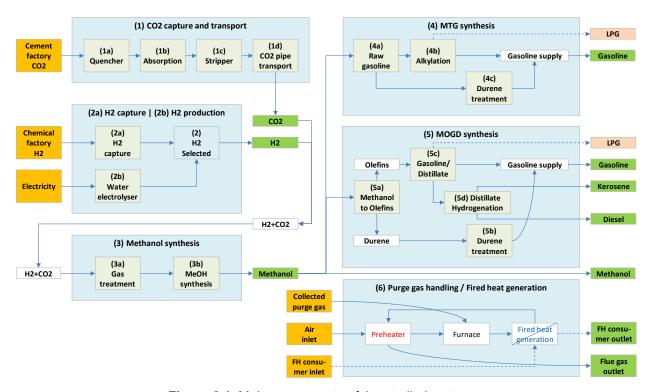


Figure 2.1. Main components of the studied system.

2.1 Hydrogen

To model the additional (optional) alkaline water electrolyser process, a model is built as demonstrated in the process **Figure 2.2**. Electricity from the grid is fed to a power converter system, where the AC current is converted to DC, usually through a transformer and rectifier process, and then supplied to the electrolyser stack. The DC current passes through a system composed of cells in series. One cell is mainly formed of cathode and anode electrodes, a diaphragm membrane, and electrolyte passing through the middle of the electrodes. The incoming electrolyte produces hydrogen gas, and OH⁻ ions in contact with the surface of the cathode, by gaining electrons. The focus ions are then transported through the electrolyte to the anode surface, where they lose electrons and produce water molecules and oxygen.

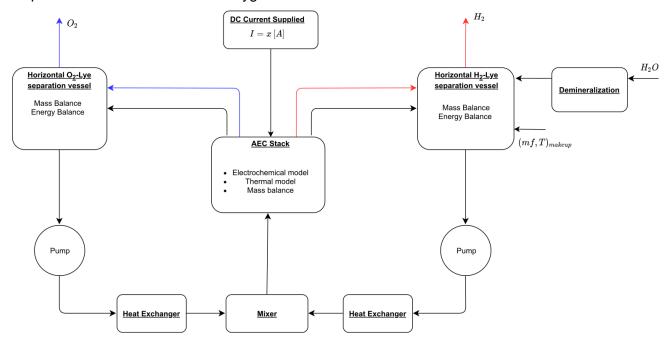


Figure 2.2. Alkaline water electrolyser process.

The produced mixture of hydrogen-electrolyte and oxygen-electrolyte is respectively transferred to horizontal gas-liquid separators, where the gases are extracted from the electrolyte (liquid). The by-product oxygen gas is usually vented out, or recirculated to the feed water tank, due to environmental issues. The end product hydrogen gas, after the separation, is sent to a purification system, composed mainly of a DeOxo, a gas-liquid separator, two heat exchangers, and two adsorber columns, one operating at regeneration phase and one at adsorption. The goal is to eliminate all the oxygen impurities, and moisture, and finally create high-purity hydrogen gas. The end product can then be transported to the purification process which can be seen in **Figure 2.1**.

The remaining electrolyte, after the separation, is pumped and recirculated back to the electrolyser stack, which is cooled with the help of heat exchangers in order to keep the temperature of the stack at the desired level, usually around 70 °C. Finally, to maintain the electrolyte concentration balance between the anode and cathode recirculation loop, the electrolyte has to mix before the next inlet to the stack.

2.2 CO₂ capture

Carbon dioxide capture model consists of two sections: pre-treatment of the flue gases and the carbon capture process. The technology is based on monoethanolamine (MEA) solution. Commercially available technology was used as a reference process in the modelling procedure. Block diagram of the complete process is shown in **Figure 2.3**.

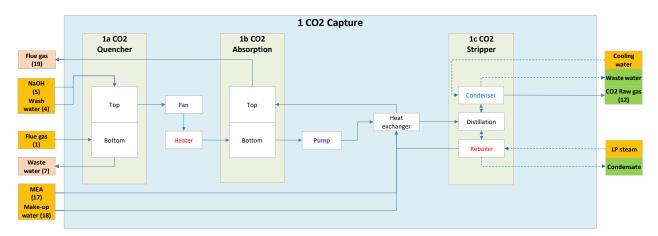


Figure 2.3. Block diagram of the CO₂ capture process.

Flue gas is first directed to a dual-purpose quench tower (1a). In the column, the flue gas is both cooled and washed in direct contact with mild lye solution. The flue gas is washed to remove acidic compounds, such as SO₂, HCl and HF. The purified flue gas exiting the quench column is then mildly pressurized to compensate the pressure drop in the capture process. Purified and compressed flue gas is then fed to the bottom and MEA solution to the top of an absorption column (1b).

In the absorption column, the flue gas and the MEA solution flow in opposite directions, and the CO_2 is absorbed into the solution via chemical reactions. As a result, the flue gas depleted of CO_2 exits the top of the column and is vented to the atmosphere. The MEA solution rich in CO_2 is collected from the bottom of the absorber and directed to a stripping column (1c) to desorb the CO_2 by boiling the solution.

Operation of the stripping column is designed so that a CO₂ capture efficiency of 85 wt% is achieved while keeping the reboiler temperature near the boiling point of water. Temperatures higher than 120 °C lead to thermal degradation of the MEA solution, thus increasing the fresh amine feed and the capture cost. CO₂ is recovered from the top of the stripping column and sent to a further treatment process. Lean MEA solution exits from the bottom and is recycled back to the absorption stage. A small portion of MEA and water is lost with the flue gas and captured CO₂, and a make-up feed is added to compensate the losses.

Prior to transporting the captured CO_2 to the Joutseno site, the CO_2 is dried and compressed. The treatment process is shown in **Figure 2.4**.

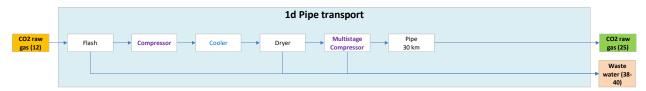


Figure 2.4. CO₂ treatment prior to pipe transport.

CO₂ is directed to the purification process directly from the stripper outlet. Excess water is removed from the gas that is then compressed to the average operating pressure of a commercial CO₂ drying unit [6]. The dryer operates with a dual-column configuration. Water in the gas flow is partially adsorbed to a desiccant bed that is regenerated with heated dry air. The adsorption technology is referred to as temperature swing adsorption since the operating pressure is kept constant and temperature is altered between the adsorption and desorption stages. Dried CO₂ is then led to a four-stage compressor that elevates the pressure of CO₂ to critical pressure of 74 bar. CO₂ can be transported efficiently with a pipeline when it is in supercritical state. Condensation of the remaining moisture occurs between the compression and cooling stages, and the knockout liquid is removed from the first three stages. Details of pipe transport of the supercritical CO₂ are discussed in **section 2.6**.

2.3 Feed gas purification

Gas purification process removes impurities form the feed gas, such as SO₂, NO_x, HCl and O₂, that act as catalyst poisons for the methanol synthesis catalyst. Based on the information obtained with the methanol synthesis offers, the allowable levels of impurities are 10 ppm of O₂, 100 ppb of SO₂, 100 ppb of NO_x, and 40 ppb of HCl. The system was modelled on a mass balance basis without taking adsorption chemistries into account. **Figure 2.5** shows the block diagram of the purification process.

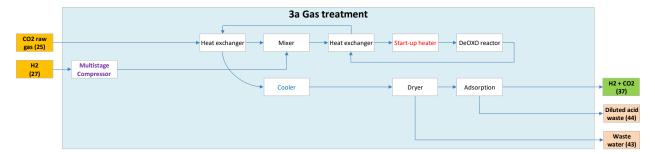


Figure 2.5. Block diagram of the gas purification process.

Hydrogen is obtained from chlorate production in 80 °C and atmospheric pressure. H₂ is then compressed to 73 bar and mixed with the transported CO₂. The mixture is sent to a DeOxo reactor for oxygen removal. In the reactor, oxygen is converted to water in reaction with hydrogen. The gas mixture depleted of oxygen is then dried with temperature swing adsorption. Regeneration of the adsorbent is carried out by using dry nitrogen gas to avoid oxygen contamination of the gas mixture. Final step of the purification process is activated carbon adsorption which removes HCl and possible SO₂ from the syngas. Impurities are adsorbed to activated carbon during the adsorption stage and liberated by water flushing in the desorption stage. As a result, a dilute acid stream is generated. The gas stream exiting the purification process meets the requirements set for syngas quality by methanol catalyst suppliers.

Hydrogen purification described here is considered when the H_2 is supplied as an industrial waste. In the case of water electrolysis as the hydrogen source, only compression of H_2 is seen necessary since commercial electrolysers are available with oxygen and moisture removal units. The level of purification requires reassessing when treating solely raw CO_2 .

2.4 Synthesis

Each synthesis process is discussed separately in the following sections. Methanol synthesis is a common first stage for all the configurations. The methanol produced in the first stage is then further processed either in the MTG process, producing primarily gasoline, or alternatively in the MTO-MOGD process, which yields gasoline, kerosene and diesel as the main products. Heat and mass balances for the different processes are also introduced.

2.4.1 Methanol

Hydrogenation of carbon dioxide to methanol is shown in **Figure 2.6** as a block diagram.

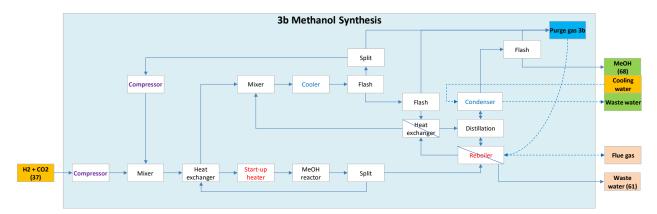


Figure 2.6. Block diagram of the methanol synthesis.

A purified mixture of CO₂ and H₂ entering the process is pressurized and heated to synthesis pressure and temperature of 73 bar and 220 °C and sent to a synthesis reactor. In the reactor, CO₂ and H₂ are partially converted to methanol and water in adiabatic conditions. Additionally, small amounts of CO are formed as a result of reverse water-gas shift reaction. The reaction system follows kinetics of a Cu/ZnO catalyst. The reactor effluent is divided into fractions to optimize heat integration within the process. Cooled reactor products are separated in high-pressure gas-liquid separation.

In the separation stage, unreacted gases are separated from the liquid products and the gases are sent back to reactor feed via recycle compressor that compensates the pressure drop in the reaction and separation cycle. A small portion of the recycle stream is purged to avoid accumulation of inert species in the cycle. The liquid product from the gas-liquid separation is sent to the second flash column that operates near ambient conditions. Remaining gaseous species are removed from the methanol-water mixture in the column. The bottom product is sent to distillation where methanol is separated from water. Methanol is recovered as a top product of the column and water as the bottom product. In the final gas-liquid separator, dissolved CO₂ is removed from the methanol product. Purge gases are collected and combusted to recover heat required in the distillation stage.

2.4.2 MTG

The process producing gasoline from methanol consists of three sub-processes: raw gasoline production (4a), gasoline alkylation (4b) and durene treatment (4c). The first stage of the process, raw gasoline production, is shown in **Figure 2.7**.

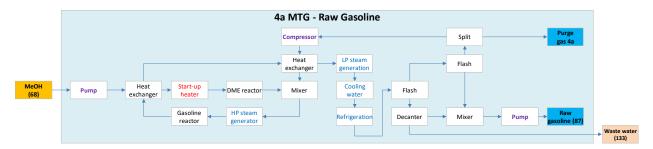


Figure 2.7. Block diagram of raw gasoline production in the MTG process.

The MTG process begins with methanol conversion to raw gasoline (4a). The methanol feed entering the process is pressurized and heated to synthesis pressure and temperature of 22 bar and 316 °C and sent to reactor train consisting of two separate reactors. In the first reactor, methanol forms dimethyl ether (DME) and water over a gamma-alumina catalyst. The reactor product is then fed to the second reactor where DME is converted to hydrocarbons and additional water over a zeolite catalyst in 360 °C and 20 bars.

The overall reaction system is divided into two reactors to manage the high adiabatic temperature increase resulted by strongly exothermic nature of the reactions. The final reactor product is cooled, and gaseous and liquid hydrocarbons are separated from water in a three-step separation stage. Non-condensable hydrocarbons are recycled back to gasoline reactor feed while purging a small portion of the gases to avoid accumulation of inert gases. The liquid hydrocarbons are collected as raw gasoline and sent to further refining.

Figure 2.8 shows the alkylation process of the light gasoline.

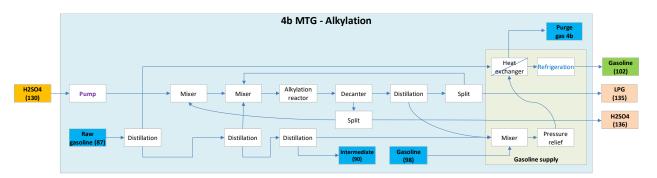


Figure 2.8. Block diagram of gasoline alkylation in the MTG process.

Properties of raw gasoline are improved by upgrading both light and heavy ends of the hydrocarbon mixture. The raw gasoline is first sent to a distillation train where remaining light gases, C₄ compounds and aromatics are separated from the mixture. Light gases are combusted to provide high-temperature heat for the process. C₄ compounds are directed to an alkylation unit (4b) where isobutane and butene are converted to isooctane (2,2,4-trimethylpentane) to increase the octane

rating of gasoline. The reaction is catalyzed by concentrated sulfuric acid by homogenous catalysis. Sulfuric acid is fed to the alkylation process in a volumetric ratio of 1 to the hydrocarbons. The alkylation reactor operates in 5 bar and 10 °C and is constantly cooled due to exothermic alkylation reactions. The acid catalyst is separated from the reaction mixture in a decanter and recycled back to the reactor feed. The hydrocarbons are sent to a distillation column to separate the unreacted C₄ compounds and the isooctane alkylate. The C₄ compounds are also recycled back to the reactor feed. About 1 wt% of the stream is purged as liquefied petroleum gas (LPG) to maintain the mass balance within the cycle. The alkylate product is finally blended to the gasoline stream.

The final process step, the durene treatment, is shown in **Figure 2.9**.

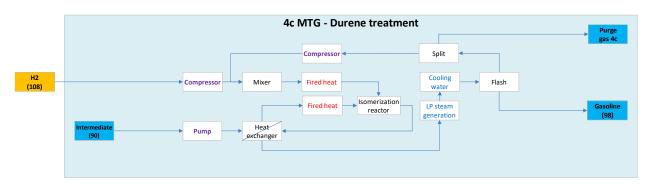


Figure 2.9. Block diagram of durene treatment in the MTG process.

Aromatic fraction rich in durene is isomerized to reduce the durene content of gasoline (4c). Durene (1,2,4,5-tetramethylbenzene) is not present in crude oil but it is formed in methanol-to-hydrocarbons processes by the rate of 10 kg/t MeOH. Durene has a high melting point of +79 °C thus causing engine running issues in cold climates if left untreated. The hydroisomerization reactor operates on 345 °C and 17 bars. The isomerization reaction is catalyzed by a modified zeolite catalyst in the presence of hydrogen gas. Hydrogen contributes to the isomerization reaction but is not consumed itself. However, hydrogenation of durene occurs in a minor scale which results in a small hydrogen consumption within the process (2 kg/t durene). After the reactor, the mixture of hydrogen and hydrocarbons is cooled and directed to a high-pressure (HP) flash for gas-liquid separation. Hydrogen is separated from the liquid hydrocarbons and recycled to the reactor feed. The liquid aromatics with reduced durene content are blended with the gasoline stream. The final gasoline product is a mixture of paraffinic raw gasoline, isooctane, and aromatics.

2.4.3 MTO-MOGD

An alternative methanol-to-hydrocarbons process is methanol-to-olefins (MTO) coupled with Mobil's olefins to gasoline and distillate (MOGD) synthesis. Coupling the process technologies enables

production of gasoline, kerosene, and diesel from methanol. The complete synthesis consists of four sections: MTO process (5a), durene treatment (5b) MOGD synthesis (5c) and distillate hydrogenation (5d). The beginning of the process is shown in **Figure 2.10**.

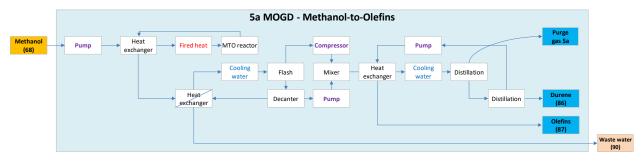


Figure 2.10. Block diagram of the MTO process.

In comparison to the MTG process, MTO produces light olefins instead of paraffins. The MTO synthesis takes place in low pressure of 2 bar and fixed temperature of 450 °C. In the reactor, methanol in converted to DME and water over a zeolite catalyst. DME further forms light olefins and additional water. The exothermic reaction heat is managed by producing HP steam. The reactor product is cooled, and gaseous and liquid hydrocarbons are separated from water in a two-step separation stage.

First, non-condensable hydrocarbons are separated from the two-phase liquid mixture. Liquid hydrocarbons are then separated from water that exits the process as waste. Both gaseous and liquid hydrocarbons are pressurized to 15 bars prior to mixing the streams. The mixture is distilled to three fractions in two subsequent distillation columns. Light gases are recovered as the top product of the first column and aromatic fraction rich in durene as the bottom product of the second. The olefin product is recovered as the top product of the second column in 10 bar and 38 °C. Light olefins, especially ethylene and propylene, are valuable raw materials to multiple chemical processes including fuel, plastic, and polymer production.

Light olefins produced with the MTO process can be converted to gasoline, kerosene, and diesel by expanding the synthesis with MOGD and durene treatment processes. The heavy gasoline upgrading process in the MTO-MOGD is shown in **Figure 2.11**.

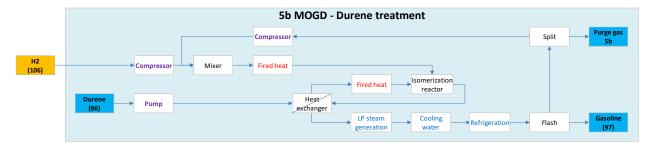


Figure 2.11. Block diagram of durene treatment in the MTO-MOGD process.

The durene treatment is carried out in the same manner as described in **section 2.4.2**. MOGD synthesis is shown in the following **Figure 2.12**.

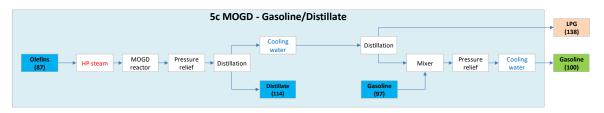


Figure 2.12. Block diagram of the MOGD synthesis in the MTO-MOGD process.

The light olefins from the MTO are sent to the MOGD synthesis (5c). The olefin feed is pressurized and heated to the MOGD reactor conditions of 200 °C and 40 bars. In the reactor, the light olefins form longer-chained olefins with carbon numbers of C_6 - C_{20} . The reaction mixture is depressurized and split by distillation to LPG-gasoline and distillate fractions. LPG is separated from gasoline in the following distillation column. Treated aromatics from process section 5b are blended with the olefinic gasoline.

Diagram of the final section of the process – distillate hydrogenation – is illustrated in Figure 2.13.

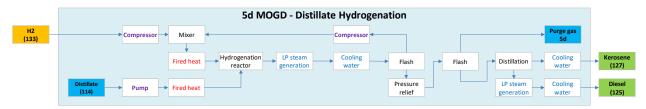


Figure 2.13. Block diagram of distillate hydrogenation in the MTO-MOGD process.

The distillate product is hydrotreated (5d) to satisfy the carbon-carbon double bonds and to improve the stability of the products. The reaction takes place in the hydrogenation reactor in 300 °C and 40 bar over a modified alumina catalyst. Hydrogen is fed to the reactor in equimolar ratio to the hydrocarbons. The paraffinic distillate product is cooled and separated from excess hydrogen in the flash column that operates in high pressure. The hydrogen is recycled back to the reactor feed

via the recycle compressor that compensates the pressure loss within the loop. Remainder hydrogen traces are separated from the hydrocarbon product in an atmospheric flash column. Finally, the kerosene-diesel mixture is distilled, and paraffinic kerosene is recovered as the top product of the column and diesel from the bottom.

2.4.4 Heat generation

Purge gases of methanol, MTG and MTO-MOGD syntheses can be utilized in process heat generation. The combustion process is similar in each synthesis, and it is illustrated in part 6 of **Figure 2.1**. The purge gases from different locations of the synthesis are collected into a single gas stream and directed to a furnace where the hydrocarbons or residual methanol are combusted with air. The feed air is supplied in 20% molar excess and pre-heated prior to entering the furnace. The gas mixture is combusted in 1000 °C and high-temperature heat (also called fired heat, FH) is recovered by transferring the heat into a medium until the flue gas is cooled down to 500 °C. The remainder heat is utilized in pre-heating the combustion air in an economizer-like configuration. The heat recovered from the combustion process covers the FH demand of both methanol-to-fuel syntheses and converts the volatile organic compound emissions to mere CO₂.

Combustion of purge gases of the methanol synthesis is even simpler. Since heat is required only in the methanol-water distillation and some of the heat demand can be covered by other means of heat integration, it is sufficient to generate only low-pressure (LP) steam within the combustion process. In such a case, it is not necessary to pre-heat the combustion air and all the combustion heat is utilized in LP steam generation. The generated species of heat are then directed to locations where the heat is consumed.

2.4.5 Mass and energy balances

General level mass and energy balances of each process are shown in the following figures. Numbering of the processes is done according to the method presented in **Figure 2.1**. In the figures, material streams are indicated with a solid black line entering the process from the left and exiting from the right. The mass flow rates are calculated with an assumption of 8000 annual operation hours. Utility flows are marked in the figures with dashed lines. Additionally, required energy enters the process from the top and removed heat exits from the bottom.

Figure 2.14 shows the mass and energy balances of the CO₂ capture and pre-treatment process.

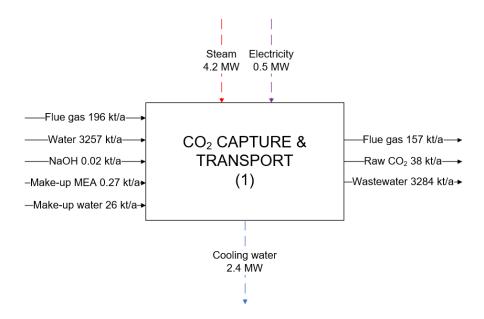


Figure 2.14. Mass and energy balance of the CO₂ capture and pre-treatment process prior to transport.

As can be seen in **Figure 2.14**, 38 kt/a of impure CO₂ can be captured from the flue gas with a CO₂ concentration of approximately 20 wt%. The process requires rather large amounts of water both in direct contact cooling and washing as well as cooling water in the condenser of the stripper column. The consumption of washing water in the quench column can be greatly reduced by optimizing the final temperature of the cooled flue gas. It is necessary to design and create a closed water circulation and purification system to reduce the fresh feed water demand of the capture process.

Balances of the gas treatment process are shown in

Figure 2.15.

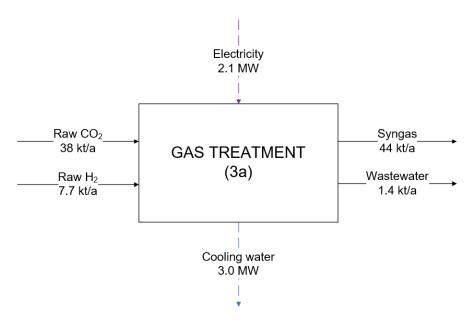


Figure 2.15. Mass and energy balance of the gas purification prior to the methanol synthesis.

Figure 2.15 shows that 38.5 kt/a CO₂ and 7.7 kt/a hydrogen feeds produce 44 kt/a of purified syngas. The composition of the treated syngas is 38.1 kt/a CO₂ and 5.2 kt/a H₂. According to the energy balance, the purification process is rather intensive in terms of electricity consumption and cooling demand that is due to the gas compression stages. The pressure increase from atmospheric pressure to over 70 bar is such high that the compression must be carried out in several stages with intercooling after each stage. It is important to notice that the gas treatment process additionally requires heated nitrogen gas for desiccant bed regeneration as discussed in **section 2.3**. The amount of N₂ can be determined in a later engineering phase and it was neglected in this study.

Figure 2.16 shows the corresponding balances for the methanol synthesis.

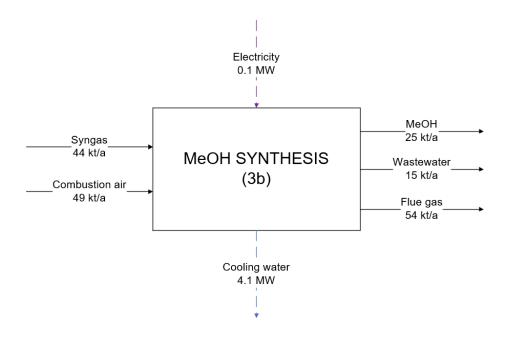


Figure 2.16. Mass and energy balance of the methanol synthesis.

The mass and energy balance of methanol synthesis in **Figure 2.16** represents the process with internal heat integration and purge gas combustion to cover the heat demand of the system. Thus, there is no need for external heat source. Electricity consumption of the process is also very small since the syngas pressure is set in the gas treatment section and only maintained within the methanol synthesis.

Inputs and outputs of the MTG synthesis are shown in Figure 2.17.

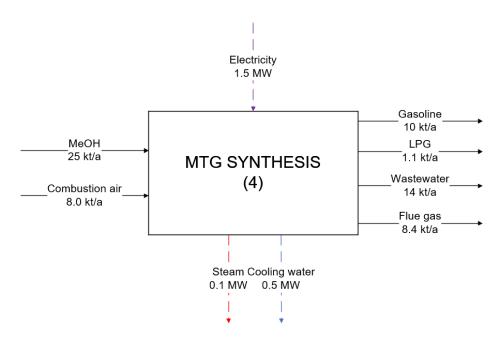


Figure 2.17. Mass and energy balance of the MTG process.

Figure 2.17 shows that the MTG process produces approximately 10 kt/a gasoline from 25 kt/a methanol which corresponds to 40 % mass yield. About 56 wt% of the methanol feed is converted to water and LPG and purge gases account for the remainder 4 wt%. In terms of fuel efficiency, 84% of the thermal power of methanol can be converted to gasoline. The high thermal efficiency can be explained by the more than twofold increase in lower heating value when converting methanol to gasoline range hydrocarbons. Net production of process heat is 0.1 MW, after taking internal heat integration and purge gas combustion into account. Electricity consumption of the MTG process is rather high due to the computation logic of refrigerant consumption. The coolant utility was calculated as electricity needed to compress the refrigeration medium after evaporation in a closed cycle. Thus, low-temperature operations, such as condensation of light hydrocarbons or alkylation of the LPG fraction to isooctane, were calculated as electricity demand.

The mass balance is shown in a simplified form in comparison to the description given in **section 2.4.2**. Sulfuric acid is not included in the mass balance since it is a liquid catalyst that circulates within the alkylation unit (4b) of the MTG process. Additionally, hydrogen consumption in the durene treatment section (4c) is insignificant in the overall evaluation of the process and it is thus neglected in the balance.

Finally, the mass and energy balances of the MTO-MOGD process are shown in Figure 2.18.

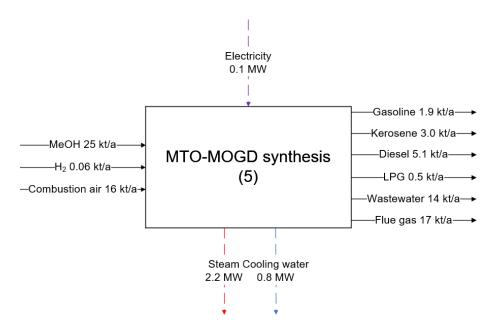


Figure 2.18. Mass and energy balance of the MTO-MOGD process.

As can be seen in **Figure 2.18**, the spectrum of output products is more diverse than in the MTG process. Gasoline, kerosene, and diesel yields are 7, 12, and 20 wt%, respectively. However, the

overall hydrocarbon yield of 44 wt% remains the same as in the MTG due to the reaction stoichiometry in the methanol-to-hydrocarbons syntheses. As gasoline is the smallest and the least valuable fraction of the product slate (when considering the future demand), neither alkylation nor hydrogenation was considered for gasoline. Additionally, durene treatment could also be excluded from the process as the treated durene does not increase gasoline yield significantly. Removal of the durene fraction does, however, decrease the octane rating of gasoline as durene and its isomers have high research octane numbers (109). The lack of the alkylation unit and the heavier hydrocarbon products lead to decreased refrigerant demand and thus to remarkably lower electricity consumption in the MTO-MOGD process than in the MTG. Excess steam is also produced in larger quantities. Energy-wise, a combined fuel efficiency (gasoline, kerosene, and diesel) of 91% can be achieved.

Figure 2.19 and

Figure 2.20 show the overall mass and energy balances of the process when fuels are produced from captured CO₂ and waste hydrogen via methanol with either MTG or MTO-MOGD.

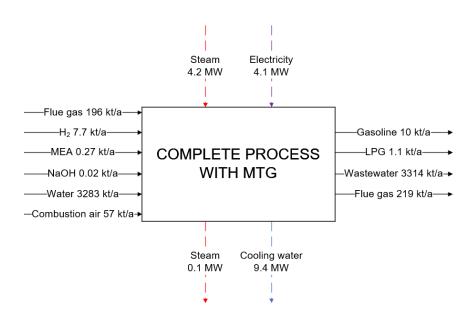


Figure 2.19. Mass and energy balance of the complete process chain consisting of CO₂ capture and treatment, gas purification, MeOH and MTG processes.

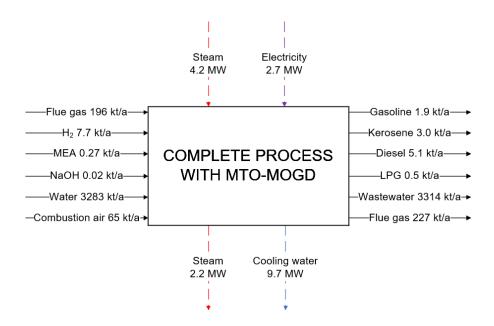


Figure 2.20. Mass and energy balance of the complete process chain consisting of CO₂ capture and treatment, gas purification, MeOH and MTO-MOGD processes.

It can be concluded by looking at the figures that the same inputs (excluding combustion air) can be converted to desired hydrocarbon products depending on the target markets. Heat consumption and production are considered separately since the excess heat supply is located at the different site than the heat demand. The situation is unique to this case, and greater synergy benefits could be gained if the excess heat from the fuel synthesis could be utilized for a partial fulfillment of the demand in the CO₂ capture process. Yet, the overall production chain would not be self-sufficient in terms of heat even if the processes were located at the same site. The optimal location for the synthesis would be near the CO₂ source so that the heat demand can be satisfied as efficiently as possible. An option for the excess heat would be electricity production in a steam turbine if no external heat consumers are available.

2.5 Water purification

Process water is the major by-product in both methanol and fuel syntheses in terms of volumes. Methanol synthesis produces water with the rate of 560 kg/t MeOH, and 56 wt% of methanol is converted to water in the fuel syntheses. The combined production rate of wastewater totals in approximately 1.1 t/t MeOH. The process water must be treated due to elevated hydrocarbon concentrations. The required level of purification depends on the final use of the water. Hydrocarbon treatment is necessary if the water is released to a municipal sewer after purification. On the other hand, if the process water is recycled to electrolysis to reduce the amount of fresh feed water, the water quality requirements are significantly more stringent. **Table 2.1** shows the water quality

required by a quoted alkaline electrolyser and the properties of wastewater collected from the MeOH and MTG processes.

Table 2.1. Alkaline electrolyser feed and demineralized water quality requirements based on an offer, and the properties of simulated process water.

		Feed water to de- mineralization	Demineralized water to electrolysis	Process water
Aluminum	μg/L	< 200	< 180	
Ammonia	μg/L	< 500		
Benzene	μg/L			760
C_1 - C_4	μg/L			1819
C ₅ -C ₈	μg/L			15
Chloride	μg/L	< 250000	< 0.03	
CO ₂	μg/L		0	5756
Copper	μg/L		< 0.6	
Iron	μg/L	< 100		
Manganese	μg/L	< 50		
Silicate	μg/L	< 15000		
Sodium	μg/L	< 200000		
Sulfite	μg/L	< 250000		
TOC	μg/L			2098
Conductivity	μS/cm	< 2790	< 0.1	
рН		6.5-9.5	6.9-7.1	5.4
Pressure	bar(a)	6-10		1
Temperature	°C	20		55
Turbidity	NTU	< 1	< 1	

In the case of directing the wastewater to a municipal sewer, the minimum requirement for water treatment is reduction of benzene concentration. Benzene is hazardous and carcinogenic chemical with a maximum allowable concentration of 1 μ g/L in drinking water [7]. It is also forbidden to release toxic chemicals to municipal sewers [8]. Total organic carbon (TOC), including hydrocarbons but not CO₂, can be readily removed from wastewater by passing the water through a bed of granular activated carbon (GAC). Exhausted GAC is regenerated by flushing the bed with hot steam. Temperature of the water must be adjusted to below 40 °C and pH to 6 – 11 prior to sending the water to the sewer [8].

If a portion of the electrolyser feed water is covered by the process water, ionic species must also be removed from the stream. Of the compounds present in the wastewater, soluble CO₂ requires addressing due to formation of carbonic acid according to **Equation (1)**. Carbonic acid further

dissociates to bicarbonate and carbonate as can be seen in **Equation (2)**. Release of protons decreases pH of the water on the acidic side.

$$CO_2 + H_2O \rightleftharpoons H_2CO_3 \tag{1}$$

$$H_2CO_3 \rightleftharpoons HCO_3^- + H^+ \rightleftharpoons CO_3^{2-} + H^+$$
 (2)

Figure 2.21 shows the shifts in carbonic acid equilibrium across the pH range. Full dissociation of carbonic acid to carbonate and bicarbonate can be achieved by adjusting the pH above 9. The pH adjustment can be carried out by base addition, but attention must be paid to the overall conductivity of the wastewater. NaOH, KOH and Ca(OH)₂ are often used in pH control. However, the use of Ca(OH)₂ is not recommended due to formation of hardness salts with carbonate ions. Potassium concentration in the feed water is not limited like sodium (**Table 2.1**), which makes KOH a potential chemical for pH adjustment. Moreover, KOH solution is used as the electrolyte in alkaline electrolysers as discussed in **section 2.1**, making it an available chemical at the site.

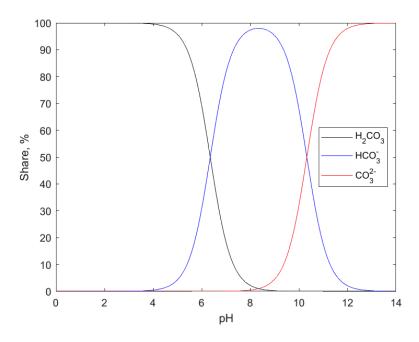


Figure 2.21. Carbonic acid equilibrium as a function of pH at 25 °C. The equilibrium curves are calculated using dissociation constants reported by Harned & Scholes [9] and Harned & Davis [10].

Commercial water electrolyser units include water treatment units for production of demineralized water from tap water. The electrolyser feed water purification unit consist of reverse osmosis (RO) filtration and electrodeionization (EDI) processes. Pre-filtration must be applied to reject larger ionic species from the wastewater prior to the RO unit since RO membranes are prone to fouling. EDI is a process combining ion exchange and electrodialysis. The technology allows continuous operation

and in-situ regeneration of the ion exchange resin without additional regeneration chemicals. The water treated with RO and EDI meets the quality requirements set for demineralized water. Pre-filtration, RO and EDI all produce reject streams rich in the compounds removed for the wastewater. The rejects are collected and treated as waste.

2.6 Feed gas transport and storage

Truck and pipeline transport were considered as candidates for CO₂ transport. The majority of existing pipelines for CO₂ are found in the United States, where they are typically applied for transporting CO₂ to oil drilling sites for enhanced oil recovery. Over 2 500 km of existing pipelines are in place in the western USA alone, together representing roughly 50 Mt_{CO2} of transport capacity annually. [11]

Drying the CO₂ prior to transportation reduces the corrosion rate and enables the use of traditional carbon-manganese steels in pipelines. Other major impurity specifications relevant to transport are listed below (originating from agreement of the first constructed CO₂ pipeline in 1970, Canyon Reef [11])

- Hydrogen sulphide (less than 1500 PPM by weight)
- Total sulphur (1450 PPM, by weight)
- Nitrogen (below 4%, by mole)
- Oxygen (10 PPM, by weight)
- Hydrocarbons (5% by mole) and dew point which does not exceed -29 °C
- Glycol

 CO_2 in pipelines is traditionally transported in pressures of around 75 - 150 bars, which exceeds the critical pressure of CO_2 of 73.8 bar as illustrated in **Figure 2.22**. When also the temperature of the fluid exceeds the critical temperature of CO_2 (31 °C), it is classified as a supercritical fluid, where the fluid exhibits properties of both liquid and gas. For instance, in supercritical state, the fluid has low viscosity (i.e. gas-like flow properties), but a high density (liquid-like property). Specifically, the high density of the fluid makes transportation more cost-effective to implement.

When the temperature of the CO₂ is below the critical temperature but pressure above the critical pressure, the fluid terminology varies, but is typically called either *dense phase liquid* or *compressible liquid*, or just plain *liquid*. Density and viscosity of CO₂ are sensitive to changes in pressure and temperature when operating close to the critical point, which is why in practical pipeline applications

the operational pressure is commonly slightly higher than the critical pressure. Another reason for using higher inlet pressures is the need to overcome the pressure losses occurring in the pipe, especially with longer distances. Typically, distances of 100 - 200 km can be reached without additional booster stations to repressurize the CO₂ [12].

Road and maritime transport typically occur at reduced pressure levels in order to reduce costs in manufacturing costs of vessels. However, operation temperatures are then also reduced to subzero temperatures in order have the CO_2 remain as a liquid. Typical densities in pipeline applications are between $700 - 1000 \text{ kg/m}^3$, and for maritime and road transport somewhat higher, $900 - 1150 \text{ kg/m}^3$.

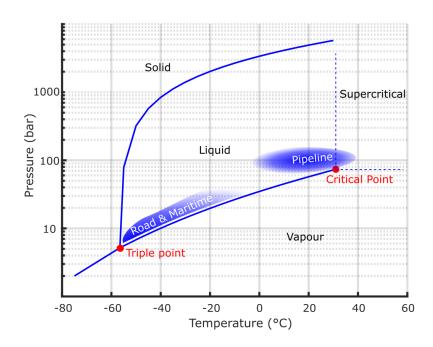


Figure 2.22. Phase diagram of CO₂ with approximation of typical transport conditions.

Storage of CO₂ is typically based on either compressed tanks in ambient temperatures (small scale) or as a refrigerated liquid in slightly elevated pressures (typically below 10 bars). In very large scale, underground caverns can be used for cost-efficient storage.

2.6.1 Truck transport cost estimation

Costs for truck transport of CO₂ are obtained from a custom-built model, which has been developed based on a cost index of road transport of goods [13]. Distribution of cost items that have been evaluated are shown in **Figure 2.23**. The largest uncertainty regarding the estimated costs most likely lies in the cost of the equipment, i.e. the truck, CO₂ tank, and the loading station. These were

assumed to have procurement costs of 280 000 €, 300 000 €, and 500 000 €, respectively. Overall, employee costs form the majority of the costs, which was based on an hourly wage of the drivers (20 €/h) and indirect employee cost (62% of direct wages). A single truck was found to be sufficient for the desired quantity of CO₂ when operated by two drivers daily.

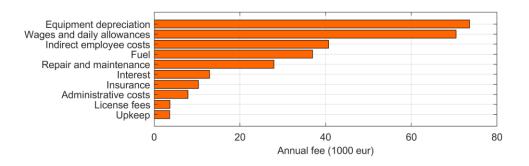


Figure 2.23. Distribution of cost items in truck transport of CO₂.

The cost of CO_2 liquefaction is included in the CO_2 capture procurement in this analysis. Compared to pipeline transport, the pressure level is considerably lower. Therefore, an additional compressor would likely be required at the destination to compress the CO_2 to synthesis pressure, which could increase the total cost of delivered CO_2 by about $1.5 \in I$ ton CO_2 . This compressor was not included in the specific costs presented in **Table 2.2**. The cost per ton of CO_2 was calculated by dividing the total sum of all cost elements (c_i) by the total quantity of CO_2 that could be transported (Q_{CO_2}) as shown in **Equation (3)**. Thus, with the current methodology, if the desired CO_2 transport quantity is exceeded, it is not reflected by an increase in the calculated specific transport cost. Another method of calculation could have been to use the annual desired CO_2 quantity as the divisor, which could increase the specific costs by about $0.5 - 1.5 \in I$, depending on how well the desired quantity matches with the quantity that could be transported with a specific combination of equipment, drivers and other such factors, which can only be adjusted in discrete steps.

Cost of transport =
$$\frac{\sum c_i}{Q_{CO_2}}$$
 (3)

Table 2.2. Total transport cost for CO₂ by truck. Liquefaction cost is excluded as it is included in the CO₂ capture costs.

Number of drivers per car Cost of transport (€/t_{CO2})

3	5.0
2	5.8
1	8.0

2.6.2 Pipeline cost estimation

Cost estimates from existing pipeline projects are predominantly from USA and Canada, where the specific cost ranges from 0.2 to 2.5 M€/km. Typically, CO₂ pipeline capacities are rather large, in the range of millions of tons of CO₂ annually. The annual quantity of material that can be transported through the pipeline is a function of pipeline diameter and flow velocity. Diameter has a significant impact on capital expenses and installation costs, whereas flow velocity is critical for determining the annual operation costs. Increased flow velocities result in larger pressure losses, but also increase the throughput. Higher pressure losses are in turn connected to a higher electricity consumption by the compressors. As such, pipeline dimensioning is an optimization problem where the capital expenses of larger diameters compete against higher operation costs through higher flow velocities.

As the scale of the pilot plant is rather small, pipeline diameter was fixed to a value of 8 cm, which was considered to be a minimum allowed pipe size for practical reasons. Flow velocity in the pipeline is also quite low even with such a low diameter size, so in practice the same pipeline could be used to transport a larger amount of CO_2 . Pipeline costs were estimated based on a model developed from the basis of realized natural gas pipeline costs [14], using the correlation is given in **Equation (4).** Total cost is obtained as a sum of different expense categories (E_i), with the coefficients being different for each category as illustrated in **Table 2.3**. The parameter L refers to pipeline length in kilometers and D to pipeline diameter in meters. The *right of way* category contains items that are associated with compensation and costs related to the pipeline passing through different regions, which may be owned by external parties such as private owners. *Miscellaneous* costs contain engineering, surveying, permitting, supervision and other such factors which are not already included in other categories.

$$E_{i} = 10^{h}(a_{0} + a_{6}\log(L) + a_{7}\log(D))$$
(4)

Table 2.3. Coefficient for pipeline cost model.

Expense category	a0	a6	a7	
------------------	----	----	----	--

Materials	3.112	0.901	1.590	
Labor	4.487	0.820	0.940	
Right of way	3.950	1.049	0.403	
Miscellaneous	4.390	0.783	0.791	

Costs for natural gas pipelines are typically used in price estimations even for CO_2 pipelines, as there is limited data available from dedicated pipelines to CO_2 , and the practical differences are relatively small between the two gases. The USD costs of the original model were converted to euros using a conversion factor of 0.83, and a cost index for steel price in pipes and tubes was used to adjust the costs from the year 2004 (index value 151.4) to the year 2021 (index value 346.3). Other relevant parameter and simulation results are shown in **Table 2.4** and **Figure 2.24**.

Table 2.4. Assumptions, intermediate technical results, and final costs for CO₂ pipeline.

Pipeline lengthkm30Pipeline diametercm8Flow velocitym/s0.3Specific pressure lossPa/m10Pressure at inletbar80Total investmentM€5Specific investmentM€/km0.17Annual CAPEX cost¹€/tonco₂9.4			
Flow velocitym/s0.3Specific pressure lossPa/m10Pressure at inletbar80Total investmentM€5Specific investmentM€/km0.17	Pipeline length	km	30
Specific pressure loss Pa/m 10 Pressure at inlet bar 80 Total investment M€ 5 Specific investment M€/km 0.17	Pipeline diameter	cm	8
Pressure at inletbar80Total investmentM€5Specific investmentM€/km0.17	Flow velocity	m/s	0.3
Total investment M€ 5 Specific investment M€/km 0.17	Specific pressure loss	Pa/m	10
Specific investment M€/km 0.17	Pressure at inlet	bar	80
·	Total investment	M€	5
Annual CAPEX cost¹ €/ton _{CO2} 9.4	Specific investment	M€/km	0.17
	Annual CAPEX cost ¹	€/ton _{CO2}	9.4
Total $cost^2$	Total cost ²	€/ton _{CO2}	17.3

¹ Calculated by using 30-year lifetime and 5 % interest rate.

² Includes the annual CAPEX cost as well as the annual operation and maintenance cost of 10 000 €/km. The CAPEX cost and total cost are provided merely to provide a reference frame, the cash flow calculation uses a different calculation procedure based on the total investment.

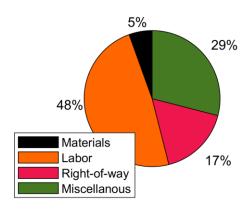


Figure 2.24. Investment cost components of the pipeline.

Numerous estimates for operational expenses of pipelines have been presented in literature. When calculated as a fixed percentage of the investment, 1.5 - 8 % are applicable. Another commonly used way is to use a fixed number per kilometer of pipe, ranging from about 5000 to 8500 USD. [12] These operational expenses were not included in the cash flow calculation in order to avoid double-counting of operational costs, as the cash flow calculation obtains operations and maintenance costs as a bulk figure for all systems and components.

The resulting pipeline cost is higher than what was estimated for road transport. This can be partially attributed to the scale of the operation, with the short transport distance having also an important part. Pipeline shows significant economy of scale but performs relatively poorly in low annual quantities. Road transport, on the other hand, has much lower up-front costs, but gains little benefit from increased scale of operations. With annual capacities of around 500 kilotons of CO_2 , the average total costs for pipeline are hovering around $2 \in /t$ according to the utilized cost model for the same transport distance. Literature sources can be found with a levelized cost range of $0.11 - 4 \in /t$ for a 25 km distance, and $1.9 - 45 \in /t$ for 300 kilometers [12]. Another important factor is that the costs of truck transport very quickly escalate with increasing transport distance. For reference, the truck transport model gives average costs of $5.1 \in /t$ for 25 km distance and over $30 \in /t$ for a distance of 300 km using the above 500 kiloton annual quantity.

2.6.3 Storage cost estimation

Estimates for the investment cost of CO₂ storages vary between 0.6 and above 3 €/kg [15, 16, 17, 18, 19]. In large scale, cavern storages can be economical, and estimates of 0.1 – 0.2 €/kg have been presented [18]. For this work, a value of 2.5 €/kg was used for the investment calculation. The size of the storage was dimensioned so that it would be adequate for 48 hours of production at nominal capacity. The selection of 48 hours was based on the assumption that truck transports would only occur during weekdays. For pipeline transport, the CO₂ storage could be designed to be significantly smaller, but for simplicity, all scenarios use the same CO₂ storage size. The resulting investment of CO₂ storage is roughly 0.8 million euros.

Hydrogen storage is considered to be remarkably more expensive. The estimate for hydrogen storage specific investment cost was set at 600 €/kg (18 €/kWh), based on a low-pressure (50 bar) storage container according to a literature reference [20]. The basis for the number is an industrial quote. Specific price for high-pressure container of 200 bars, according to the same reference, is estimated to be 1 900 €/kg. Cavern storages could have significantly lower specific prices, but they can be somewhat more challenging to implement in proximity of existing industrial sites.

It was assumed that only a small buffer storage would be installed for hydrogen, which corresponds to roughly 3 hours of operation at nominal capacity. The investment cost for hydrogen storage is thus about 1.2 million euros as is evident in **Table 2.5**.

Table 2.5. Summary of storage tank sizes and costs.

Material	Quantity stored (t)	Purchase price (M€)
CO ₂	230	0.8
H_2	2	1.2

The production of green hydrogen is essentially a conversion process from electricity. As the price of electricity on the market is fluctuating on an hourly basis, it could potentially have a temporally linked correlation with the availability of hydrogen. This will likely be an important aspect both for pilot sites and actual full-size industrial units of the future. Fluctuating production of hydrogen should then be taken into account in the dimensioning of the plant components: synthesis processes could for instance be designed to be smaller than what would be required for peak hydrogen production. Storages could then be used to decrease the average cost of utilized hydrogen. If the hydrogen storage costs remain at such high levels, in practice it means that only storages which have a high annual number of discharge cycles are economically feasible. The dynamic performance of the plant and its interconnections with storages are topics which should be investigated further.

2.7 Process components and manufacturing

The processes introduced so far contain well-known technologies with high technology readiness levels (TRLs). The sections of the process are commercially available from multiple suppliers. MTO-MOGD is the only part of the process which has been developed only to a pre-commercial stage. Tabak and Yurchak have reported that a pilot facility with an annual fuel production capacity very close to the case Joutseno (approximately 9 kt vs. 10 kt) was run successfully in the 1980s [5]. It would therefore be possible to commercialize the MTO-MOGD technology yet today. Suppliers of full-scale commercial technologies with specifications are listed in **Table 2.6**.

Table 2.6. List of commercial technology suppliers.

Technology	Supplier	Technology type	Reference
Electrolysis	Cummins	Alkaline, PEM	[21]
	Green Hydrogen Systems	Alkaline	[22]
	Hydrogen Pro	Alkaline	[23]
	ITM Power	PEM	[24]
	McPhy	Alkaline	[25]
	NEL Hydrogen	Alkaline, PEM	[26]
	Siemens	PEM	[27]
	Sunfire	Alkaline, SOEC	[28]
CO ₂ capture	Air Liquide Engineering & Construction	Cryogenic	[29]
	Aker Carbon Capture	Amine	[30]
	Carbon ReUse	Water	[31]
	GE Power	Amine, oxy-combustion	[32]
	Mitsubishi Heavy Industries	Amine	[33]
	Shell	Amine	[34]
	Toshiba Energy Systems & Solutions Corporation	Amine	[35]
MeOH synthesis	Air Liquide Engineering & Construction	Syngas/CO ₂ to MeOH	[29]
	BSE Engineering	n.a. ¹⁵	[36]
	Carbon Recycle International	CO ₂ to MeOH	[37]
	Johnson Matthey	Syngas to MeOH	[38]
	Mitsubishi Gas Chemical	Syngas to MeOH	[39]
Fuel synthesis	Chemieanlagenbau Chemnitz	MTG	[40]
	ExxonMobil	MTG	[41]
	Haldor Topsøe	MTG, syngas to gasoline	[42]
	Sunfire	Fischer-Tropsch	[28]

As is evident in **Table 2.6**, alkaline water electrolysis and amine-based CO₂ capture technologies are the most widely available among the vendors. Methanol synthesis technology is available with a syngas feed consisting of either carbon monoxide or carbon dioxide. Of the fuel synthesis technologies, both MTG and Fischer-Tropsch (FT) routes are available. It is important to notice that FT suppliers are not comprehensively represented in the list as FT was not in the scope of this project. The references given in the table are directed to the homepages of the suppliers where more information about their technology can be found and requested.

Table A1 in Appendix A shows a list of process equipment required in each process step. Valves, additional equipment related to distillation columns (reflux pumps, heat exchangers and decanters)

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¹⁵ Information not available on the company webpage.

and equipment for purge gas combustion and heat generation were excluded from the table. The equipment are organized to the table in an order that follows the direction of interpreting the block diagrams shown in **sections 2.2-2.4**.

Material requirements of the process equipment listed in the table vary between specific pieces of equipment. Chemical contact and operation temperature limit the use of regular carbon steel in some equipment. In general, equipment that are in contact with corrosive chemicals, namely MEA solution, methanol, hydrogen, or sulfuric acid, must be manufactured of more resilient materials. Stainless steels are suitable in most of these cases, but acid-resistant metal alloys are required in sulfuric acid handling. Additionally, stainless steel is considered necessary instead of carbon steel with operating temperatures above 400 °C, and highly heat-resistant metals in >850 °C operation. Hastelloy C was considered for both sulfuric acid contact and high temperature operation.

A summary of the equipment listed in **Table A1** is given in **Table 2.7**. The pieces of equipment are classified based on their basic function. For instance, absorption, adsorption, and distillation columns are listed as "columns". Dual operation of adsorption columns and reactors is also considered in the number of the equipment.

Table 2.7. Number of equipment of the overall process with either MTG or MTO-MOGD as the fuel synthesis

Equipment type	MTG	MTO-MOGD
Centrifugal pumps	5	6
Columns	14	15
Gas/liquid separators	7	7
Heat exchangers	26	34
Liquid/liquid separators	2	1
Multi-stage compressors	3	4
Reactors	12	12
Single-stage compressors	6	7
Total	75	86

Although many of the components used in the P2X environment are quite common in other industrial applications, there is still room for development in many aspects. Innovations in manufacturing and design are crucial for increasing the competitiveness of P2X. Scale-up of production is one of those aspects, for which there are fundamentally two approaches. Either the bulk production of identical components in series, or by designing and manufacturing larger equipment and modules. Practical weight and size restrictions come into play at some stage for the latter approach, which leads to the fact that an optimal solution utilizes both approaches in certain extent.

Detailed design of the plant and individual components was outside the scope of this project. Developed process analysis tools and the understanding obtained in this project can still be capitalized later on. The physical dimensions and requirements of vessels and equipment form the starting point of construction design, which can then be taken further to analyze the extent of subcontracting, raw material selection and availability of desired sizes, for instance.

Recently, LUT has taken steps to increase its competence in the manufacturing and design of electrolysers, which is a natural continuum to this project. At this stage, manufacturing of electrolysers still involves some manual labor steps, and global production capacity is likely to increase manyfold in the coming decades. These types of initiatives could bridge the gap between theoretical understanding of processes and manufacturing of equipment and components.

3 Business models

In addition to the techno-economic analysis carried out in this work, a preliminary screening of P2X markets and potential business models were also analyzed. Market survey was conducted as expert interviews to get insights of future P2X fuel markets. The results create the basis for business model development and profitability modelling. The purpose was creating understanding about the ecosystem around P2X fuel production, what kind of business models could be created and how the demand and pricing of P2X fuels will develop in future markets to support the profitability analysis.

3.1 Market expert survey

Market survey was conducted as semi-structured interviews where 12 interviews were made, in 6 organizations, and 13 people were interviewed in total (see **Table 3.1**). Interviews were conducted during May-June 2020. Interviewees are experts in the fields of oil and energy industry, representing both the supply and demand side, including manufacturing and engineering companies. The interviewees are well aware of the fuel market and have insights of the future developments in fuel markets. The structure of interviews and interview questions are presented in Appendix B. Semi-structured interviews comprised four themes and 11 questions in total. The discussed themes were P2X products and supply, demand, price, and business models/sales contracts. The aim was to investigate the potential and development of P2X fuel markets now and in future, and to create an understanding about the pricing principles of fuels for the basis of profitability analysis.

Table 3.1. Background information of expert interviews

Date of interview	Characterization of interviewees' company	Number of interviewees
15.5.2020	Energy company	1
19.5.2020	Research institution	1
28.5.2020	Airline company	1
1.6.2020	Oil refining and marketing company	2
2.6.2020	Manufacturing and engineering company	1
3.6.2020	Energy company	1
3.6.2020	Energy company	1
8.6.2020	Manufacturing and engineering company	1
11.6.2020	Airline company	1
17.6.2020	Energy company	1
22.6.2020	Manufacturing and engineering company	1
23.6.2020	Manufacturing and engineering company	1

3.1.1 Definition of future markets of P2X fuels

First theme discusses why P2X products are interesting and what are the benefits and disadvantages compared to the competing fuel alternatives. The produced products in discussion were P2X technology based synthetic fuels including a) hydrogen, b) methanol, c) gasoline, d) diesel, and e) kerosene. Competing fuel alternatives for P2X fuels were named by the experts to be fossil fuels, biofuels, advanced biofuels, battery technology and hydrogen. However, it was stated that P2X fuels cannot compete with fossil fuels because "they will always be the cheapest choice". The main competition would be with advanced biofuels, in short-term, and battery technologies and hydrogen in the long run. It was also noted that in certain segments, such as aviation, liquid fuels are necessary for long time and the electricity/batteries are feasible only in short-distance flights. It was also mentioned that P2X fuels are the "only sustainable solution" for fossil fuel and by this it was meant that other liquid fuels cannot be as sustainable as P2X fuels due to the endless discussion about the source and sufficiency of biofuels. **Table 3.2** summarizes the main findings what are the main benefits and challenges of P2X fuels and why they are seen as an interesting solution in fuels markets.

Table 3.2. Pros & Cons of P2X fuels.

	Pros	Cons
Product	 Drop-in fuel, no limits in blending Distribution infrastructure exists (similar to e.g. liquid fossil fuels) 	
Raw mate- rial	 Endless raw material: water, (green) CO₂, renewable energy Do not compete with food production (compared to biofuels and advanced biofuels) 	 The need of (green) electricity The source of CO₂, the low carbon content of air
Technology	Technology is developing (e.g. electrolysers)	 Resource efficiency Technology needs to be tested in plant/industry scale
Price	If included in regulation, the price will be at good level for a long time	 High price There is no market unless P2X products are treated equal to advanced biofuels (regulation & premium price) Only way to be profitable is to get fossil fuel price + premium
Segment specific notes	 Distribution infrastructure e.g. in road transport Liquid fuels are needed in certain segments for a long time (e.g. aviation) Environmental awareness increases demand/interest in multiple sectors 	 Distribution infrastructure in certain segments (e.g. aviation, marine) Regulation is needed at global level (e.g. marine, aviation) High price reflects in high prices for consumers (flying tickets, cruises)

3.1.2 Demand development of P2X fuels

According to interviews, the main critical factors for the demand development of P2X fuels were named to be inexpensive green electricity and regulation. It was said that there is no market before P2X fuels are included in EU level regulation, e.g. RED II directive, and thus to be included in distribution obligations and treated similarly to advanced biofuels. This allows to use premium price. If P2X fuels are included in regulation, demand exceeds the supply for a long time (both advanced biofuels and P2X fuels). Challenge is at global level, and thus at least EU level decisions need to be made. There could also be regional regulations, but the global level regulation is needed as well. Ambition and right actions to get rid of fossil fuels are needed.

In early phase, the demand is close to the end-users of fuels and brand and sustainability pressures are remarkable in certain customer segments, such as aviation and marine. Also, in road traffic has the pressure to decrease fossil fuels but in traffic the brand pressure is not as remarkable as in aviation and marine, where especially the flights and cruises can be seen luxury and consumers are more and more environmentally conscious (e.g. in Germany).

Remarkable change in demand is expected to happen around 2030, which means that during next 10 years, prerequisites for P2X fuel production need to be implemented and tested to enable the full-scale production. The interviewees had two different visions of the speed of demand growth and some of interviewees thought it would take more likely 15-20 years before P2X fuels can significantly replace fossil fuels.

According to the majority of interviewees, the development in demand can be presented as follows: During the next

- 5 years, nothing will really happen
- 10 years, demand will slightly grow
- 15 years, demand will increasingly grow
- 20 years, demand will keep growing

However, this development requires that right decisions are made today. Although the market pull is not high in the next 5-10 years, the decisions made today are prerequisite to success in 15 years. Regulation was seen a key to launch and increase the production to industry scale, which enables economics of scale and the production costs can be minimized.

Next, some segment specific observations and highlights are discussed:

Aviation

In aviation social pressure is significant driver in the transition to "the green aviation". Flying can be seen as luxury and the demand of sustainable aviation fuels is partly relying on the customers' willingness to pay more to compensate the emissions of flying. According to interviews, the airplanes do not fly only with batteries or hydrogen for a long time, and liquid fuels are needed at least in long distance flights. That makes P2X based kerosene interesting.

The main challenges in sustainable aviation fuels and especially P2X fuels is the sufficient volume of fuel production. There needs to be enough P2X technology-based kerosene available so that it

can be considered a reasonable alternative as a sustainable fuel. In aviation, the fuels need special standardization and certification which causes the challenges and restrictions for the location of fuel production. The price of P2X based kerosene also reflects as higher fuel prices and means higher price for flying tickets. In aviation, airlines operate globally which sets challenges for regulation that needs to treat airlines fairly.

Marine

Internationality and exemption from taxes set challenges in marine for P2X based fuels, especially if the price of fuels is considered. Thus, global actions are needed. Another challenge was named to be the distribution and refueling infrastructures, because not all the fuels are available at harbors. Vessels may be transferred to the other side of the world during vessel's long lifetime and similar requirements for distribution and refueling infrastructure are needed across the world. It was also mentioned that the availability of methanol and biodiesel is limited and thus, LNG is the most popular fuel in new vessels. However, usually the vessels are capable of changing the fuel from LNG to diesel if needed. The price is also challenge as the price for LNG is around 500-600 €/t and the synthetic fuels should not cost more than 10-20% over LNG price.

The main drivers for P2X fuel demand in marine can be seen as the environmental and sustainability targets (e.g. by 2050, 50% reduction in CO₂ emissions). First, cruisers could be interested in P2X fuels if compared to freight where the low fuels costs are the most important factor. Cruises can be seen as luxury and unnecessary environmental load and consumers might be interested in paying a little bit higher ticket prices, as the cost per ticket is not that remarkable if there are several thousands paying customers in cruise. The most interesting P2X based fuels were seen as follows: 1) diesel, 2) methanol, 3) hydrogen.

Road traffic

In road traffic, especially in heavy traffic, the liquid fuels are competing with gas fuels in future. Whereas in passenger car traffic, electricity/batteries are competing with renewable liquid fuels. The advantage of P2X fuels is the existing infrastructure but the competition is with the advanced biofuels that already are included in distribution obligations. With the aid of regulation, for example, Finland, Sweden and Norway have promoted the biofuels to road traffic instead of e.g. aviation.

3.1.3 Price development of P2X fuels

Price development of P2X fuels is strongly depending on the regulation and the production volumes of competing fuels. The evaluation of P2X fuels' prices is challenging because there is no price or market at the moment. However, interviewees strongly believed that P2X fuels would be or at least should be included in regulation and get the premium price, and thus compete with advanced biofuels.

Therefore, the price comparison should be made to advanced biofuels, and not to fossil fuels, because fossil fuels will always be the cheapest option. According to interviews the price is expected to be at same level with advanced biofuels, which means about threefold fossil fuel price.

Other assumption for price of P2X fuels were related to the actual CO₂ reduction calculations, and to that reduction, the premium can be paid (fossil price plus premium based on CO₂ reduction). The price for CO₂ reduction has been around 300-400 €/t CO₂.

However, in addition to the regulation, demand will define the market price rather than production costs. It can be expected that the price will remain high for relatively long time because there is limited amounts of competing products and market entry takes time.

Other factors affecting to the price development of P2X fuels can be named as: decreasing production costs over time when economies of scale can be achieved and cost of renewable energy (electricity) decreases.

3.1.4 Business models / Selling contracts

Interviewees were asked what kind of business models or what kind of selling contracts exists in fuel markets if considering especially new (pilot) plants producing carbon dioxide free synthetic fuels. It was said that there can be different types of contracts in fuel markets, long and short contracts (e.g. from six months to ten years) or contracts of buying only certain amounts of fuel occasionally. However, when it is a question of new market or new fuel products, the contracts may be long contracts and purchasers are willing to commit to buy for example the total production during the next years. Usually in new markets the contracts are offtake agreements and in mature markets the contracts are short ones. Often the prices are bound to the changes in fuel markets.

3.2 Ecosystem analysis

The term business ecosystem is used to describe a network of varying actors that interact with each other. The actors can be profit or non-profit organizations. The purpose of the ecosystem map is to visualize an ecosystem by illustrating connections between ecosystem actors. The nodes represent companies and the lines represent connections between the companies (**Figure 3.1**). Companies can analyze their own business, and the strength and success of their suppliers, partners and competitors by using ecosystem approach [43].

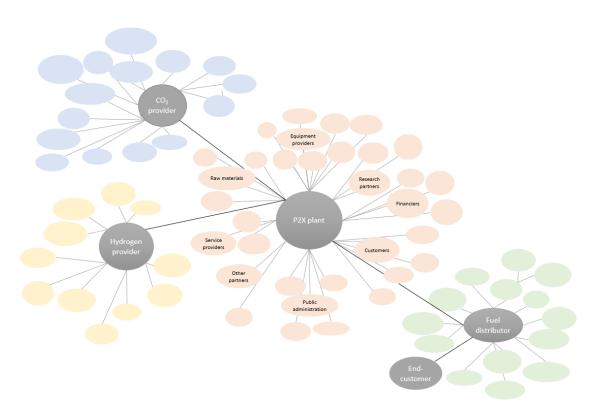


Figure 3.1. P2X Ecosystem map (general view).

Main raw material providers of P2X Joutseno plant are Kemira (hydrogen) and Finnsementti (CO₂). In addition, water, electricity, and steam are needed. Potential technology suppliers for electrolysis, CO₂ capture, MeOH and fuel synthesis are listed in **Table 2.6**.

Service providers for operation, maintenance, logistics and transportation are needed to support the company's manufacturing operations. The P2X Joutseno plant co-operates also with the public authorities like City of Lappeenranta, Finnish Government, Ministry of Economic Affairs and Employment of Finland (TEM), European Union, and Regional Council of South Karelia. Potential research partners are LUT University, St1, Wärtsilä and Hannes Snellman. Financiers represent both

the public and private sectors: TEM, financial institutions, and private investors. Potential customers for the plant's products have been identified through market research. Main customer segment is fuel distributors (road traffic, aviation, and harbor/marine). Other potential customer segments could be the adhesive and plastic industries.

This kind of ecosystem analysis offers big picture for detailed business models and profitability analysis following. It also gives possibilities to take account different interests of various actors in real business cases. Sometimes it can help to find evolutionary collaboration options and relationships during the planning process.

3.3 Business model scenarios

Business model canvas (BMC) was chosen to be the framework for describing the different business model scenarios that could be possible in the P2X Joutseno project. BMC was used because it provides a complete view to a business model in a single figure and because the framework is widely known and used both in academia and industry. The purpose of the business model scenario work was to identify possible routes for commercializing the project outcomes, but not going too much into details on how the business model would be implemented. The information available was not detailed enough for building a business model that could be used in the actual implementation phase.

While BMC is a valuable tool for describing different scenarios, it has a few shortcomings. First, it is a static description of the operational business and therefore does not include the investment phase of the project except in interest costs. Second, it does not show the value transactions between all members of the partner network. Third, it would require numerous iterations to create a business model canvas that could be used in operational business, because in each of the scenarios there are lots of assumptions that have not been validated.

The chosen six business model scenarios are:

- 1. Joutseno pilot plant
- 2. Global P2X production plant
- 3. Methanol production plant
- 4. Olefin production plant
- 5. P2X pilot platform
- 6. P2X plant engineering consultancy

Each of the scenarios is next described with their respective initial BMCs.

3.3.1 Joutseno Pilot plant

The BMC for first scenario, Joutseno Pilot plant, is presented in **Figure 3.2** This scenario concentrates on the business case of the pilot plant to be built in Joutseno. In this scenario, the hydrogen used in the process is sourced from a partner rather than generated on-site. The production partners have been identified in the project and that makes this scenario the most applicable for implementation. The success of this scenario is based on low cost of hydrogen and positive application of RED II regarding synthetic fuels.

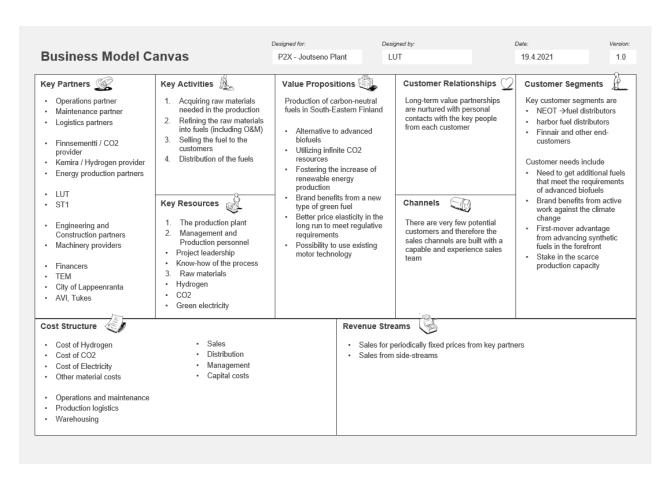


Figure 3.2. Joutseno Pilot plant.

The value proposition of this business model scenario is to produce carbon-neutral fuels for road and marine transport and aviation. Additionally, the scenario provides both brand benefits and first-mover advantage for customers investing early in synthetic fuel production. The value creation process involves collaboration between a wide range of companies and organizations. The cost

structure has been described in detail in this report and possible revenue streams depend on numerous factors that are difficult to quantify exactly, as described earlier in this chapter.

3.3.2 Global P2X production plant

The second scenario, BMC for global P2X production plant (see **Figure 3.3**), is identical with the first one, except that it aims in building an industrial scale plant for bulk production of synthetic fuels. It includes a lot more speculation regarding partners, customers, and location and sources of green electricity and CO₂. However, it provides a basis for building a scalable production plant that is required to lower the production costs of synthetic fuels to be more competitive. The pre-requisite for this scenario too is that synthetic fuels are treated equally with advanced biofuels in regulation. There are many open issues in this scenario including the decisions regarding which fuels would be the most profitable to produce and regional differences in regulation that affect the demand of synthetic fuels.

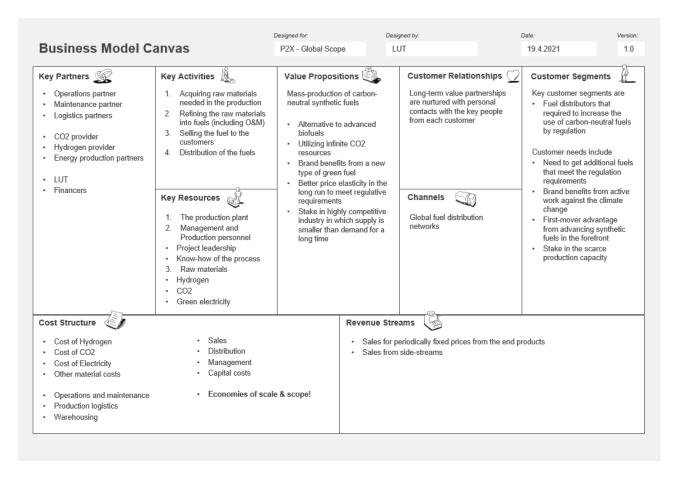


Figure 3.3. Global P2X production plant.

Main differences between Joutseno pilot plant BMC and the global scale BMC are in the scale of production and sales of the end products. This scenario aims at 30x production scale compared to

the Joutseno plant, meaning that there would have to be very large demand for synthetic fuels for a price that would be lower than in the pilot plant, but still rather high compared to competitors. The main advantage of this business model is the opportunity of building on economies of both scale and scope. The plant is capable of producing large amounts of fuels and the output can be directed to the ones that are most profitable.

3.3.3 Methanol production plant

The third business model scenario, BMC for methanol production plant (see **Figure 3.4**) alters the approach of the pilot plant considerably. In this scenario the production process aims in producing methanol instead of refined fuels, which makes the process considerably less complex and expensive. Naturally, methanol as the end product is aimed at different markets. Possible target markets would be plastics, adhesives and other chemical industries that would benefit from carbon-neutral methanol in their own production processes.

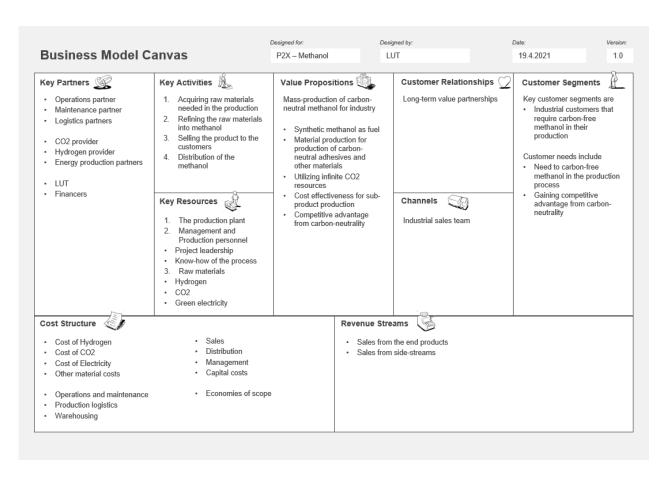


Figure 3.4. Methanol production plant.

The main difference of this BMC compared to previous ones is in the value proposition and targeted customer. Providing carbon-neutral methanol as a material for industrial production is less

appealing to synthetic fuel production, but it appears to be in high demand as carbon reduction is very hot topic in all industries. As the production process is simpler than the previous one, this scenario could be very feasible.

3.3.4 Olefin production plant

This scenario, BMC for olefin production plant (see **Figure 3.5**) aims in between the previous ones: refining methanol further but ending at olefin stage rather than continuing to the drop-in fuels. This too would make the investment and production costs much lower than in the first two scenarios. The customers for the plant would be refineries that are in demand of carbon-neutral olefins to produce more synthetic fuels. This scenario benefits from existing refineries and could provide a shortcut to producing synthetic fuels with lower investment costs compared to fully functioning P2X plant.

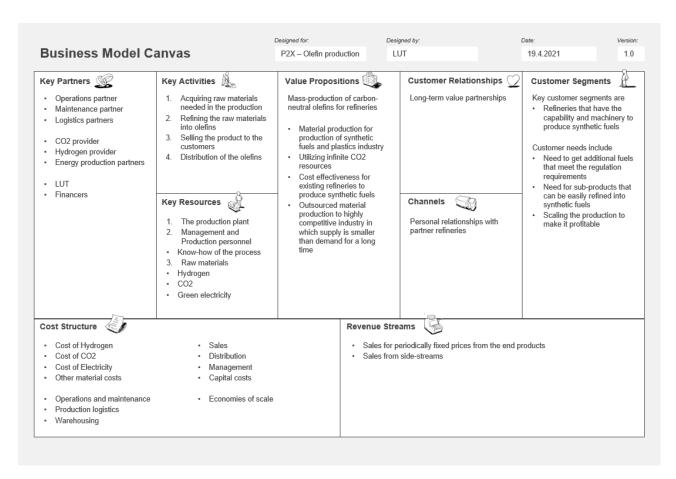


Figure 3.5. Olefin production plant.

Main difference of this BMC compared to the methanol production BMC is the scope of customers. In this scenario, the customer basis comes from fuel refineries, and there are such synergies

between the two processes that it could provide a good opportunity for a fuel producer to invest in olefin production plant situated close to their refinery.

3.3.5 P2X pilot platform

The fifth scenario, BMC for P2X pilot platform (see **Figure 3.6**) is very different from the previous ones. It aims at utilizing the P2X Joutseno plant as a piloting platform in which companies could test and develop their P2X technology in real life working environment. The investment would be much lower than a fully functioning plan – somewhere close to 4 M€. This scenario can help organizations make investments in P2X technology easier by reducing the uncertainty of building industrial-scale processes by testing them before deciding to invest in them.

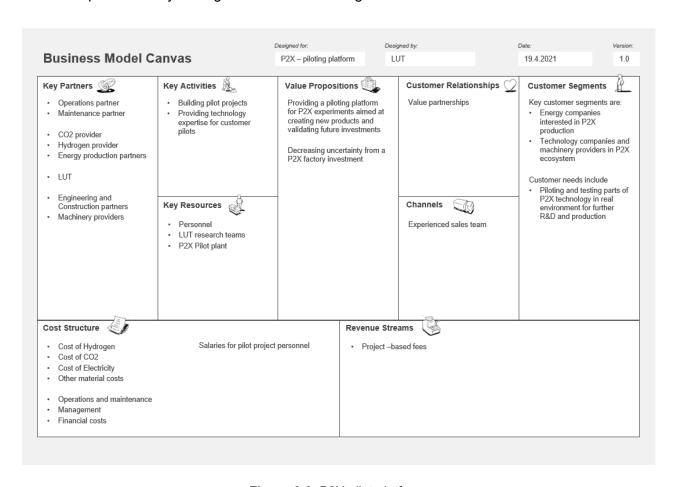


Figure 3.6. P2X pilot platform.

This BMC description is different to the previous ones in almost all aspects. The value proposition is to provide an industrial testbed to decrease uncertainty within P2X investments. Possible customers include energy companies, technology companies and machine providers in the P2X ecosystem. The value creation process concentrates on building and maintaining a functioning plant and facilitating industrial testing and experimentation for customers.

3.3.6 P2X plant engineering consultancy

The final scenario, BMC for P2X plant engineering consultancy (see **Figure 3.7**), describes a consulting business opportunity that builds on the cumulative expertise that is going to be obtained in building the pilot plant and P2X research at LUT. The business does not require utilization of the plant but is based on engineering competence of specialists in different areas of P2X production process.

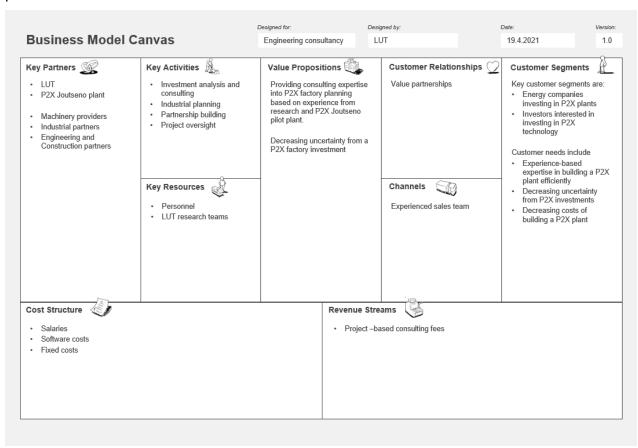


Figure 3.7. P2X plant engineering consultancy.

The value proposition of this sixth BMC is similar to the previous one: to decrease uncertainty from a P2X investment. Approach is rather different, though. In this scenario, the value creation comes from engineering competence rather than providing a testbed and in addition to investment planning, the expertise of personnel can be utilized also in actual engineering of P2X plants. This is a rather straightforward engineering consulting business model.

4 Profitability

Profitability analysis of P2X Joutseno pilot plant was done by developing an investment model using discounted cash flow method. The profitability model was realized as an Excel tool and it combines the elements of CAPEX costs, OPEX costs, pricing principles and demand expectations from market survey (see **section 3.1**). The components affecting to the development of profitability model are presented in **Figure 4.1**.

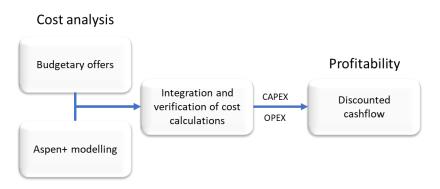


Figure 4.1. Development process of profitability model.

Cost analysis started with Aspen Plus modelling and requesting of budgetary offers¹⁶ from equipment suppliers. Investment cost estimates were calculated based on the simulation models according to methodology presented in **section 4.1**. After the integration and verification of cost calculations based on Aspen modelling and budgetary offers, CAPEX and OPEX costs were determined and used as input data in the profitability model. Revenues in profitability model are based the presumptions that P2X fuels can get premium price (fossil price plus premium) and the market for P2X fuels exists (included in regulation). These presumptions for revenue streams are based on the results of market survey and assumes that there is market for P2X fuels in future. Other input data in profitability analysis are discussed in **section 4.2**.

P2X Joutseno investment, Base case -model analyses the profitability of MTG production process where the end product is gasoline. CO₂ would originate from cement industry and hydrogen from chemical industry as a unused residue of current production. The profitability model is developed for a 20-year time period, that is usual for projects in plant investments in general. It has also been assumed that there is no residual value at the end of the time period, which is related to the

¹⁶ The budgetary offers include information under NDA and are not discussed in this report

assumed useful life for this kind of plant. The profitability model takes into account the time value of money and the profit requirements from financing.

The profitability model applies discounted cash flow method, calculates number of key figures such as Net Present Value (NPV) and Internal Rate of Return (IRR), and makes sensitivity analysis with key variables. **Section 4.2** describes in detail the structure of the investment model. The calculated key figures are discussed in detail in **section 4.3** and sensitivity analysis in **section 4.4**. The structure and data contents of the model has been developed in several collaboration workshops and discussions between business and technology teams.

The developed model can be fitted or extended for analyzing other technology variations and processes as well. P2X Joutseno investment, Base case -model was further developed during the research project and **section 4.5** describes the further developed model and different scenarios that were calculated with that further developed model.

4.1 Aspen

Aspen Process Economic Analyzer (APEA) tool was used to determine the purchased costs of major process equipment based on the Aspen Plus simulation models. The APEA tool estimates the costs by performing initial dimensioning of the equipment and comparing the results against a comprehensive reference database. The costs are given on US\$ $_{2018}$ and U.S. Gulf Coast basis, and they were converted to Finnish prices with a currency rate of 0.87 US\$ $_{2018}$ / \in $_{2020}$ and a location factor of 1.2 [44]. Accuracy of the equipment cost estimates is approximately $\pm 30\%$. The purchased major equipment costs were converted to inside battery limits (ISBL) costs with **Equation (5)** by taking several installation factors into account [45]. Of the components, the equipment and piping connected to them are subject to the material selection that is determined with a material factor. The factor describes the relation of carbon steel to more refined and expensive materials. **Equation (5)** can be simplified to the form of **Equation (6)** by a material-dependent installation factor $f_{tot,j}$. Values of the factors used in the calculation are given in **Table 4.1**.

$$C = \sum_{i=1}^{n} C_{e,i} [(1 + f_{p}) f_{m} + (f_{er} + f_{el} + f_{i} + f_{c} + f_{s} + f_{l})]$$
 (5)

$$C = \sum_{i=1}^{n} C_{e,i} \cdot f_{\text{tot,j}}$$
 (6)

where C ISBL cost, M€

- C_e Purchased major equipment cost, M€
- i Number of equipment
- n Number of processes
- i Material selection

Table 4.1. Installation and material factors used in Equation (5)and (6). In the table, CS stands for carbon steel, SS for stainless steel and HC for Hastelloy C **[45]**.

	j	CS	SS	HC
Piping	f_p	8.0	8.0	8.0
Equipment erection	f_{er}	0.3	0.3	0.3
Instrumentation and control	\mathbf{f}_{i}	0.3	0.3	0.3
Electrical	f_{el}	0.2	0.2	0.2
Civil	fc	0.3	0.3	0.3
Structures and buildings	f_s	0.2	0.2	0.2
Lagging and paint	f_{l}	0.1	0.1	0.1
Material factor	f_{m}	1.0	1.3	1.6
Sum of factors	\mathbf{f}_{tot}	3.2	3.7	4.3

Table 4.2 shows the estimated purchased major equipment costs and calculated ISBL costs with the three different equipment and piping materials. The equipment costs do not include valves, trays or packings for distillation columns, or any equipment related to utility systems. The costs are tabulated for each process separately and for the complete process with either MTG or MTO-MOGD fuel synthesis.

Table 4.2. Purchased equipment costs obtained from the simulation models and ISBL costs calculated with Equation (6).

Process	Purchased cost of major equipment, M€	ISBL cost _{cs} , M€	ISBL cost _{ss} , M€	ISBL cost _{HC} , M€
CO ₂ capture (1)	4.3	13.7	16.0	18.3
Gas treatment (3a)	3.4	10.8	12.6	14.5
MeOH (3b)	2.6	8.3	9.7	11.1
MTG (4)	3.7	11.7	13.7	15.6
MTO-MOGD (5)	6.9	22.0	25.7	29.5
Total _{MTG}	13.9	44.5	52.0	59.5
Total _{MTO-MOGD}	17.1	54.8	64.1	73.3

As can be seen in the table, compression ratio and overall complexity of the processes are translated to higher equipment costs. CO₂ capture, for instance, is rather simple process with few process equipment but compression to the transport conditions is expensive due to high investment costs of the compressors. The effect of compressors can be also observed in the case of methanol synthesis as the process includes compressors with only mild pressure increases even if the MeOH

process contains more equipment in total. On the other hand, MTO-MOGD is the most complex process with the most synthesis steps and equipment. Material selection also clearly affects the investment when comparing the range of ISBL costs. It should be noted that more resilient materials are required only in some areas of the processes, but the ISBL costs with stainless steel can be considered as average values that are neither overly optimistic nor pessimistic.

4.2 Modelling the profitability

This section describes the structure of investment model developed as an Excel tool. The developed model applies discounted cash flow method, calculates number of key figures such as NPV and IRR, and makes sensitivity analysis with key variables.

The Excel model comprises of five sheets including source data, construction phase, cash flow calculation, key results, and sensitivity analysis. P2X Joutseno investment, Base case -model analyzes the profitability of MTG production process, where the end product is gasoline and feed-stocks originate from cement industry (CO₂) and chemical industry (residual hydrogen which is formed as a by-product of current production).

Source data (Sheet 1)

Source data combines all essential input data, including

- Operation time (h/a)
- Annual production amounts of end products and by-products (from Aspen modelling, see section 2.4.5)
- Production ratio %, availability
- Technical investment costs, including investments in hydrogen, CO₂, MeOH and MTG syntheses, auxiliary systems, electricity connection fees, infrastructure (roads etc.), buildings, engineering, interest and expenses during construction, bank's fees, land lease before the start-up, and permitting
- Reserve (%)
- Working capital addition (cash reserve)
- Financing, including investment subsidy (%) (TEM), debt (%), equity (%)
- Selling prices (€/t) for end products and by-products
- Costs and expenses during operation, including land lease, operation costs as percentage
 of actual revenue, maintenance costs as percentage of technical investment, electricity

consumption and price, steam consumption and price, hydrogen consumption and price, carbon dioxide consumption and price, real estate tax, insurance costs, administration costs (percentage of actual revenue)

- Other source data, such as rate of inflation, income tax %, number of debt amortization, debt rate, straight-line depreciation (years), residual value, cost of equity and change % of WACC (weighted average cost of capital).

Input data to annual production amounts and annual consumptions of electricity, steam, hydrogen and carbon dioxide are based on Aspen modelling and are discussed in detail in **section 2.4.5**. Input data to technical investment costs are based on budgetary offers and knowledge of expert in project team. Input data to selling prices of end products are based on market analysis (**section 3.1**) and the knowledge of experts in the project.

Input data to prices of raw materials (electricity, steam, hydrogen, and CO₂) are based on the knowledge of experts in the project and existing market prices.

Construction phase (Sheet 2)

Construction phase describes the cash flow and financing of the construction phase. Construction phase lasts 24 months and is divided into 6 months of engineering and 18 months of actual construction. The total technical investment costs are divided into this 24-month period and creates the monthly cash flow and financing need.

It was assumed that engineering phase takes first 6 months and spends 10 % of total technical investment. The remaining 90 % of total technical investment is divided to the construction phase that lasts the rest 18 months.

Financing consist of investment subsidy (TEM), debts and equity. In addition to the total technical investment, base cash (during construction) and interest costs during construction are included in the net cash flow of the construction phase.

In construction phase, also the interest and expenses during construction phase are calculated and they need to be taken into account in the total investment costs.

Cash flow (Sheet 3)

Cash flow sheet describes the calculation of cash flow during operation phase of the plant. Time period is 20 years, and all base investment costs are allocated to the first year. The model presents two types of cash flows: discounted net cash flow and investor's cash flow.

Discounted cash flow follows the traditional investment appraisal methods and comprises the elements of investment costs (CAPEX costs), revenues and OPEX costs and thus they formulate the net cash flow. Total investment costs are defined in the source data and in the cash flow sheet, the assumed subsidy (TEM) is reduced from the total investment costs, and this is the investment cost in cash flow. Revenues are based on the sales of the end and by-products. OPEX costs include annual costs, such as operation and maintenance (O&M) costs, electricity costs, steam costs, hydrogen costs, CO₂ costs, real estate tax, insurance costs, land leases and administration costs. In discounted cash flow, WACC is used as the interest rate. Based on discounted cash flow, key figures such as NPV, IRR, payback time (with and without interest) and Benefit-Cost ratio (B/C ratio) are calculated.

Investor's cash flow is based on profit that is calculated from operating margin (that is same as net cash flow) of each year and decreased by debt amortization and debt interest costs (**Equation (7)**).

$$Profit = operating margin - debt amortization - debt interest costs$$
 (7)

Investor's cash flow regards as an investment the investor's equity and the cash flow is based on the profit. The shares of subsidy, dept and equity are defined in source data sheet. Based on the investor's cash flow, key figures such as IRR (investor), Investor's Return on Equity (ROE), Debt-service coverage ratio (DSCR), Dividend % and Moneyback are calculated.

Results (Sheet 4)

Results sheet collects the results of key figures and presents the results from two views: Total investment view and Investor view. Total investment view collects the key figures resulted from discounted cash flow and includes IRR, NPV, payback time and B/C ratio. It also gives the decision criteria for the different key figures (e.g. if IRR > WACC, the investment is profitable). Investor view collects the key figures in which the investor is interested and are based on the investor's cash flow. It presents the key figures such as IRR (investor), ROE (average), Moneyback and DSCR. Results sheet also presents figures demonstrating the investment cash flow, the components of technical investment, OPEX costs, and the development of revenues.

Sensitivity analysis (Sheet 5)

Sensitivity analysis is conducted as one-variable sensitivity analysis. Base case is calculated with certain input data values and then essential variables are selected (e.g. electricity price, hydrogen price, operation time, end-product price etc.). Input data values have been changed by one variable at a time. The range of changing variable has been selected to be realistic expected minimum and maximum values. Sensitivity analysis is made for each key figure, but IRR (investor) has been selected to be investigated more carefully.

4.3 Analysis of results

Investment profitability model describes the cash flow of the investment project and calculates numerous key figures that can be used to evaluate the profitability of the investment.

The selected key figures that evaluate the profitability of total investment are NPV, IRR, Payback time and B/C ratio. According to the decision criteria for each key figure, the P2X Joutseno investment is profitable with selected input values (see **Figure 4.2**). It needs to be acknowledged that the input values include 40 % subsidy (TEM), and the remainder is financed 70 % dept and 30 % equity. In addition, the total investment included 15 % reserve and the revenues are based the premium prices for the end products. The interest rate in discounted cash flow is WACC, that takes the financing, the shares of equity and debt, and their profit requirements into account. The profitability of investment can be evaluated by comparing IRR of investment to the WACC. Because the IRR exceeds WACC, the investment can be considered profitable. Parallel results can be noticed from NPV of the investment and from **Figure 4.3** that illustrates the net cash flow, discounted cash flow and discounted cumulative cash flow during 20 years time period and indicates that NPV is around 21 million euros.

B/C ratio shows whether the total discounted benefits overrun the total discounted costs of investment, but it also shows the ratio of the benefits overrunning the costs. Thus, it compares the cash flow and the size of investment. The decision criteria for B/C ratio gives the similar results as the other key figures that measure the profitability, but it needs to be acknowledged that the value is relatively low. That means that the benefits are relatively low compared to the size of investment.

In Investor's view, the key figure of IRR (investor), the investor decides the profit requirement for the investment. In principle, the IRR (investor) is compared to the cost of equity that was defined in this case 6 %. Thus, the investment seems to be profitable also from investor's point of view.

ROE tells what kind of profits investor earns to invested equity and Moneyback shows how soon invested money flows back to the investor. DSCR considers how high is firm's operating cash flow compared to its obligations (i.e. interests and repayments) for debt financier.

The selected key figures cover different aspects to profitability of the project. Based on input data and assumptions total investment seems to be profitable with both absolute and relative measures. Investor's view is positive as well, i.e. earnings to equity are adequate and risks can be managed.

Total investment view						
IRR	7,1 %	>	3,20 % profitable			
NPV	20 776 847 €	>	0 profitable			
Payback	10,6 ye	ears				
B/C	0,4	>	0 profitable			

Investor view		
IRR	12,1 %	
ROE (average)	18,9 %	
Moneyback	3,8x	
DSCR	1,8x	

Figure 4.2. The profitability of P2X Joutseno investment (Base case), results of key figures from total investment point of view and key figures from investor's point of view.

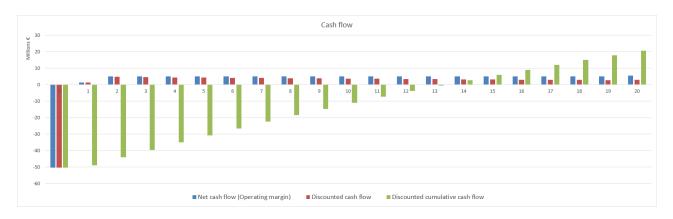


Figure 4.3. Cash flow of P2X Joutseno investment (Base case).

4.4 Sensitivity analysis

Based on one-variable sensitivity analysis, the most critical factors for the profitability of the investment can be analyzed and the results of sensitivity analysis can be used to consider risk factors of the investment. The most critical variables for the profitability of P2X Joutseno investment (Base case), can be interpreted from **Figure 4.4**. The most critical factors are:

- Selling price (gasoline),
- Operation time,
- Hydrogen price and
- Total investment

It can be noted that the electricity price is not as significant as it might be expected because of the source of hydrogen. When the hydrogen is purchased, it won't be produced by electrolyser, which consumes a huge amount of electricity. In this base case, where the source of hydrogen is the residual hydrogen from chemical industry, the actual price of hydrogen is thus more remarkable than the electricity price.

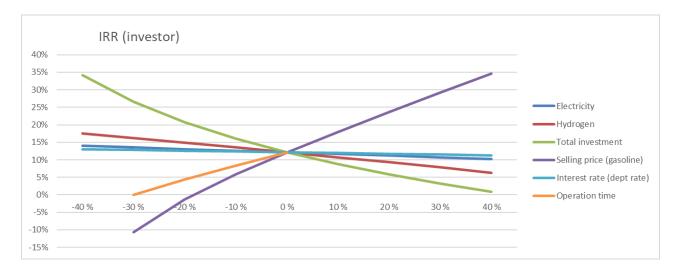


Figure 4.4. One-variable sensitivity analysis, changing variables.

However, Figure 4.4 does not take into account the realistic changes of each variable, but the scale may differ depending on the changing variable. For example, it can be assumed that the price of electricity cannot increase by 100% from the value in base case but realistic scale could be 20-50 €/MWh. On the other hand, the price of hydrogen may have wider and the least certain range in the input values. That is why the IRR (investor) has been investigated more carefully with realistic range of input values for the essential variables. This sensitivity analysis in one variable has been presented in Figure 4.5, which shows that the most critical factors are hydrogen price, price of gasoline and operation time. It can be assumed that these variables also include the biggest risks and uncertainty which values realize. For example, there is still discussion about the possibility to get the premium price for the P2X technology-based fuels and what are the criteria (e.g. green carbon dioxide, source of hydrogen etc.).

				Base case			
Electricity price €/MWh)		20	30	40	50		
IRR (investor)		14,4 %	13,3 %	12,1 %	11,0 %		
Hydrogen price (€/MWh)			10 (0,3 €/kg)	15 (0,5 €/kg)	20 (0,6 €/kg)	25 (0,8 €/kg)	30 (1 €/kg)
IRR (investor)			16,7 %	12,1 %	7,3 %	2,1 %	-3,9 %
Total investment (reserve)	-30 %	-15 %	0 %	15 %	30 %		
IRR (investor)	43,9 %	27,4 %	18,2 %	12,1 %	7,8 %		
Gasoline (€/tn)	1000	1200	1300	1400	1600	1800	
IRR (investor)	-9,1 %	3,0 %	7,7 %	12,1 %	20,5 %	28,4 %	
Debt rate			1 %	2 %	3 %	4 %	5 %
IRR (investor)			13,3 %	12,1 %	11,0 %	10,0 %	9,0 %
O&M				2% & 3%	3% & 4%	4% & 5%	
IRR (investor)				12,1 %	7,8 %	3,3 %	
Operation time		6000	7000	8000			
IRR (investor)		2,2 %	7,4 %	12,1 %			
Investment subsidy (TEM)			30 %	40 %	50 %		
IRR (investor)			9,1 %	12,1 %	15,9 %		
			·				

Figure 4.5. One-variable sensitivity analysis: effects of variables to IRR (investor).

4.5 Scenario descriptions

During the research project, the Joutseno Base case was further developed in the P2X investment model as more details were obtained from Aspen modelling and other analyses. Also, the other process pathways (MeOH, MTO-MOGD) were developed. Comparison of the different scenarios is shown in **Table 4.3**. The base case was technologically based on MTG process, but the improved profitability of the MTG 2.0 case is mostly attributable to the increased sale prices of products. The assumed basic prices of products are given in

Table 4.4. Prices are based on an estimate of the fossil selling price of the product with an additional premium of 300 €/tonCO₂ and an emission reduction level of 90 %.

Table 4.3. Summary of scenario performance and main differences. Investment prices include a 15% contingency reserve.

Case	Description and comments	Total in- vestment (M€)	Investment subsidy (M€)	tor IRR	NPV (M€)
Base case	Initial first draft for plant profitability analysis	67.6	26.4	12.1	20.8
Base case electroly- sis	Initial first draft for plant profitability analysis using electrolyser-sourced hydrogen	117.5	40.1	-	-166.2
MTG 2.0	Basic route to drop-in-fuels. Compared to the base case, most critical changes are Upgraded product prices and investments Utility consumptions revised (e.g. electricity) Catalyst renewal cost included	82.8	28.6	24.7	53.0
MeOH	 Final product is methanol No drop-in-fuel synthesis in investment and catalyst cost Product price assumed to be 400 €/t. Highly dependent on the assumed selling price of MeOH, for instance 500 €/t results in IRR of 25% and NPV of 41 M€. 	62.0	21.4	9.0	7.2
MTO- MOGD	Alternative synthesis pathway including kerosene and diesel as end product.	99.3	34.6	23.0	56.9

Table 4.4. Product selling prices and mass yields.

Product	Selling price (€/t)	MTG 2.0	MeOH	MTO-MOGD
Methanol (t/a)	400	0	25000	0
Gasoline (t/a)	1583	9500	0	1750
Kerosene (t/a)	1677	0	0	3000
Diesel (t/a)	1712	0	0	5000
LPG (t/a)	512	1000	0	500
Purge (t/a)	0	500	0	750
Annual sales (M€)		15.5	10	16.6

None of the cases with electrolyser-sourced hydrogen were profitable with the standard input values (net present values ranged from -100 M€ to -150 M€). The largest factors for this are electricity price, and the sales obtained from the products. From

Table 4.4, the annual sales are about 10-15 M€, whereas the electricity purchase prices on an annual level amount to 14 million euros (assuming total electricity price of 40 €/MWh including grid fees). Thus, the operation margin becomes so slim that it is simply not profitable. Total electricity price would have to be about 10 €/MWh to reach an investor IRR of 9.2 % with the MTG technology, assuming that all other factors remain constant.

Profitability of the cases where the hydrogen is obtained from electrolysis can be improved by several different ways, so that the lowering of the electricity price is not the only factor. Investment costs of the electrolysers could also decrease significantly during the following years [46], but it does not still address the key issue of operational expenses. Electrolyser efficiency was assumed in the calculation to be somewhat conservative (63 %_{LHV}), which could be as high as 69 % in state-of-the-art systems. Another important point is the prices of the products, which includes the potential by-products. Alkaline electrolysers produce significant quantities of low-grade heat (around 70 °C), which could boost the potential income if a suitable application is found. Oxygen is another by-product that could be utilized for additional sales. Furthermore, the product that the hydrogen is used for should ideally be very valuable. Finally, the smaller the total investment is, the less critical it is to be running at nominal capacity at all times, which could potentially open up avenues of operating only during the low-cost hours, reducing the average electricity price.

To reiterate, the profitability is fundamentally defined by the additional value that is obtained by converting electricity to products. From a marketability point of view, it would be preferable if the end product's price would not have a strong dependence on hydrogen. The introduction of this sustainable hydrogen-based product into the market would then be less dramatic in terms of overall price change because the increased cost of hydrogen is diluted by the marketed product.

5 Life-cycle assessment

Estimation of greenhouse gas (GHG) emissions from fuel production in the P2X pilot plant was made using **life-cycle assessment (LCA)**, which is a standardized methodology for calculation of environmental impacts associated with products or processes throughout their lifetime. LCA should be performed according to ISO standards [47, 48] and taking into account the guidelines for carbon capture and utilization [49, 50].

The goal of the study is to estimate the environmental impact of fuels (methanol and gasoline) produced using P2X technology and compare it to the impacts from conventional fuels. The environmental impact is estimated in terms of greenhouse gas (GHG) emissions. The study is aiming to answer the questions:

- what is the difference between GHG emissions of P2X and conventional fuels?
- what is the origin of the environmental impact of P2X fuel production?
- what are the benefits of waste hydrogen stream utilization?

The functional unit was defined as 1 MJ of fuel produced, which is in line with the LCA guidelines and the revised renewable energy directive 2009/28/EC (RED II) suggestion to use energy content as a base for comparison of GHG emissions from fuels.

The study is performed for two fuels (methanol and gasoline) and includes estimations of the emissions from the production stage of the fuels (from cradle-to-gate) (**Figure 5.1**). Although it is recommended to cover the entire life cycle of the product (from cradle-to-grave), in this case, cradle-to-grave approach is excessive. Assuming that the compared fuels have identical chemical structures and composition, and their final application is unknown, the GHG emissions from the use phase of such fuels will be also similar. The difference in the GHG emissions occurs in the production phase only, and therefore a cradle-to-gate LCA modeling was made for this case.

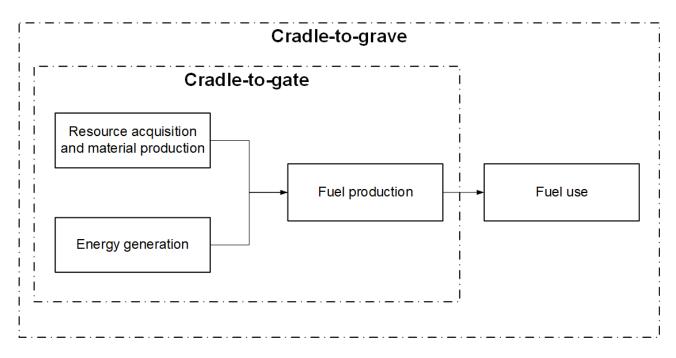


Figure 5.1. System boundaries of cradle-to-gate and cradle-to-gate approaches.

5.1 Methodology

Estimation of the GHG emissions was made based on the modeling in GaBi Software (version 10.0.1.92), using data from the commercially available technologies and Aspen modelling. Auxiliary processes and energy generation were modelled using the GaBi database or literature sources. A description of the processes used in the modelling can be found in **section 5.1.3** for methanol and **section 5.3** for gasoline.

Life cycle impact assessment was made using the IPCC AR5 method for the impact category Global Warming Potential (GWP). Biogenic emissions were not included in the estimation. For the comparison, fossil fuel comparator values provided by the RED II Directive were used. Since the comparator values include emissions from the production and use of fossil fuels, the use stage of fuels has been included in the comparison. A detailed explanation can be found in the **section 5.1.2**.

The system boundaries of the P2X plant utilizing waste hydrogen from the Kemira plant are presented in **Figure 5.2**. Carbon dioxide captured from the cement plant's plant's flue gases is liquefied and transported from Lappeenranta to Joutseno, where P2X fuel production is located. Hydrogen is supplied from the waste stream of the Kemira plant. Block "P2X fuel production" (**Figure 5.2**) includes methanol synthesis for the P2X methanol production case. For the gasoline case, this block includes methanol and MTG processes. The scope of the study includes all the relevant

processes, such as energy generation, material acquisition, water treatment, and waste utilization. Additional purification and storage of gases were not taken into account in the study.

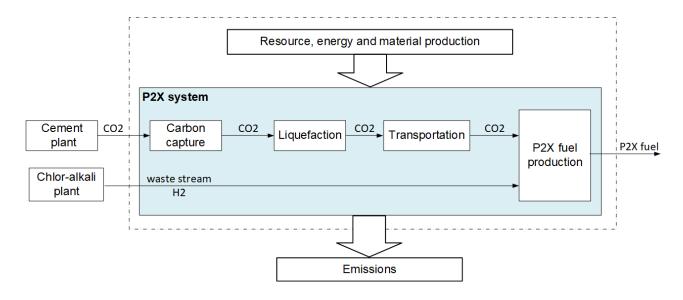


Figure 5.2. System boundaries of the analyzed P2X pilot plant.

Considering that energy sources have a high impact on the emissions level, four scenarios were analyzed for each P2X fuel (**Table 5.1**). The scenarios represent different energy sources for electricity and steam generation, so the impacts from energy sources with low GHG emissions (renewable sources: wind energy and biomass) and sources with relatively high GHG emissions (electricity grid and natural gas) can be estimated. Description of energy sources considered in the modelling can be found in **section 5.1.3**.

ScenarioElectricity sourceSteam sourceGrid/NgasFinnish energy gridNatural gasGrid/BiomassFinnish energy gridBiomassRE/NgasWind energyNatural gasRE/BiomassWind energyBiomass

Table 5.1. Electricity and heat sources considered in the scenarios.

5.1.1 CO₂ emissions as a CO₂ source

Although CO₂ emissions captured from the cement plant are utilized in a product, they cannot be subtracted from the cement plant emissions. According to the European Emissions Trading System (EU ETS), captured CO₂ emissions can be excluded from the cement plant carbon footprint only if they are stored in geological formations. In this case, attribution of captured CO₂ to the P2X fuel

will lead to double counting of the emissions, when the emissions are calculated in both cement and P2X fuel (**Figure 5.3 a**). To avoid double-counting of the emissions, CO₂ captured from the cement plant, should not be accounted as a part of the GHG emissions from P2X fuel (**Figure 5.3 b**).

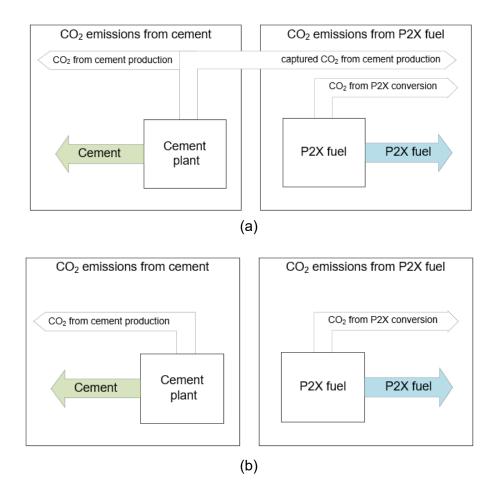


Figure 5.3. Attribution of CO₂ emissions. (a) double counting of the emissions (b) captured emissions are excluded from the CO₂ emissions attributed to the P2X fuel.

CO₂ captured from the cement plant for the P2X process, releases during the fuel production as fugitive emissions, and the fuel use as combustion emissions. Therefore, in this study, both fugitive and combustion emissions have been subtracted from the total GHG emissions of P2X fuels.

5.1.2 Comparators

The fossil fuel comparator for biofuels provided by the RED II Directive was used for the comparison and estimation of GHG emissions savings. Because the directive does not provide different comparators for different types of fuel, the same value (94 g_{CO2eq}/MJ) was used for methanol and gasoline. The comparator includes total emissions (production and use) from a fossil fuel.

The difference between the RED II comparator and GHG emissions from methanol and gasoline produced by conventional routes is illustrated using literature data (**Table 5.2**). Values for the methanol represent methanol production from natural gas by steam methane reforming (SMR).

Table 5.2. Literature values for GHG emissions from methanol and gasoline (gco2eq/MJfuel).

Fuel	Production		Combustion		TOTAL
Methanol	30.2	[51]	68.9	[52]	99.1
Biomethanol	10.4-16.2	RED II	-		10.4-16.2
Gasoline	5.8 -10.2	[52]	73.4	[52]	79.2-83.6
RED II comparator					94

GHG emissions from biomethanol production are also varying due to the different feedstock and production technologies. The total GHG emissions from biomethanol are significantly lower than the comparator because only the production stage is taken into account. Although the threshold for the GHG savings provided by the RED II Directive assumes a comparison of total emissions, biogenic emissions from the combustion of biofuels can be considered as zero, and only the emissions from the production can be used for comparison.

Although the combustion emissions from both biofuels and analyzed P2X fuels can be considered as zero, the principles that underlie it are different. Combustion of biofuels releases almost the same amount of CO₂ that was previously sequestered in biomass, therefore net CO₂ emissions are zero. In the case of CO₂ captured from the cement plant, the combustion emissions are not taken into account because they are allocated to the cement plant, so the process is not considered to cause net emissions – only recirculation of emissions that would otherwise be emitted directly. In practice, both processes emit emissions: biofuel emissions are sequestered back to biomass over the next years and decades, whereas in the P2X case the emissions are first captured for a brief time and then re-released during the fuel use stage.

Considering the above explanations, for the correct estimation of GHG emissions from the P2X based on the LCA model, only emissions related to the P2X process should be taken into account for comparison (**Equation (8)**).

$$E_{\text{P2X fuel}} = E_{\text{production}} - E_{\text{fugitive}} - E_{\text{use}}$$
 (8)

where

E_{P2X fuel} total GHG emissions from P2X fuel that are used for comparison, g_{CO2eq}/MJ

E_{production} GHG emissions from P2X fuel production, g_{CO2eq} /MJ

E_{fugitive} fugitive CO2 emissions that originate from captured CO2, g_{CO2eq} /MJ

E_{use} GHG emissions from P2X fuel use, g_{CO2eq} /MJ

GHG emissions savings can be calculated by comparing them against a benchmark as shown in **Equation (9)**.

$$Savings_{GHG} = \frac{E_{fossil\ comparator} - E_{P2X\ fuel}}{E_{fossil\ comparator}}$$
(9)

where

Savings_{GHG} reduction of GHG emissions from fuel production and use, %

E_{fossil comparator} GHG emissions from fossil fuel comparator, g_{CO2eq}/MJ

The threshold for recycled carbon fuels is not set by the RED II Directive yet, but for renewable fuels of non-biological origin, the GHG savings should be 70%. This means, that the emissions from the P2X fuel are 70% lower than emissions from fossil comparator. A negative value of the savings means that the emissions from the P2X fuel are higher than those from fossil comparators.

5.1.3 Process description and assumptions

The description of the processes included in the LCA model can be found in previous chapters. The important assumptions and possible differences are explained below.

<u>Steam supply</u>. Steam supply was modeled using the GaBi database, which provides data for the production and supply of process steam from a heating plant to final consumers. The data cover a steam production process relevant for Finland. The steam is produced with 95% efficiency from natural gas or solid biomass in the "Natural gas" and "Biomass" scenarios respectively (**Table 5.1**). The fuels are modelled for a specific Finnish consumption mix and consider the properties of the average regional fuel mix. Data for fuels covers all relevant processes including energy carrier exploration (for natural gas), feedstock production and processing, transport to the power plants, steam production, as well as the power plant construction and end-of-life. A detailed description of the processes included in the steam supply can be found in the database [53, 54].

Possible utilization of waste heat for carbon capture and heat integration in methanol synthesis are not included in the model. The influence of such heat utilization is similar to the sub-scenarios with a biomass heat source.

<u>Electricity supply.</u> Two options were considered for the electricity supply: the Finnish electricity grid and wind generation. GHG emissions from the Finnish electricity grid mix were calculated using data on electricity supply by energy sources in 2019 (**Figure 5.4**). Unit processes from the GaBi database were used to estimate the emissions from each electricity source as well as for distribution losses. The data covers all relevant processes for electricity production, including fuel production, technical characteristics of power plants, transmission, and distribution losses, as well as power plants construction and end-of-life. The GWP of the electricity mix from the modeled grid is 169 gco₂/kWh.

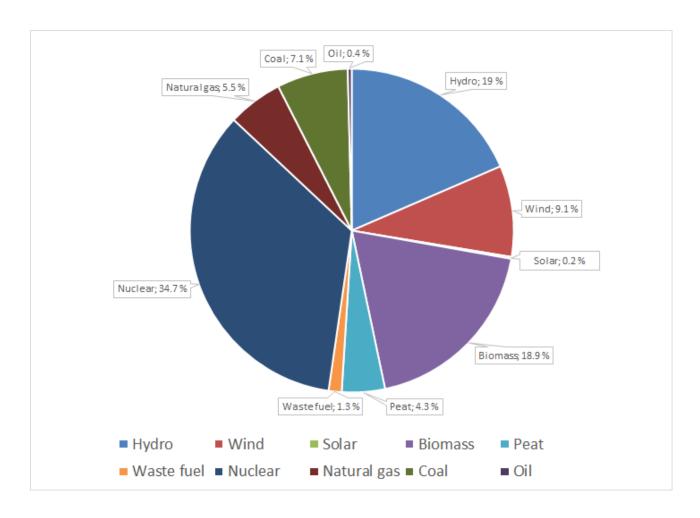


Figure 5.4. Supply of electricity by energy source for Finland, 2019 [55].

The emissions from the electricity grid mix used in the calculations are higher than the emission factors reported for 2019 by the European Energy Agency (111 g_{CO2}/MJ) [56] or those calculated based on a methodology developed by the Finnish Statistics and Fingrid (87-101 g_{CO2}/MJ) [57] . The difference is due to different methodologies used for the emissions calculation in the database and the mentioned sources. For example, in the methodology used by the Fingrid, allocation of the emissions from combined heat and power plants is made based on the volumes of energy, and in the GaBi database, allocations are made based on exergetic content. Furthermore, in the Fingrid calculations, hydroelectric, nuclear, wind, and solar power are defined as emission-free, and the environmental impacts associated with the life cycle of energy plants and infrastructure are not into account. Whereas in the GaBi database, these emissions are taken into account.

It is important to use similar principles for the estimation of emissions from different processes, so in order to adhere to one methodology throughout the study, the emissions calculated based on the database (169 g_{CO2} /kWh) was used. However, the difference in the emissions from the electricity can lead to a significant difference in the results, and the influence of the alternative values for the electricity grid emissions was taken into account in the analysis of the results.

Data for wind electricity is also based on the GaBi database processes, which consists of a mix of onshore and offshore wind electricity generation relevant for Finland. The data covers production and end-of-life utilization of wind turbines as well as transmission, and distribution losses. The GWP of the electricity from the modelled wind grid is $8.85 \, g_{CO2}/kWh$.

<u>Cooling water supply.</u> The design of the cooling water supply should be developed in the later stages; therefore, some assumptions are necessary. The analyzed P2X system requires cooling water for direct contact and non-contact cooling. These systems set different requirements for the cooling water quality, therefore water of process quality i.e. demineralized water was considered for the direct contact cooling. For non-contact cooling, the water of tap quality was considered.

Equipment. According to the RED II Directive, emissions from manufacturing the machinery and equipment shall not be taken into account in GHG emissions calculations. However, LCA standards suggest including it, and emissions from the equipment manufacturing are included in some processes from the GaBi database. Estimation of the emissions from equipment manufacturing for carbon capture and fuel synthesis was made based on the weight and material of the equipment assuming that a major part of the environmental impacts originates from the production of the material. The construction of buildings was not taken into account. For water electrolysis estimation of impact from the equipment was made based on a detailed LCA study [58].

<u>Transportation</u>. Transportation by truck was modelled for CO₂ transport from the capture site to the methanol production plant. The transportation distance is approximately 27 km for a one-way trip. The return trip is assumed to be done by an empty truck.

The process was modelled using GaBi database unit processes for a truck and fuel supply. Assuming that approximately 20 tons of CO₂ should be transported per trip, a diesel-driven truck with a 22-ton payload capacity was considered in the modelling. The emissions level from the truck was modelled in compliance with Euro 6 standard. Truck production and end-of-life treatment were not included in the process.

Fuel supply was modelled assuming an average European diesel mix with 6.4 wt% of biocomponents. The dataset from the GaBi database includes the entire diesel supply chain from well-drilling and crude oil production to the refinery and fuel transportation from the refinery to a filling station.

5.2 Methanol production

Processes included in the system boundaries of the P2X methanol production are presented in the detailed flow chart below (**Figure 5.5**). The boundaries include the main P2X processes (carbon capture and methanol synthesis), as well as additional processes (CO₂ liquefaction and transportation), energy generation, and auxiliary processes, such as chemical production and water supply.

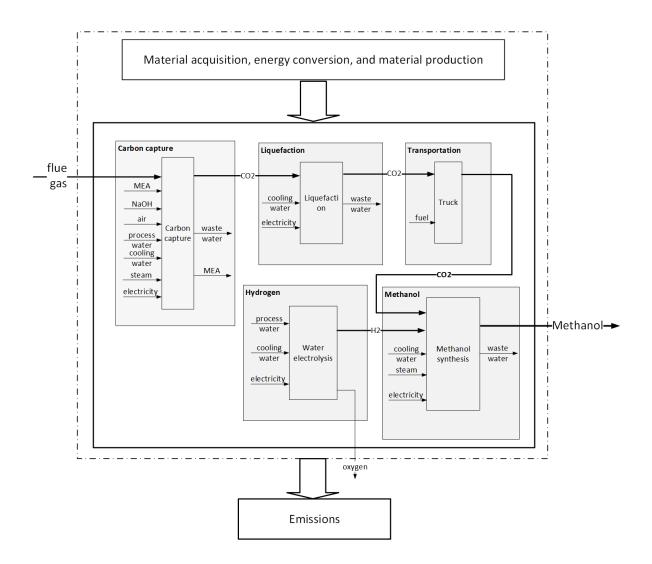


Figure 5.5. System boundaries of P2X methanol production.

5.2.1 Results

For the case of the analyzed P2X pilot plant, the GHG emissions from methanol production can be estimated in range from 4.1 to 7.3 g_{CO2}/MJ if a low-emission heat source is available for steam generation. The GHG savings from methanol production, in this case, are 92.2%-95.6% compared to fossil alternatives. The difference in the numbers is due to electricity sources – a lower emissions level can be achieved if renewable electricity from wind is used.

Heat integration for methanol synthesis (section 2.4.4) and waste heat utilization from the cement plant for carbon capture can be even more beneficial than the use of biofuels. The reason is that GHG emissions from the waste heat can be considered zero, whereas steam production from biomass includes emissions from biomass production and processing. Although the waste heat integration was not included in the LCA model, the emissions for this case can be estimated in range

from 3.8 to 6.5 gCO2/MJ, which leads to savings of 93.1 - 96%. However, the utilization of heat from the cement plant should not reduce the amount of heat supplied by the cement plant for other purposes, such as district heating. For the scale of this particular pilot plant, the amount of excess heat available from the cement plant was estimated to be adequate without needing to alter the current use of heat, but increasing the scale of the plant could lead to different conclusions.

Total GHG emissions and GHG savings from the P2X methanol production using other energy sources are presented in **Table 5.3**. The contribution of the main processes to the GHG emissions of P2X methanol are shown in **Figure 5.6**.

Table 5.3. GHG emissions and emission savings from P2X methanol production utilizing waste hydrogen (gco2eq/MJ_methanol). GHG savings are compared to 94 gco2eq/MJ_fuel.

		Scenarios				
Process	Grid/NGas	Grid/Biomass	RE/NGas	RE/Biomass		
Carbon Capture	18.2	1.8	18.0	1.6		
Methanol synthesis	15.3	4.6	12.8	2.1		
Liquefaction	0.6	0.6	0.1	0.1		
Transport	0.3	0.3	0.3	0.3		
Total emissions	34.41	7.33	31.18	4.10		
Emission savings	63 %	92 %	67 %	96 %		

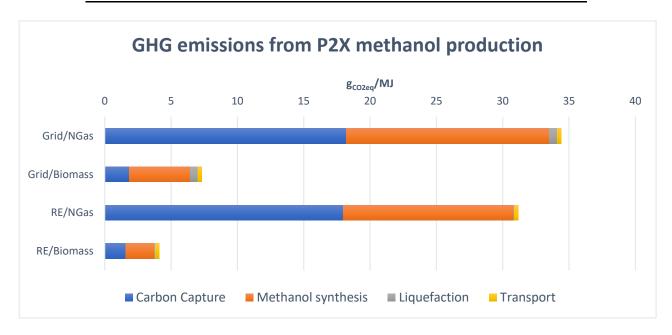


Figure 5.6. Contribution of the main processes in the GHG emissions from P2X methanol production utilizing waste hydrogen.

In all analyzed scenarios, P2X-methanol has a lower GHG emissions level than the fossil comparator (Table 5.3) and the processes related to carbon capture and methanol synthesis causes the main part of the emissions. The main parameter contributing to the emissions is the origin of heat. Utilization of heat produced from natural gas leads to an increase in the GHG emissions from methanol to $31.2 - 34.4~g_{CO2eq}/MJ$ fuel. Other processes cause smaller impact on the emissions level. In the scenarios with low-emission heat (Grid/Biomass, RE/Biomass), water supply and electricity are contributing to the most to the emissions.

Despite a significant difference in the emissions from the electricity grid and wind power, utilization of wind power instead of the grid mix leads to a relatively small reduction of the emissions (~3gCO2eq/MJ_methanol). Thus, in case of P2X methanol, the difference between the emission values used in this study and reported by the statistics will not significantly change the results.

5.3 Gasoline production

Processes included in the scope of the P2X gasoline production are presented in the detailed flow chart below (**Figure 5.7**). All the processes used in the P2X gasoline production are similar to those used in the P2X methanol. The difference is the MTG process added for gasoline production.

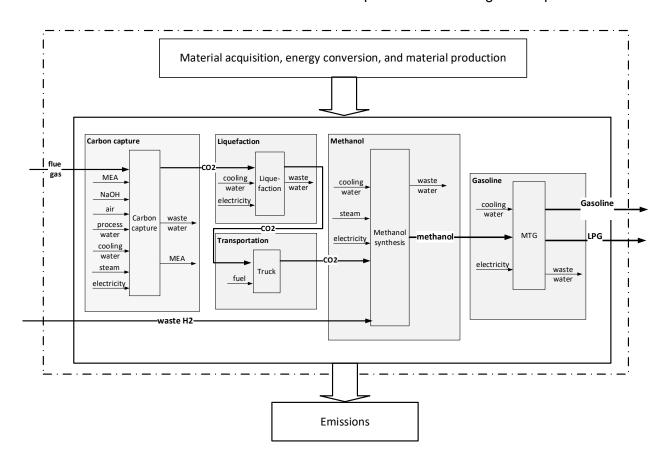


Figure 5.7. System boundaries of P2X gasoline production.

The methanol-to-gasoline process was modelled based on the Aspen model and heat integration is included in this process. Therefore, the process requires only methanol, electricity, and cooling water for the synthesis. However, MTG is a multi-functional process producing two products. Therefore, GHG emissions from this process should split between gasoline and LPG, because both are valuable products with energy content. Allocation of the emissions was made based on the total energy content of the products, assuming energy densities of 43.2 MJ/kg for gasoline and 46 MJ/kg for LPG. This means, that about 10% of GHG emissions from the MTG process are attributed to LPG.

5.3.1 Results

The results of GHG emissions estimation for the MTG process can be seen in Table 5.4.

Table 5.4. GHG emissions from P2X gasoline production utilizing waste hydrogen (g_{CO2eq}/MJ_gasoline) and GHG saving compared to 94 g_{CO2eq}/MJ_fuel.

Process	Grid/NGas	Grid/Biomass	RE/NGas	RE/Biomass
Carbon Capture	19.9	2.0	19.7	1.8
Methanol synthesis	16.7	5.0	14.0	2.3
MTG	4.7	4.7	0.5	0.5
Liquefaction	0.6	0.6	0.1	0.1
Transport	0.3	0.3	0.3	0.3
Total emissions	42.3	12.7	34.6	5.00
Emission savings	55 %	86 %	63 %	95 %

In all the analyzed scenarios for the P2X gasoline production the GHG emissions per MJ of fuel are more than 50% lower than the emissions from fossil fuel alternative. The influence of the main processes on the total GHG emissions (**Figure 5.8**) is similar to the methanol case – the system is the most sensitive to the heat source. Savings in GHG emissions can be achieved when either renewable electricity or emissions-free hydrogen is used. The share of GHG emissions from the MTG process is lower than from carbon capture and methanol synthesis. A possible reason for this is that MTG requires only electricity and does not require an external heat supply because of the internal heat integration.

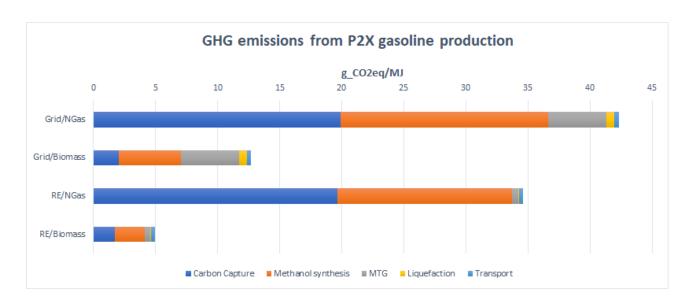


Figure 5.8. GHG emissions from P2X gasoline production utilizing waste hydrogen.

5.4 Production using electrolyser-sourced hydrogen

The utilization of waste hydrogen is beneficial for P2X fuel production because of zero GHG emissions attributed to hydrogen. However, if the amount of waste hydrogen is not enough or otherwise available, hydrogen can be produced by water electrolysis. The introduction of water electrolysis to the P2X fuel production can significantly increase GHG from the process due to the high electricity consumption of the electrolyser. To estimate the influence of hydrogen supply from water electrolysis, GHG emissions from P2X fuel production using water electrolysis were also analyzed for methanol and gasoline. The system boundaries of the analyzed system presented in **Figure 5.9**.

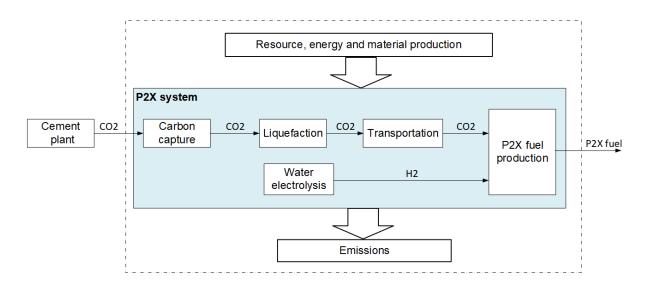


Figure 5.9. P2X fuel production with water electrolysis.

<u>Water electrolysis</u>. Water electrolysis was modeled based on an alkaline electrolyser. The multifunctionality of water electrolysis should be taken into account when calculating the GHG emissions from the process. The electrolysis has two products: hydrogen and oxygen and the emissions from the process should be split between them. If oxygen is not utilized and considered as waste flow, then all the emissions from electrolysis are allocated to hydrogen. If oxygen is utilized, then the allocation is needed. The allocation of the emissions in the case of energy production is recommended to be done based on the energy content. Since the oxygen energy content is zero, all the emissions are assigned to hydrogen in this case as well.

Table 5.5. GHG emissions from P2X fuels production utilizing water electrolysis (g_{CO2eq}/MJfuel) and GHG saving compared to 94 g_{CO2eq}/MJfuel.

		Scenarios				
Process		Grid/NGas	Grid/Biomass	RE/NGas	RE/Biomass	
Methanol production	Total emissions	129.90	102.82	37.87	10.79	
	Emission savings	-38 %	-9 %	60 %	89 %	
Gasoline production	Total emissions,	146.73	117.12	41.90	12.29	
	Emission savings	-56 %	-25 %	55 %	87 %	

As can be seen from **Table 5.5**, if hydrogen is supplied from the electrolysis, emission savings can be achieved only if renewable electricity is used. Negative emissions savings in the scenarios with the electricity supplied from the grid mean that the GHG of the fossil fuel is lower than the emissions from the P2X fuel. It is important to mention that in this study the emissions from the electricity grid were calculated considering approximately 35% of electricity supplied from renewable sources and 25% from nuclear power¹⁷. Comparison with other grid mixes can lead to a more significant influence of electricity sources on the emissions from water electrolysis.

5.5 Conclusions from life-cycle assessment

The study aimed to estimate GHG emissions from the fuel production in the P2X plant and compare them to the emissions from fossil fuels. The P2X plant is supposed to utilize waste hydrogen from the Kemira plant to produce either methanol or gasoline. To estimate the benefits of waste hydrogen utilization, the case of hydrogen supply from the water electrolysis was also analyzed. In addition, the influence of electricity and steam supply from different sources was analyzed in four scenarios

¹⁷ GWP of 169 g_{CO2}/kWh, which includes the fuel emissions as well as other emissions such as power plant construction and transmission losses as outlined in section **Error! Reference source not found.**.

(**Table 5.1**). **Figure 5.10** shows a comparison of GHG savings from methanol and gasoline production for the case of waste hydrogen utilization (Kemira) and production of hydrogen (Electrolysis). The savings were estimated comparing the emissions from the P2X fuel with the comparator value (94 g_{CO2eq}/MJfuel) defined by the RED II (Directive 2009/28/EC). Since the GHG savings threshold for the recycled carbon fuels is not defined yet, the threshold for RFBNO (70%) is shown with a dashed line. In addition, for comparison, GHG emission savings from an average case of biomethanol are also presented in the figure.

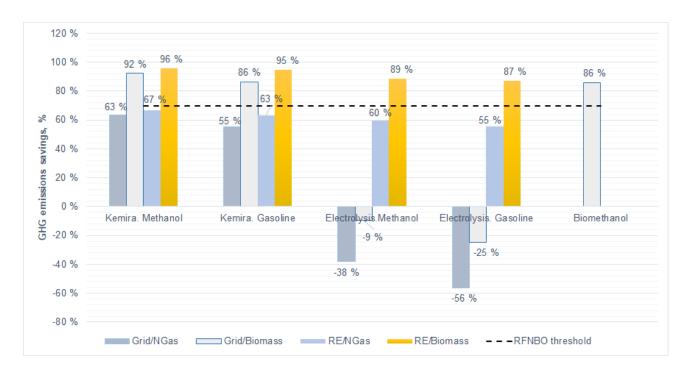


Figure 5.10. GHG emissions reduction from P2X fuel production for cases of waste hydrogen utilization (Kemira) and hydrogen supply from water electrolysis (Electrolysis). The scenarios for energy sources include electricity from the grid (Grid), electricity from the wind (RE), process steam from natural gas (Ngas) and process steam from biomass (Biomass).

The level of the emissions reduction is similar for the P2X methanol and gasoline cases. This can be explained by the low energy requirement for the MTG process, where internal heat integration was taken into account.

Methanol and gasoline produced using P2X can reach the same level of GHG emission savings as biomethanol if the origin of the electricity is renewable, and the heat is sourced either from internal heat integration between process components, or from sources with low GHG emissions, such as biomass. Potentially even greater emission savings could be achieved in cases where there is waste hydrogen available from existing processes, like in the case of this project.

A key contributor to the emissions level from P2X systems is the hydrogen source. The utilization of hydrogen from a waste flow (**Figure 5.10** Kemira) leads to a significant GHG emissions reduction regardless of the energy sources used in the production process. Whereas hydrogen production by water electrolysis (**Figure 5.10** Electrolysis) requires significant amounts of electricity and, therefore, electricity supply from renewable sources is necessary to achieve emissions levels lower than those of comparators.

Overall, the results indicate, that GHG emissions from P2X methanol production are lower than the comparators if either more than ~45% of electricity comes from a renewable source, or more than ~55% of hydrogen comes from a waste stream. For gasoline, these values are ~55% and ~50 % respectively. However, as was already mentioned, these calculations are valid only if the origin of the rest of electricity is an electricity mix with a significant share of renewable and nuclear energy.

Finally, it is important to interpret the result bearing in mind that captured CO₂ utilized in the P2X fuels was attributed to the cement plant. If captured carbon is attributed to P2X fuels, GHG emissions from P2X fuels will be higher than fossil comparators. However, in this case, the GHG emissions from the cement plant will be lowered by the corresponding amount.

6 Regulation

During the project execution, EU made a big turn towards fostering green economy. It was augmented by the COVID-19 recovery plan, which is formed primarily from the temporary instrument NextGenerationEU coupled with long-term EU-wide budget adjustments. The 2018 recast Directive (RED II) was therefore opened for revision to bring it in line with the European Green Deal, 2030 Climate Target Plan, and other strategical targets.

The thorough analysis of the RED II on P2X Fuels¹⁸ was carried out by Julia Ranta in her master's thesis "Implications of the recast Renewable Energy Directive on Power-to-X fuels" [59]. In brief, some of the findings are summarized and commented in the next sections.

6.1 RED II and EU regulation

RED II sets binding EU overall target for 2030 of at least 32% of energy from renewable sources. It covers in transport sector with binding target of 14% of energy from renewable sources, a specific sub-target for advanced biofuels of 3.5%, and two non-biogenic fuel categories: renewable liquid and gaseous transport fuels of non-biological origin (RFNBOs) and recycled carbon fuels (RCFs). For heating and cooling sectors RED II presents new rules.

It also sets forth strengthened sustainability criteria for bioenergy and an extended guarantee of origin (GO) system covering all renewables. Additionally, RED II aims at simplifying administrative procedures (one-stop-shops, time-limits, digitalization).

For carbon dioxide, there are fossil and biogenic point sources, and direct air capture. Regulation for fossil emissions in made by EU ETS [60]. Carbon capture and storage, at present, is releasing the emitter from paying the emission price.

According to RED II, greenhouse gas emissions savings threshold for RFNBOs is 70%. However, the methodology for assessing greenhouse gas emissions savings from RFNBOs is to be determined in a delegated act by 31 December 2021.

¹⁸ Synthetic fuels, e-fuels, Power-to-Liquids (PTL), etc.

A major factor in emission reduction is also the source of electricity. Depending on the origin of the electricity, it has great impact on end-product classification and reduction calculation.

6.2 Grid Electricity

For grid electricity, emission burden is calculated based on the renewable energy's average share of electricity production in the country, as measured two years prior to the production year.

6.3 Electricity from direct connection

For direct connection (like wind, solar farm) electricity may be counted as fully renewable, if the installation fulfills the following conditions:

- The plant comes into operation simultaneously or shortly after the installation producing RFNBOs.
- Grid electricity is not used for production. The plant can be either not connected to the grid
 at all, or if a grid connection exists, it must be proven that the consumed electricity is supplied directly from renewable sources without additional input from the grid.

6.4 Green grid electricity

Electricity taken from the grid may be treated as renewable if it is produced exclusively from renewable sources, noting that "renewable properties and other appropriate criteria has been demonstrated, ensuring that the renewable properties of that electricity are claimed only once and only in one end-use sector."

6.5 Additionality

"Recital 90 states that the electricity used for producing RFNBOs should be derived from a renewable origin to ensure their contribution towards the GHG emissions reduction targets. In the context of RED II, the renewable sources are identified in Article 2(1) of RED II. Moreover, Recital 90 necessitates an element of additionality." [59]

Absolute additionality requires that the share of renewable electricity in voluntary markets is purchased from a new production facility that is not benefitting from any existing renewable energy support schemes and where the electricity produced is not considered towards national targets.

6.6 Conclusions and discussion

As a result, firm carbon reduction calculations can be made for P2X Joutseno case only after publication of the delegated at the end of year 2021.

As seen at this point there is need for quick revision of RED II. EU Green Deal and RED II need to be aligned. The regulation should support innovation-friendly approaches.

6.7 Unnecessary, double regulation

There is no need to double regulate the system, i.e. place restrictions on the source of electricity as well defining guidelines for the emission reduction that should be achieved by e-fuels. For instance, by expanding the ETS system and decreasing the amount of emission allowances on the market, fossil production would be driven out of system due to increasing costs. Recycling of CO₂ into products should be promoted to rapidly decrease fossil emissions into the atmosphere, with the assumption that the lifecycle emissions of the recycled product are better than the fossil reference product.

Regulation of the source of electricity unnecessary: new production will be built as demand grows. A large share of production could be built based on power purchase agreement contracts bilaterally. Fossil electricity production will be forced out of the system by increasing ETS costs and cheap renewable energy from wind and solar.

The regulation seems to be addressed to solve the problems in the energy system in the Central European countries, especially Germany and partly ignoring the energy systems in the Nordic Countries.

6.8 Consequences of RED II

Recycling CO₂ emissions could reduce in proportion the pumping of fossil oil or digging coal out of the ground. RED II focuses on cleanness of the end-product and neglects focus of recycling and reducing CO₂ emissions. The requirement for additionality, green grid electricity (as measured two years before) and electricity from direct connection complicates the implementation of these facilities, which results in less recycled CO₂ and thus limits the emission reduction potential.

Isolated electricity systems and production units could also reduce the efficiency and robustness of the electricity system. The directive does not take into account the system balancing opportunities like batteries, carbon-neutral liquid fuels, or demand response. This could isolate the new renewable electricity production instead of embracing the potential benefits that system integration could offer.

In EU there is already proper ETS scheme in place. The system should be expanded and used. By increasing the price of CO_2 emissions per ton, costs would drive fossil-based sources of the system. Similarly, recycling of the fossil emission would not be a long-standing investment due to threat of termination of the CO_2 source. The downside of the EU ETS is that has been rather slow in the past to react to a surplus of emission rights on the market. Balancing between the predictability and stability of the regulation tool against its effectiveness and impact is not a simple task. Adjustments take years to take effect.

Potential consequences of the EU regulation are

- delays the implementation of P2X fuel production investments
- investments will go outside the EU (Norway, USA, Australia, Africa, etc.), decreasing the security of supply of energy and fuels
- investments will concentrate only in specific regions within EU (Sweden, France), causing inequality among the member states
- price of the biofuels will surge due to lack of substitutes and increasing demand, leading to increased deforestation and loss of biodiversity on a global level
- electrification and hydrogen economy become too expensive to implement and, as a consequence, the EU member states may not be able to meet the climate goals in the given timeframe
- market based P2X businesses fail to realize, or they require substantial support programs and high taxation
- interest for technology development is low, causing players outside the EU to take the technological and market lead

7 Conclusion and discussion

Power-to-fuels production technology is available and ready. Technology-related challenges are linked to scaling up the production and improving the efficiency. Electrolysis technology deviates from conventional industrial processes and could thus face more challenges in upscaling the technology compared to other parts of the production chain. The technology itself is more than hundred years old, but at the present, both its individual unit sizes and annual production quantities are moderate.

The other driver for the P2X products' growth is regulation and market demand: carbon-neutral fuels need to be regulated equally to biofuels, having their own blending liability. Regulation creates the market, as it has made for biofuels, and confirms the existence and predictability of the business for investors.

Electric fuels possess some clear advantages over conventional fuels and their alternatives. Required raw materials are essentially water, renewable energy, and CO₂, which are much more evenly spread out and accessible than conventional fuel reserves. Production plants of e-fuels have relatively low footprint requirements in comparison to biofuels that additionally require arable land for biomass crops. Even very harsh environments can be made suitable for P2X, and the products can be put to use immediately, using the existing infrastructure and conventional machines and systems.

Low-cost sustainable electricity will be a prerequisite for successful implementation of large-scale production facilities. It will be a challenge to achieve a profitable operation environment with electrolyser-sourced hydrogen, and a combination of factors is likely required, e.g. valuable end product, utilization of by-products (oxygen, heat), adequate number of operational hours, and technological improvements. On the other hand, few technological solutions are available and capable of solving climate-related challenges in global scale to the extent that P2X technologies can. Falling short of climate targets should not be an option, so necessary steps should be taken to pursue the possibilities of the technology.

In the regulative environment, EU should have a clear target. This target should be the reduction of greenhouse gas emissions in the atmosphere. Regulation should be simple to understand and focus on this as the main target. It is essential that potential hindrances of regulation are cleared to enable the growth of the P2X technology.

At present, regulation takes place in many areas, such as waste, recycling, fuels, and emission directives. Simultaneously, the technology is getting more complicated, and regulation expands to the entire system. The regulation of system level transition requires understanding of a very complex system itself and cannot be done by sub-optimization of parts of the system and market. This has led to a situation where EU officers from different sides of the organization pursue to the same target. As an outcome, the regulation is getting more and more complicated and understanding it becomes a major source of competitive advantage for firms.

For further research on e-fuels and P2X production, see the listed initiatives in section 8.

8 Proposals for future research

It came evident along the research work that there are multiple areas for further research such as:

- Development of the fuel synthesis and catalysts
- Refinement of e-fuels for various end use purposes and obtaining necessary approvals
- Heat integration of the various components and their potential links to external systems such as heat pumps
- Processing of wastewater
- Gas purification
- Hydrogen/CO₂ production, compression, storage, and transport
- Dynamic operation of the plant and proper dimensioning of storages
- Digital twin of the process
- Business opportunities in P2X and market development
- Benefit-cost analysis of the business ecosystem actors
- Potential for local manufacturing of components necessary for P2X plants

Long-term stability and activity of the catalysts is important for industrial systems both in methanol and methanol-to-fuels processes. Determination of catalyst performance requires pilot systems that can be operated for long periods of time. Especially the catalysts in the MTO-MOGD synthesis require experimental testing to gain first-hand operational experience. Digital twin systems developed to describe the fuel syntheses would allow examining the effect of individual or combined process variables without implementing any physical changes to the process. For instance, the models would provide virtual information about catalyst degeneration, wearing of consumable parts, and potential safety hazards.

Since the level of impurities is crucial for the long-term activity of the catalysts, experimental verification of the feed gas purification methods is also important. This can be conducted by laboratory experiments. Development of analytical methods and analysis of impurity levels in available gases (from industry or from gas suppliers) is also of great importance.

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Appendices

APPENDIX A:

Table A1

List of equipment in the simulation model and their operating conditions. In the table, p = pressure, T = temperature, H = height, D = diameter, A = heat transfer area, P_{th} = thermal power, and P_{el} = electrical power. Vertical lines separate inlet and outlet values, or condenser and reboiler duties in distillation columns.

Equipment	p, bar	T, °C	H, m	D, m	A, m²	P_{th} , kW	P _{el} , kW
CO₂ capture (1a-c)							
Quench column	1.1, 1 1, 1	150, 10 10, 15	11	2.5			
Flue gas fan	1 1.1	10 19					53
Heater	1.1	19 40			9.4	123	
Absorption column	1.1, 1.1 1.1, 1	40, 40 67, 43	42	2.5			
Pump	1.1 1.6	43 42					1.6
Heat exchanger	1.6, 1.1 1.6, 1.1	42, 103 98, 40			138	4717	
Distillation column	1.6 1.2, 1.2	98 25, 107	24	1.6		-1798 4153	
CO ₂ treatment (1d)							
Flash column	1.2	25	0.9	3.7			
Compressor	1.2 7	25 185					207
Cooler	7	185 35			3.1	-210	
Dryer	7	35	1.5	0.45			
Compressor	7 74	35 30					218
Gas treatment (3a)							
Compressor	1 73	80 30					1660
Heat exchanger	73, 72 73, 72	20, 240 40, 186			1.5	226	
Heat exchanger	73, 72 73, 72	11, 255 25, 240			0.3	63	
Start-up heater	72	25			0.9	288	
Deoxo reactor	73 72	25 255	1.5	0.42			
Cooler	72	186 30			14	-819	
Dryer	72	30	1.8	0.87			
Adsorption column	72	30	1.8	0.75			
MeOH synthesis (3b)							
Compressor	72 73	30 31					5.1
Heat exchanger	73, 64 72 63	35, 280 220, 69			257	5108	
Start-up heater	72	220			122	5108	
MeOH reactor	72 64	220 280	4	0.02			
Cooler	69	81 30			70	-2115	
Flash column	69	30	3.7	1.1			
Compressor	69 73	30 36					134

Flash column	1.2	24	3.7	1.1			
Heat exchanger	64, 1.2 64, 1.2	213, 20 103, 80			17	1086	
Distillation column	1.2 1	80 64, 100	28	1.5		-2026 2277	
Flash column	1	64 30	3.7	1.1			
MTG synthesis (4)							
Pump	1 22	30 32					8.0
Heat exchanger	22, 21 22, 21	32, 863 316, 265			4.6	1483	
Start-up heater	22	32 316			57	1483	
DME reactor	22 21	316 435	3.5	1.4			
Cooler	21	426 360			4.3	-145	
Gasoline reactor	21 20	360 863	3	1.3			
Heat exchanger	21	62, 265 252, 257			0.3	18	
Cooler	21	257 135			289	-1260	
Cooler	20	135 30			14.5	-381 	
Cooler	20	30 10			6.2	-55	
Flash column	20	10	0.9	3.7			
Flash column	10	10	0.9	3.7			
Compressor	10 21	10 61					3.7
Decanter	20	10	3.7	0.9			
Pump	10 20	10 12					1.9
Distillation column	20	12 -46, 131	13	0.5		-6.8 109	
Heat exchanger	10, 1 10, 1	-39, 29 23, 28			0.5	1.3	
Cooler	1	28 25			0.6	-6.2	
Distillation column	20 5	131 44, 104	9.1	0.5		-37 25	
Distillation column	5 1	104 31, 169	4.9	0.5		-91 72	
Pump	1 5	20	4 =				0.5
Alkylation reactor	5	31 10	1.5	1.1			
Decanter	5	10 37	4.3	1.4		00414000	
Distillation column	5	37 9, 58	9.8	1.1		-234 1306	
Pump	1 17	169 172			0.0	00	0.6
Heat exchanger	17, 16 17, 16	172, 345 263, 268			0.3	20	
Heater	17	263 345			1.1	21	0.0
Compressor	1 17	0 309			0.5	40	2.0
Heater	17	76 345	4 5	0.7	0.5	12	
Isomerization reactor	17 16	345	1.5	0.7	44	55	
Cooler	16 16	268 135			11	-55	
Cooler	16	135 30	0.0	2.7	8.0	-24	
Flash column	16 14	30	0.9	3.7			0.7
Compressor	14 17	30 47					0.7
MTO-MOGD synthesis (5)	112	30					0.4
Pump Heat evelonger	1 2 2				58	1741	0.4
Heat exchanger		30, 450 430, 86					
Heater MTO reactor	2 2	430 450	15	1 2	4.0	41	
	2	450	4.5	1.3	0.5	22	
Heat exchanger Cooler	2	30, 86 40, 83			0.5 14		
Cooler Flash column	2	83 30 30	27	0.9	14	-249	
i iasii coiullili	۷	3U	3.7	0.9			

Decanter 2 30 2.7 0.9 Pump 2 15 30 33 1E-0 Heat exchanger 40, 15 40, 15 45, 125 95, 100 1.3 45	7
·	7
Heat exchanger 40, 15 40, 15 45, 125 95, 100 1.3 45	
Cooler 15 100 50 3.1 -110	
Distillation column 15 50 7, 60 5.5 0.5 -24 21	
Distillation column 15 10 60 38, 289 6.7 0.5 -169 155	
Pump 10 40 38 45 6.0	
Pump 10 17 290 291 0.03	3
Heat exchanger 17, 16 17, 16 291, 345 315, 320 0.5 0.6	
Heater 17 315 345 0.5 1.6	
Compressor 1 17 25 309 0.3	
Heater 17 82 345 0.5 1.0	
Isomerization reactor 17 345 0.8 0.3	
Cooler 16 320 135 1.1 -6.3	
Cooler 16 135 30 0.5 -2.3	
Cooler 16 30 10 0.5 -0.4	
Flash column 16 14 10 3.7 0.9	
Compressor 14 16 10 21 0.03	3
Heater 40 95 200 2.2 161	
MOGD reactor 40 200 4 1.3	
Distillation column 5 176 104, 207 5.5 0.5 -23 33	
Cooler 5 104 50 0.8 -29	
Distillation column 5 50 4, 81 8.5 0.5 -18 19	
Cooler 1 35 30 0.4 -3.0	
Pump 5 40 207 213 5.4	
Heater 40 213 300 3.3 71	
Compressor 1 40 25 145 15	
Heater 40 110 300 0.4 8.7	
Hydrogenation reactor 40 300 3 1.5	
Cooler 40 300 135 26 -137	
Cooler 40 135 30 2.3 -68	
Flash column 40 36 30 3.7 0.9	
Compressor 36 40 30 42 0.2	
Flash column 1 32 3.7 0.9	
Distillation column 1 32 189, 297 7.3 0.6 -20 207	
Cooler 1 297 135 16 -81	
Cooler 1 135 30 1.8 -42	
Cooler 1 189 30 1.1 -66	

APPENDIX B: Market interview questionnaire

Interview for market assessment/analysis

Introduction: P2X

LUT University studies P2X (power-to-x) technology -based synthetic fuels and establishment of pilot plant.

The purpose of interview is to find out the market price and demand of synthetic fuels and thus, create

understanding about the pricing principles of fuels for the basis of profitability analysis. For more infor-

mation, please see the monthly newsletter <u>Link to Newsletter</u>

At the end of this document, the figure about the production process of synthetic fuels is presented. It can

be assumed that the used electricity is green/carbon dioxide free.

The produced products are a) hydrogen, b) methanol, c) gasoline, d) diesel, e) kerosene

Theme 1: Products and supply/offering

1) What does make P2X technology -based carbon dioxide free synthetic fuels interesting compared to com-

peting products? Benefits and challenges.

Theme 2: Demand

2) Which operators and actors do want these end products, i.e. carbon dioxide free synthetic fuels (hydro-

gen/methanol/gasoline/diesel/kerosene)?

3) What does affect to the demand? The special characteristics of each fuel regarding the demand.

a) hydrogen, b) methanol, c) petrol/gasoline, d) diesel, e) kerosene

4) How will the demand of fuels change/develop during the next a) 5 years, b) 10 years, c) 15 years, d) 20

vears?

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5) How does the regulation/legislation (e.g. taxation, distribution obligation) affect to the demand? How will the regulation develop/change in the future and how should it change in order that it would increase the demand of synthetic fuels?

a) National regulation, b) EU-level, c) Other actors (e.g. USA)

Theme 3: Price

6) Insights of market price: Estimation for the development of average prices (without taxes: excise tax, value added tax) / How much can synthetic (carbon dioxide free) fuel cost?

7) Estimation for price development: How would you estimate that the price of synthetic fuels develops/changes during the next a) 5 years, b) 10 years, c) 15 years, d) 20 years?

8) How does the producer define the price? Does it make any difference to whom the fuel is sold or to which purpose of use it is sold? a) hydrogen, b) methanol, c) petrol/gasoline, d) diesel, e) kerosene

9) How do the possible subsidies for green fuels or penalties for using fossil fuels affect to the prices of fuels?

10) What other factors may affect to the price of synthetic fuels?

Theme 4: Business model/Sales contracts:

11) What kind of sales contracts can be made with a fuel producer and a buyer? How the long-term customer relationship is established and sustained?

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