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ENHANCING POWER-TO-X HYDROGEN PLANT PROFITABILITY THROUGH OPTIMIZED SOLUTIONS

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ABSTRACT

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The Power-to-X (P2X) concept is built around energy conversion and storage technologies, and the term is often associated with renewable energy production management and levelling solutions. In the P2X concept, energy is converted to a storable or usable form X, which in this work is hydrogen, meaning that P2X is specified as Power-to-Hydrogen (P2H2). The purpose of the work was to perform a profitability study that examines three different production scenarios' effects on the P2H2 production plant's profits. The investigated production scenarios included production capacity increase, participation in electricity reserve markets, and the sale of district heat generated from waste heat, in addition to the base operation. Along with the study of the production scenarios, a comprehensive literature review of the P2X concept, the related market needs, and the optimization with mixed-integer linear programming (MILP) used in the research was included in the work.

The profitability study of the P2H2 production plant was conducted for Valmet Automation Oy in cooperation with Energy Opticon AB, Woikoski Oy, and Tampereen Energia Oy. The research was done with the Energy Optima 3 (EO3) optimization application from Energy Opticon AB. The system to be studied was first modelled in the optimization tool, which was used for calculating the results of the research questions. Woikoski Oy helped with the modelling and dimensioning of the hydrogen production plant by providing some of the necessary initial data and parameters. Tampereen Energia Oy, on the other hand, assisted in determining the price of the district heat purchased by an energy company. Some of the initial data needed for the work was obtained also from the literature.

The initial data needed for the research can be divided into three groups. The first of these consists of the information required by the P2H2 production plant, which is for the alkaline (AWE) electrolyzers, hydrogen compressor, hydrogen storage, hydrogen demand, and the power purchase agreement needed by the plant. The second group consists of the information required for the electricity reserve market. These include the information for the automatic frequency restoration reserve (aFRR) and the manual frequency restoration reserve (mFRR) regulation products. The last data group consists of the information needed by the heat pump and district heating demand.

The results were generated with year-long optimizations with an hourly resolution, which used input data from 2021 and 2022, such as electricity prices and demand for district heating determined according to the outside temperature. In terms of electricity prices, 2021 presented a relatively steady period, while 2022 was significantly more volatile and exceptional. In order to provide a basis for comparison of the generated results, optimizations were also carried out for the hydrogen production facility without additional functionalities.

The results of the work showed that, within the framework of the assumptions made, each production scenario generated additional income in both years under review. Each of the three scenarios studied made a more significant increase in profit during the exceptional year, i.e., 2022. Each research scenario was stated as advantageous and profitable in its own way when the production is planned with optimization and the process is controlled accordingly. Production capacity increase brings flexibility to the plant's use, participating in the reserve market is a low-threshold investment, and district heat sales improve the plant's overall efficiency. The conducted research and utilized tools yielded valuable insights into operating the facility and its constituent parts, including comprehension of the power purchase agreement's significance and potential enhancements to the production plant's capabilities.

Keywords: P2X, optimization, MILP, profitability study, energy carrier, green energy

TIIVISTELMÄ

Arttu Halminen: Power-to-X vetylaitoksen kannattavuuden parantaminen optimoiduilla ratkaisuilla
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Power-to-X (P2X) -konsepti rakentuu energian muunnos- ja varastointitekniikoiden ympärille, ja termi liitetään usein uusiutuvan energian tuotannon hallinta- ja tasoitusratkaisuihin. P2X-konseptissa energia muunnetaan varastoitavaan tai käytettävään muotoon X, joka tässä työssä on vety. Tällöin termi P2X tarkentuu muotoon Power-to-Hydrogen (P2H2). Työn tarkoituksena oli tehdä kannattavuustutkimus P2H2-tuotantolaitokseen lisättävistä toiminnallisuuksista. Lisättävät ja tutkittavat toiminnallisuudet olivat tuotantokapasiteetin lisääminen, osallistuminen sähkön reservimarkkinoille sekä hukkalämmöstä tuotetun kaukolämmön myynti. Lisäksi työhön sisällytettiin kattava kirjallisuuskatsaus P2X-konseptista, siihen liittyvistä markkinoista sekä tutkimukseen käytetystä optimoinnista, johon kuuluu lineaarinen sekalukuohjelmointi (MILP).

P2H2-tuotantolaitoksen kannattavuustutkimus tehtiin Valmet Automation Oy:lle yhteistyössä Energy Opticon AB:n, Woikoski Oy:n ja Tampereen Energia Oy:n kanssa. Tutkimus tehtiin Energy Opticon AB:n Energy Optima 3 (EO3) -optimointisovelluksella. Tutkittava järjestelmä mallinnettiin ensin optimointityökalussa, minkä jälkeen sovellus laski tulokset esitettyihin tutkimuskysymyksiin. Woikoski Oy auttoi vedyn tuotantolaitoksen mallintamisessa ja mitoittamisessa toimittamalla osan tarvittavista lähtötiedoista ja parametreista. Tampereen Energia Oy auttoi puolestaan energiayhtiön ostaman kaukolämmön hinnan määrittämisessä. Loput työhön tarvittavista lähtötiedoista saatiin kirjallisuudesta.

Tutkimukseen tarvitut lähtötiedot voidaan jakaa kolmeen ryhmään. Näistä ensimmäinen koostuu P2H2-tuotantolaitoksen tiedoista, jotka koskevat alkalielektrolysaattoreita (AWE), vetykompressoria, vedyn varastointia, vedyn kysyntää ja laitoksen tarvitsemaa sähkönostosopimusta. Toisen ryhmän muodostavat sähkön reservimarkkinoiden tarvitsemat tiedot. Näitä ovat tiedot automaattisen taajuuden palautusreservin (aFRR) ja manuaalisen taajuuden palautusreservin (mFRR) säätötuotteista. Viimeinen ryhmä koostuu lämpöpumpun ja kaukolämmön kysynnän tarvitsemista tiedoista.

Tulokset muodostettiin vuoden pituisilla tunnin tarkoilla optimoinneilla, joissa käytettiin vuosien 2021 ja 2022 lähtötietoja, kuten sähkön hintaa ja ulkolämpötilan mukaan määritettyä kaukolämmön kysyntää. Sähkön hintojen osalta vuosi 2021 edusti suhteellisen tasaista ajanjaksoa, kun taas vuosi 2022 oli huomattavasti epävakaampi ja poikkeuksellisempi. Tulosten vertailun pohjaksi optimointeja tehtiin myös vedyn tuotantolaitokselle ilman lisätoimintoja.

Työn tulokset osoittivat, että tehtyjen oletusten puitteissa jokainen lisätty toiminnallisuus tuotti lisätuloa molempina tarkasteluvuosina. Kukin kolmesta tutkitusta toiminnosta oli tuloksiltaan merkittävämpi poikkeusvuonna eli vuonna 2022. Jokainen lisätty toiminnallisuus todettiin omilla tavoillaan hyödylliseksi ja kannattavaksi, kun tuotanto suunnitellaan optimoimalla ja prosessia ohjataan sen mukaisesti. Tuotantokapasiteetin lisääminen tuo laitoksen käyttöön joustavuutta, sähkön reservimarkkinoille osallistuminen on matalan kynnyksen investointi ja kaukolämmön myynti parantaa laitoksen kokonaishyötysuhdetta. Tehdyt tutkimukset ja käytetyt työkalut antoivat arvokkasta tietoa laitoksen sekä siihen kuuluvien komponenttien tärkeydestä, kuten sähkönostosopimuksen merkityksestä ja mahdollisista tuottantolaitoksen kehityskohteista.

Avainsanat: P2X, optimointi, MILP, kannattavuustutkimus, energian kantaja, vihreä energia

PREFACE

This master's thesis has been done on an exciting and topical subject area, which has been pleasant to research, internalize, and work on. Along with the work, I have also learned much about planning, organizing, and scheduling. In addition, cooperation with the parties involved in the research has increased communication skills and understanding of the importance of the roles of the different stakeholders. Therefore, I would like to express my great gratitude towards Valmet Automation Oy, Woikoski Oy, Tampereen Energia Oy and Energy Opticon AB for the research and the results achieved.

I would also like to thank the university supervisors Professor Matti Vilkko and University Teacher Veli-Pekka Pyrhönen for their work guidance. Through them, a clear vision for the goals and content of the work and a coherent track of how to reach them was achieved.

Most importantly, I would like to thank Valmet Automation Oy's thesis supervisor, Jyri Kaivosoja, for his cooperation and supportive guidance. Jyri's guidance method was balanced excellently between offering valuable visions, perspectives, and help and giving space for independent work.

Tampere, 6 September 2023

Arttu Halminen

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LIST OF ABBREVIATIONS

aFRR	Automatic Frequency Restoration Reserve
BECCS	Bioenergy with Carbon Capture and Storage
CCS	Carbon Capture and Storage
CCU	Carbon Capture and Utilization
CCUS	Carbon Capture, Utilization and Storage
CHP	Combined Heat and Power
COP	Coefficient of Performance
CSTR	Continuous Stirred-Tank Reactor
DAC	Direct Air Capture
DC	Direct Current
DSO	Distribution System Operator
EO3	Energy Optima 3
FCR	Frequency Containment Reserve
FFR	Fast Frequency Reserve
FRR	Frequency Restoration Reserve
GCT	Gate Closure Time
GHG	Greenhouse Gas
GOT	Gate Opening Time
HVDC	High-Voltage Direct Current
IEA	International Energy Agency
LP	Linear Programming
MILP	Mixed-Integer Linear Programming
Mtoe	Million Tons of Oil Equivalent
mFRR	Manual Frequency Restoration Reserve
Nm^3	Normal Cubic Meter
NP	Nondeterministic polynomial
NTP	Normal Temperature and Pressure
NTPL	Nonthermal Plasma
PPA	Power Purchase Agreement
PSA	Pressure Swing Adsorption
P2G	Power-to-Gas
P2H	Power-to-Heat
P2H2	Power-to-Hydrogen
P2L	Power-to-Liquid
P2X	Power-to-X
SMR	Steam Reforming of Natural Gas
SPE	Solid Polymer Electrolyte
STEPS	Stated Policies Scenario
STP	Standard Temperature and Pressure
TSO	Transmission System Operator
RWGS	Reverse Water-Gas Shift

1. INTRODUCTION

The modern day's energy and transport system is mainly based on fossil forms of energy carriers, which cannot be seen as a sustainable solution for the long term. Constantly tightening environmental regulations direct the growing competition in the green energy field toward inventing more efficient and commercially profitable energy solutions. Partially due to these environmental regulations, solar and wind power have significantly increased their share in global energy production (IEA, Renewables, 2021). However, solar and wind power are weather-dependent energy sources, so their energy production is highly varying and sometimes challenging to forecast. This variation in energy production creates a great demand for flexibility in the network, which is aimed to be balanced with, for example, energy conversion and storage technologies. The collective term used for these conversion and energy-storing technologies is called Power-to-X (P2X), in which low-cost and usually green electricity is directed through a set of conversion, storage, and reconversion pathways. (Burre, Bongartz, Roh, & Mitsos, 2019)

In Power-to-X technologies, the energy is stored in a so-called energy carrier (X). These conversion technologies can be divided by their intended use, such as Power-to-Fuel and Power-to-Syngas, or by a form of energy like Power-to-Gas (P2G), Power-to-Liquid (P2L), and Power-to-Heat (P2H). Many of these conversion technologies have hydrogen produced by electrolysis working as the primary energy carrier, which then can be used directly or further refined to other energy carriers such as fuels or chemicals. Thus, in addition to the P2X technologies presented above, Power-to-Hydrogen (P2H2) is another commonly referenced conversion technology. (Varvoutis, Lampropoulos, Mandela, Konsolakis, & Marnellos, 2022). P2X solutions have gathered lots of interest because of their many potential advantages. For example, they can facilitate the replacement of fossil fuels with carbon-neutral alternatives, provide long-term storage of renewable energy, accelerate society's transition to carbon-neutral energy production, and they can balance the gap between varying renewable energy production and a grid load. However, P2X solutions are still a relatively new area of technology and, therefore, also contain many challenges, such as higher energy costs, significant investments in infrastructure, low efficiency in hydrogen storage, and high weight and volume of hydrogen storage facilities (Daiyan, MacGill, & Amal, 2020).

The objective of this thesis is to carry out a study on the economic viability of introducing new functionalities to the P2H2 production facility under review. The examined research scenarios include increasing production capacity, participating in electricity reserve markets, and selling district heat generated from waste heat. Thus, the research questions are formulated as follows:

- What is the effect of increasing the production capacity on the profitability of using a P2H2 plant?
- What is the effect of participating in the electricity reserve market on the profitability of using a P2H2 plant?
- What is the effect of selling district heat generated from waste heat on the profitability of using a P2H2 plant?

The thesis is done as a case study for Valmet Automation Oy to accelerate the development of the existing Valmet DNA Energy Management system for P2X industries and to understand and meet the new market expectations for future-proof automation systems. To achieve the objective of the work, cooperation is made with the companies Energy Opticon AB, Woikoski Oy, and Tampereen Energia Oy. The research is carried out with Energy Opticon AB because their optimization application Energy Optima 3 (EO3) is an essential part of the Valmet DNA Energy Management system. In the EO3, the investigated P2H2 production plant is modelled, and the results for the research questions are generated. The modelling of the P2H2 production facility is done with Woikoski Oy, which supplies part of the initial data needed for the work. Tampereen Energia Oy, on the other hand, helps in determining the price of the district heat purchased by an energy company. Some of the initial data is also taken from literature. The research uses data from the years 2021 and 2022, such as electricity prices and the outside temperature needed to determine the demand for district heating. In terms of electricity prices, 2021 represents a relatively steady period, while 2022 is volatile and exceptional.

To support a better understanding of the goals, needs, and context, the work also conducts an extensive literature review of the P2X operating field, the related markets, and the optimization with mixed-integer linear programming (MILP) used for the research. To complement, the work introduces two studies that also used MILP-based optimization. The first of the studies use a stochastic MILP approach to exploit the electricity market arbitrage enabled by the storage of electricity from wind power. Besides the achieved profits, the research compares the advantage brought by the stochastic method compared to the deterministic and non-coordinated model. In the second study, MILP-based optimization is used to implement the medium-term production plan of a chemical company. The research provides valuable information on the efficient ways of driving production processes, process bottlenecks, and product prioritization based on profitability.

This work's literature review consists of three chapters, which are 2, 3, and 4. Chapter 2 introduces the application field of the work. The chapter begins by introducing the four potential energy carriers of the P2X field (hydrogen, methanol, methane, and ammonia) and their markets. In addition to this, the chapter presents carbon capture and related market needs, the operating principle of the electricity network and the electricity market, and the definition of green energy and its guarantee of origin. Chapter 3 limits the focus of the work to the Power-to-Hydrogen solution and examines the sub-processes of the energy conversion chain and their characteristics. Chapter 4 presents the fundamental idea of optimization theory and the general theory underlying the problem formulation. In addition to this, the chapter provides a more in-depth introduction to mixed-integer linear programming, which is related to the hydrogen system's optimization modelling. After the literature review, the thesis introduces the optimization case and defines the configuration settings and the limitations in Chapter 5. Finally, the results of the optimization scenarios, the conclusion of the work, and the potential subjects of further research are presented in Chapters 6 and 7.

2. APPLICATION FIELD AND THE RESEARCH DRIVERS

The entire P2X concept and its stakeholders consist of power production systems, such as renewable energy production, power conversion and storage technologies, and demand for the final product (energy carrier). Creating a functional and profitable P2X system requires competitive power purchase agreements, efficient conversion and storage technologies, and sufficient demand for produced end products and services. (Incer-Valverde, Patiño-Arévalo, Tsatsaronis, & Morosuk, 2022) Of these three areas, this chapter focuses on the review of final products and services and the power purchase agreement.

First, four potential energy carriers (hydrogen, methanol, methane, and ammonia) and their markets are introduced. After this, the carbon capture, utilization and storage, and emissions market, which are part of the P2X concept and connected to the production of methanol and methane, are presented. In addition to these, the operating principle of the Finnish electricity network and market, as well as the definition of green energy and the guarantee of origin, are reviewed.

2.1 Demand sector overview of potential energy carriers

The analyzed energy carriers are hydrogen, methanol, methane, and ammonia. Each of them has their own demand, and this section presents what the demand for each carrier consists of. The section does not compare the market profitability of the carriers to each other and instead focuses on presenting each type separately. The section presents the typical industrial uses for each carrier, the change in demand over time, and their future outlook.

2.1.1 Hydrogen

Hydrogen is versatile in its uses, both as a raw material and as an energy source. The demand for hydrogen currently mainly consists of oil refining and ammonia production, although it can be widely applied to various purposes, such as industrial production, transportation, and heating. The production of hydrogen is well known and controlled in the industry, but most of the hydrogen that is still manufactured is produced from fossil energy sources. However, modern hydrogen production will be returned to in more detail in Chapter 3. (IEA, The Future of Hydrogen, 2019)

In addition to the current hydrogen-utilizing processes, upgrades and technologies are being developed in both industry and transportation, which make it possible to switch from fossil feedstock to utilizing hydrogen. The steel industry serves as one example, as the direct reduction of iron with hydrogen is being developed for this environment, which would replace the fossil coal used at the moment. As already stated earlier, hydrogen is a versatile building block as it can also be used to produce synthetic raw materials and fuels, such as methane, methanol, gasoline, kerosene, or diesel. Due to its properties, hydrogen is, therefore, able to participate in carbon capture and utilization (CCU) operations because, in addition to hydrogen, carbon dioxide is also needed to produce synthetic fuels. Unfortunately, these CCU operations do not change the carbon balance because the carbon dioxide used in the process is released back into the atmosphere in the short term. (Sivill, et al., 2022)

The production of raw materials and fuels from hydrogen produced by electrolysis is a potential target for hydrogen refining, as they can effectively utilize the already existing infrastructure. However, a general challenge in hydrogen processing is the low efficiency that occurs in all conversion situations. Thus, hydrogen produced with electricity and the electric fuels produced as derivatives are not directly competitive compared to fully electrified transport. However, hydrogen produced with electrolysis and its further refined products is more profitable and even competitive if at least the waste heat and oxygen generated in the hydrogen conversion process could be utilized. Waste heat can be collected and connected, for example, to a district heating network, while the oxygen produced as a by-product could replace the oxygen produced by distillation used in the steel and chemical industries. Other sites suitable for utilizing oxygen are, for example, increasing the efficiency of energy production combustion processes, the pharmaceutical industry, and welding. The current uses of hydrogen are presented in Figure 2-5, which illustrates and summarizes the overall demand for the selected energy carriers. (Sivill, et al., 2022)

The production of hydrogen, its uses, and the infrastructure used for transportation have developed significantly over the years, which is reflected in the increased demand for hydrogen. The global demand for hydrogen in 2020 was around 90 Mt, which means a 50% increase from the turn of the millennium. The increase in demand has largely been due to the refining and industrial use of hydrogen. Although the demand for hydrogen has grown, its segmentation has remained relatively the same. The utilization of hydrogen in new technologies and applications has been slow, but its use in hydrogen-powered transportation and as part of electricity production and storage has been a clear direction of development and research for a while. However, the hydrogen economy is expected to grow significantly in the next few years, as hydrogen technologies suitable for industry and consumers, which enable transportation, provide heating of buildings, and evolve energy production, are constantly being developed. The global distribution of hydrogen demand, the development course, and the future forecast are shown in Figure 2-1. (IEA, Global Hydrogen Review, 2021)

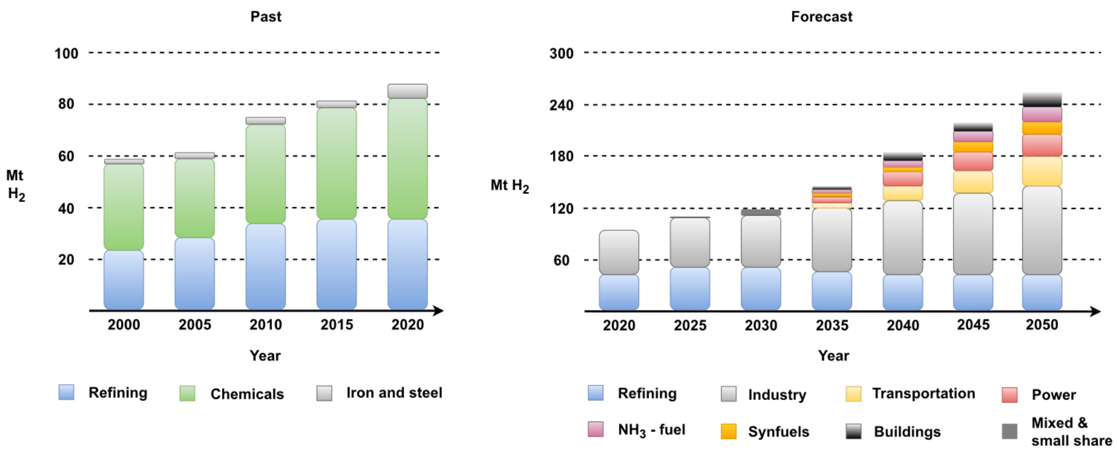

Figure 2-1: *Past and future of hydrogen demand structure. Based on source (IEA, Global Hydrogen Review, 2021).*

The Figure 2-1 shows how hydrogen consumption is expected to almost triple by 2050. In that case, the demand for hydrogen would be around 250 million tons. The forecasts presented in the Figure have been created based on the goals and pledges made by governments belonging to the International Energy Agency (IEA). Finland, like 29 other countries, is a member of the IEA. (IEA, Global Hydrogen Review, 2021)

2.1.2 Methanol

Interest in alternative fuels has grown significantly as fossil fuels keep getting more expensive, and preventing climate change requires concrete measures to reduce traffic pollution, for example. The hydrogen economy is a possible solution, but hydrogen production, storage, and transportation still need development. Methanol has been proposed as one competitive alternative, especially regarding transportation. Methanol production is inexpensive compared to other alternative fuels, and its storage is also easier and cheaper due to its liquid form. Methanol can also utilize existing infrastructure and thus can be treated like fossil fuels already in use. (Deka, Osman, Baruah, & Rooney, 2022)

In addition to its properties suitable as a fuel, methanol is an important starting material in many industrial productions. It is commonly used in household products, essential components of automobiles, and in manufacturing valuable chemicals. These chemicals include, for example, formaldehyde, olefins, acetic acid, and many compounds needed for producing dyes and pharmaceuticals. In addition to these, methanol is used in the production of fertilizers and plastics. Along with its diverse product portfolio, methanol is considered a clean energy carrier, as its combustion processes have low emissions. When methanol is produced through carbon capture, utilization, and storage, and renewable sources, such as hydrogen produced by solar and wind power, it becomes a carbon-neutral energy carrier, which aligns with climate change policy to reduce greenhouse gas emissions. The current uses of methanol are also presented in Figure 2-5, alongside hydrogen and other energy carriers. (Araya, et al., 2020)

Although methanol has many uses, clear visions of the future have been planned for it. A more significant part of the total methanol demand than before is believed to be bound to olefins and biofuels. In the production of both refined products, methanol replaces more and more oil-based starting materials. Consequently, as the demand and possibly also the availability of petroleum-based substances decreases in the future, the usage rate of methanol will naturally increase due to its right type of properties. The increase in usage rate is already noticeable in biofuels. For example, in China, methanol fuels have been developed for a long time, such as M100 (100% methanol) and M85 (85% methanol and 15% gasoline), which have been successfully used since 2005 (Ho, Peng, Yun, & Mao, 2022). The future of methanol can also be seen as closely tied to the hydrogen economy and the solutions needed for it. As stated earlier, the challenge of a functioning hydrogen system is both infrastructure and storage. Thus, methanol could also be considered a hydrogen storage solution, as it is a very efficient hydrogen carrier. Namely, methanol packs more hydrogen into one alcohol molecule than the corresponding volume of hydrogen gas itself. Methanol is liquid in NTP (normal temperature and pressure) conditions, so it can be handled, stored, and transported using traditional fuel transfer networks and methods. With the help of methanol reformers, hydrogen can be produced when needed or at the point of use. The current and predicted global demand for methanol and its distribution is shown in Figure 2-2 (Suseno & Umar, 2021). (Schorn, et al., 2021)

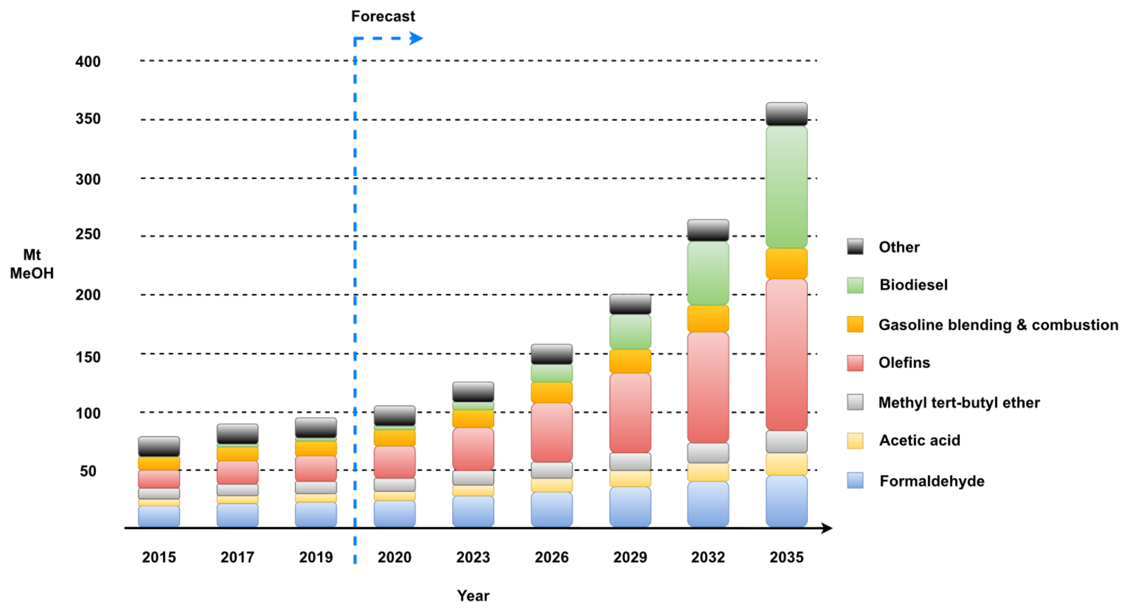

Figure 2-2: *Past and future of methanol demand structure. Based on source (Suseno & Umar, 2021).*

The Figure 2-2 illustrates how the demand for biodiesel and olefins is believed to grow considerably during the next decade, when they will cover the largest part of the total demand. Thus, the future of methanol looks promising, as its total demand is expected to nearly triple by 2035. In that case, the demand for methanol would be around 360 million tons.

2.1.3 Methane

Along with hydrogen and methanol, methane has its own broad demand, and, like methanol, it can also act as a carrier of hydrogen in addition to carrying energy. As with methanol, the methane conversion process is simple, and methane is an easy-to-use substance. In addition, it is possible to utilize the already existing gas infrastructure for methane. (Qi, et al., 2022)

In general, methane and natural gas have almost the same demand base. The only significant difference between the two is that methane can be produced from renewable sources and can be used as energy carrier. However, when connected to the gas network, the substances presented are mixed in an almost indistinguishable way, so their markets are practically the same. Like other energy carriers, the uses of methane are summarized in Figure 2-5. Methane and natural gas are both colorless and odorless, but methane is a reasonably clean gas, while natural gas contains ethane, propane, carbon dioxide, and water vapor, which makes its combustion process less clean. Methane production is also supported by the rising price of fossil raw materials, which directly affects the price of natural gas. (Qi, et al., 2022)

Methane works well as a fuel for power plants, as it burns very cleanly. Burning methane does not release, for example, sulfur, heavy metals, or other solid pollutants. In addition, the combustion reaction of methane produces a lot of thermal energy. Therefore, its combustion properties make it ideal for energy production. However, methane is not a completely problem-free fuel because, despite its good properties, it is itself the second largest (after carbon dioxide) greenhouse gas contributing to climate change. In addition to this, carbon dioxide is released in the process of burning methane, which is why the process design should possibly consider filtering or recovering carbon dioxide. Despite this, methane is widely used in energy production, especially in CHP power plants (combined heat and power) and boilers, where relatively good efficiencies are achieved by burning methane. In CHP power plants, the efficiency in terms of electricity production is around 50%, while in heat production, this type of power plant can reach up to around 80% level (EPA, CHP Benefits, 2022). However, power plant types, such as thermal boilers, which focus entirely on converting energy into heat, can reach up to 90% efficiency. (Obaideen, et al., 2022)

In addition to power and heat production, methane has also attracted public interest as an energy source for transport. It has many advantages compared to fossil liquid fuels, mainly because of the simple structure of methane, whose molecular structure consists of only one carbon atom. Thanks to the homogeneous structure of methane, its emissions are low, the amount of emission components is small, and the particle emissions are minor. If methane is produced from renewable sources utilizing carbon capture, then in addition to its low emissions, it can also be considered a neutral solution in terms of net effects on the carbon balance. This is because the amount of carbon dioxide bound in carbon capture can be equal to the amount released from burning methane (Enapter, 2021). Furthermore, the removal of nitrogen oxides formed during the combustion process in the vehicle engine is more effective with methane than with conventional fuels because conventional fuels produce liquid emissions. The filtration of this flue gas mixture in the catalyst is less efficient than the filtration of completely gaseous methane emissions. Finally, the properties of methane enable higher efficiency in combustion engines, better cold operation properties, and suitability for versatile engine solutions. Thus, methane, along with the other presented energy carriers, turns out to be a potential fuel alternative. (AMF, 2023)

The future of methane seems to be found in the production, processing, and use of green methane and biomethane. Green methane is further refined from hydrogen produced from renewable sources, also using carbon dioxide collected by carbon capture presented in section 2.2 (Enapter, 2021). Biomethane, which can be compared to green methane in terms of its environmental classification, is produced either by refining biogas by removing carbon dioxide and other impurities or by gasifying solid biomass, followed by methanation. The demand for methane classified above is expected to increase significantly in the future in the areas of industry, energy production, transportation, and heating of buildings and residential use, which is illustrated in Figure 2-3. (IEA, Outlook for biogas and biomethane, 2020)

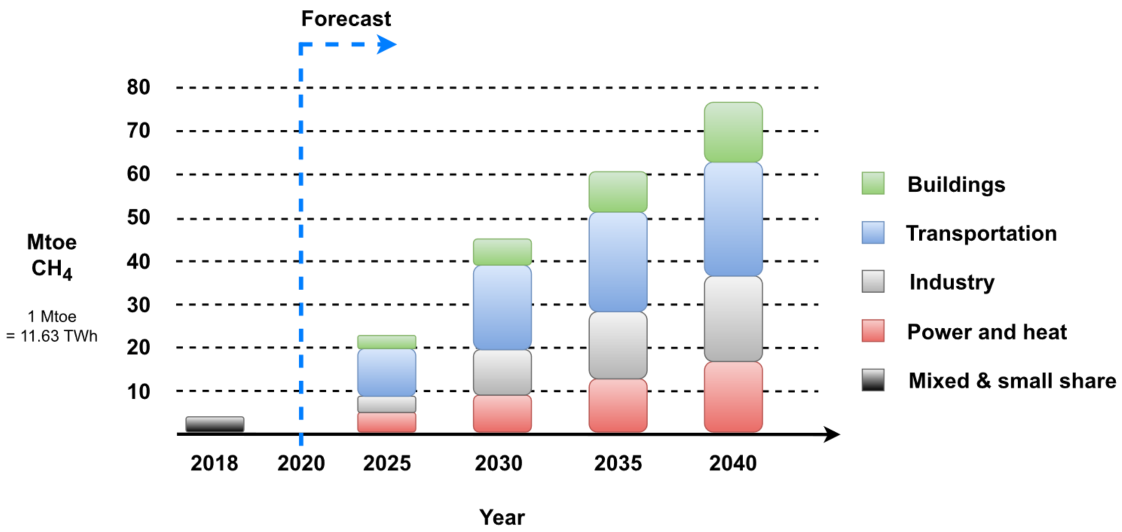

Figure 2-3: *Past and future of biomethane demand structure. Based on source (IEA, Outlook for biogas and biomethane, 2020).*

The forecast presented in the Figure 2-3 is based on the Stated Policies Scenario (STEPS), which creates a picture of where today's political goals and plans, including national political announcements and pledges, would steer the energy sector. In the situation described in the Figure, the demand for biomethane is gradually replacing the demand for natural gas, which is partly why the growth in the demand for biomethane is believed to be rapid. In 2040, the amount of demand for biomethane is believed to reach around 75 million tons of oil equivalent (Mtoe), in which case transportation is expected to be the biggest demand target. (IEA, Outlook for biogas and biomethane, 2020)

2.1.4 Ammonia

Finally, along with other energy carriers, ammonia is one of the targets to be examined because its production from hydrogen is simple, and the conversion process is well-known and developed. Ammonia is used a lot in the industry, but its greatest demand is found in the production of agricultural fertilizers. In industry, ammonia is used as a fuel in energy production, as a key raw material in the production of chemicals, as the main substance in cleaning agents, as fuel in engines, and as a refrigerant in cooling systems (Erdemir & Dincer, 2021). In agricultural fertilizers, ammonia is a very important raw material, and 80% of its production is used to manufacture different fertilizer products. These include, for example, urea, ammonium nitrate, and calcium ammonium nitrate. At the moment, interest in ammonia has also risen as a target for hydrogen storage and further processing. (Yüzbaşıoğlu, Avşar, & Gezerman, 2022)

The global use and demand for ammonia are mainly through agricultural systems. It is the starting material of all mineral nitrogen fertilizers and most of the ammonia is converted into urea and other nitrogen fertilizers before use. The use of ammonia itself is currently less than 3% of the total demand, but its share is expected to increase in the future. Over the years, the use of ammonia in agriculture has experienced a clear increase due in part to population growth and the resulting increase in food production. Although ammonia is used a lot for nitrogen fertilizers, and other fertilizer derivatives, a large part of the global demand also consists of the needs of industry and the applications included in them. As in agricultural fertilizer products, a lot of ammonia is used to produce nitric acid, which in turn is used to make different forms of ammonium nitrate. In addition to fertilizers, these can also be used as explosives in mining, quarrying, and tunneling, as well as in the manufacture of other chemical products. Accordingly, urea is also used for industrial purposes in addition to fertilizers. About a fifth of the produced urea is used as an intermediate product in the production of durable resins and as a chemical agent to reduce nitrogen oxide emissions from power plants and diesel engines. Furthermore, ammonia is also used to make acrylonitrile, which is an intermediate for several durable chemical products such as plastics, rubbers, and fibers. The current uses of ammonia are presented in Figure 2-5, which also summarizes the demand sector of the examined energy carriers. (IEA, Ammonia Technology Roadmap, 2021)

Along with the typical demand, ammonia is considered a potential future hydrogen storage and further processing target in the green energy production and transmission chain. Ammonia's advantages over hydrogen are its better liquefaction temperature (-33 °C with ammonia and -253 °C with hydrogen), higher volume energy density (circa 50% more when compared to the liquid states), and the infrastructure related to transport and storage is more developed (Lamb, Dolan, & Kennedy, 2019). In addition, ammonia's general advantages include low production costs and the fact that it can also be used as a carbon-free fuel, for example, directly in large gas turbines. However, the future visions of ammonia are not limited to hydrogen storage or the power sector. It is also seen as a possible fuel in the maritime sector. Ammonia-powered combustion engines for maritime use are constantly being developed, and at least some of the maritime technology companies expect to make them commercially available by the mid-2020s. The development of ammonia demand and its future outlook is illustrated in Figure 2-4, where the possibility of demand brought by maritime, or power generation is not taken into account. The information in the Figure is again based on IEA's STEPS forecast, where political goals, announcements, and pledges guide the future vision. (IEA, Ammonia Technology Roadmap, 2021)

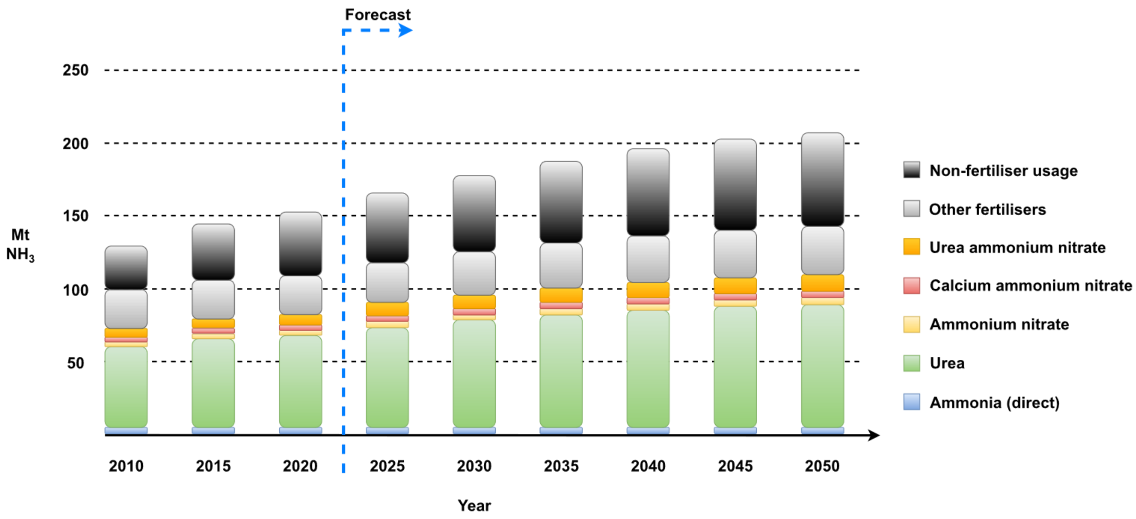

Figure 2-4: *Past and future of ammonia demand structure. Based on source (IEA, Ammonia Technology Roadmap, 2021).*

The Figure 2-4 shows a moderate but solid growth in the demand for ammonia in the future, where the largest areas of utilization are assumed to be urea and non-fertilizers. By 2050, the total demand for ammonia is believed to be around 205 million tons.

2.1.5 Energy carrier summary

All the examined energy carriers have a clear and broad demand at the moment. In addition, each carrier is assumed to be part of future green energy production and storage in one way or another. The future of all energy carriers also looked promising due to their growing demand and expanding field of application. All the energy carriers have in common their possible future as low-emission fuel in transportation and energy production. Figure 2-5 summarizes the overview of the demand sector, illustrating the overlapping uses of the investigated substances and the connections between them.

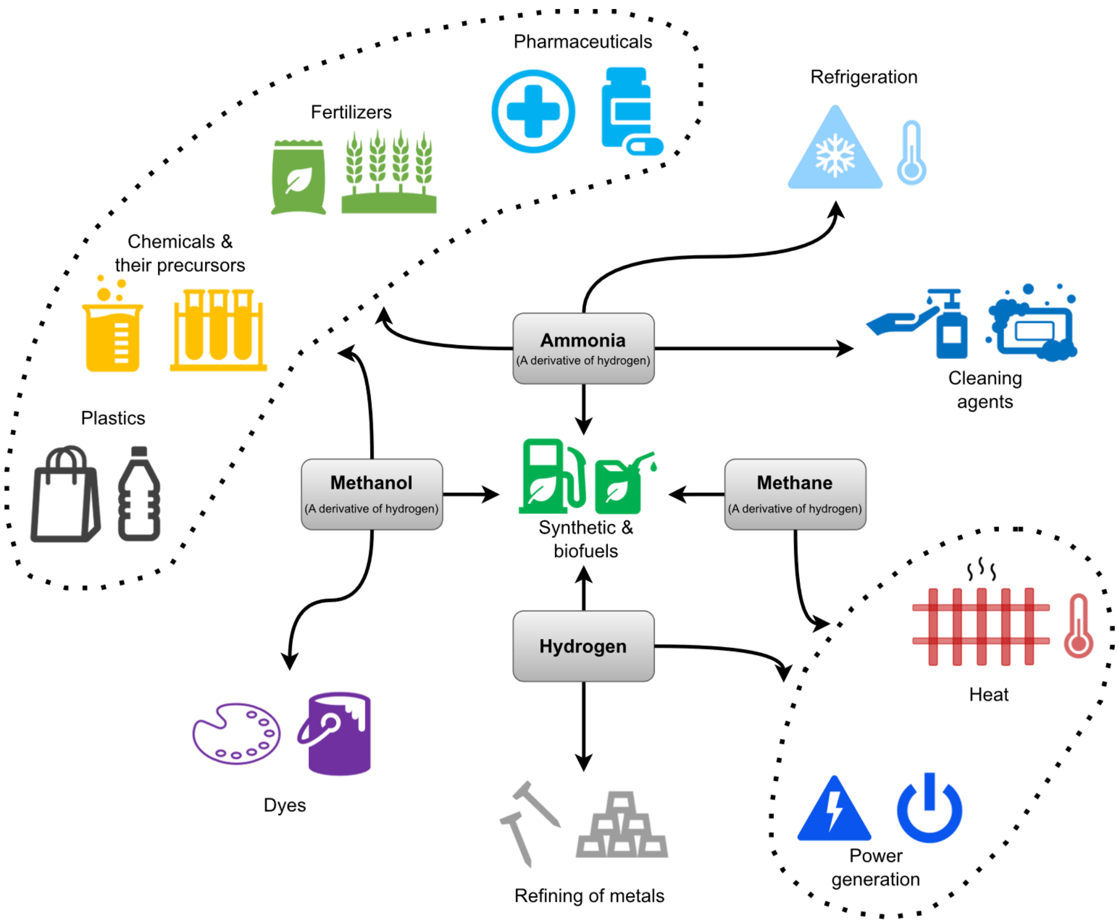

Figure 2-5: *Energy carriers' demand and connections.*

As seen from the Figure 2-5, the demand sector for each energy carrier is broad, and each of them is distributed in many areas of the economy, from energy production to the manufacture of pharmaceuticals. However, energy carriers are divided into two categories, which could be characterized as energy production, and intermediate and final products of industry. Of these, methanol and ammonia contribute more to the production of intermediate and final products, while hydrogen and methane contribute to energy production. Although the carriers can be divided into categories, they are united by the development projects of synthetic and biofuels and the future outlook in green energy production and storage.

2.2 Carbon capture, utilization and storage and related markets

Carbon dioxide recovery is commonly referred to as carbon capture. It is often divided into topics such as carbon capture and storage (CCS), carbon capture and utilization (CCU), and their combined area carbon capture, utilization, and storage (CCUS). In CCS, for example, the carbon dioxide contained in the emissions of power plants, factories, and industrial plants that operate with carbon dioxide-releasing fuels is collected and stored while reducing the plants' emission load and moving production toward net-negative greenhouse emissions. In CCU, on the other hand, the possibilities of further use of the collected carbon dioxide are examined, in which case the focus of attention is the utilization of carbon dioxide in various production and manufacturing processes. (Gabrielli, Gazzani, & Mazzotti, 2020) CCU is an essential part of the P2X energy conversion chain, for example in the production processes of green methanol and methane, as presented in previous chapters. In this section, the concept related to CCS and CCU is presented, as well as their future outlook in the carbon-neutral economy and the emission trading enabled by carbon capture, storage, and utilization.

2.2.1 Carbon capture, utilization and storage

The structure of the CCS concept includes carbon capture, long-term storage solutions, and a transportation network. The capture process can be divided into three typical categories, which are pre-combustion, post-combustion, and oxy-combustion processes. The separation of carbon dioxide and other substances, which are part of the presented processes, are based on, for example, absorption, membrane separation, adsorption, and chemical looping techniques. (Madejski, Chmiel, Subramanian, & Ku´s, 2022) In the case of the term CCS, the focus of attention is not only on the capture of carbon dioxide but also on its existing long-term storage technologies and methods. CCS does not apply short-term storage solutions for carbon dioxide, which are used with, for example, CCU, but instead, research and applications are focused only on permanent storage solutions. Carbon dioxide is naturally stored in oceans and forests, but its capacity is not sufficient to contain the increase in atmospheric carbon dioxide concentration. Consequently, the manual storage of carbon dioxide has become one of the global projects against climate change. However, storing carbon dioxide is a challenge because the carbon dioxide emissions caused by the storage process and the leaks in the storage solutions must be lower than the amount of carbon dioxide to be stored. Therefore, for example, the storage location should be as close as possible to the capture site to minimize emissions from carbon dioxide transportation. (Kearns, Liu, & Consoli, 2021) Currently, carbon dioxide storage methods can be divided into at least three types, which are geological storage, mineralization, and offshore storage. However, the last of these is a controversial storage type due to the risks associated with its environmental impact. (CTNC, 2023)

CCU and CCS are overlapping concepts in terms of carbon capture and transportation. In addition to these, CCU focuses on the usage of carbon dioxide as a feedstock in the production of chemical substances, synthetic fuels (such as methanol and methane), and building materials. In CCU, carbon dioxide emissions can also be limited by the direct use of it, for example, by converting carbon dioxide into products and permanently binding it into building materials such as concrete. With CCU, it is also possible to offer electricity storage options by producing, for example, synthetic methane or methanol by further refining carbon dioxide with hydrogen produced from renewable sources, as presented in the previous section. Thus, CCU can also participate in sector coupling by helping to integrate renewable energy into the gas network while keeping infrastructure upgrade costs at a minimum. (Gao, et al., 2020)

In addition to the previously introduced carbon dioxide binding products and the energy grid integration solution, CCU is also used in fertilizer industry applications, where it plays a central role in the production processes of melamine- and urea-based products and resins. Furthermore, CCU is also an essential component in the production of calcium carbonate, lime, and calcium ammonium nitrate. Along with the many uses of carbon dioxide, its utilization would also significantly increase emissions trading in the EU, for example. Through trading, it would have a positive effect on actions against climate change. In general, however, CCU is less advanced in its development and implementation than CCS, which is why more attention should be paid to it so that the entire CCUS chain would work as effectively as possible. Figure 2-6 presents and summarizes the operation of the entire CCUS chain and clearly illustrates the research and application fields of CCS and CCU. (IOGP, 2019)

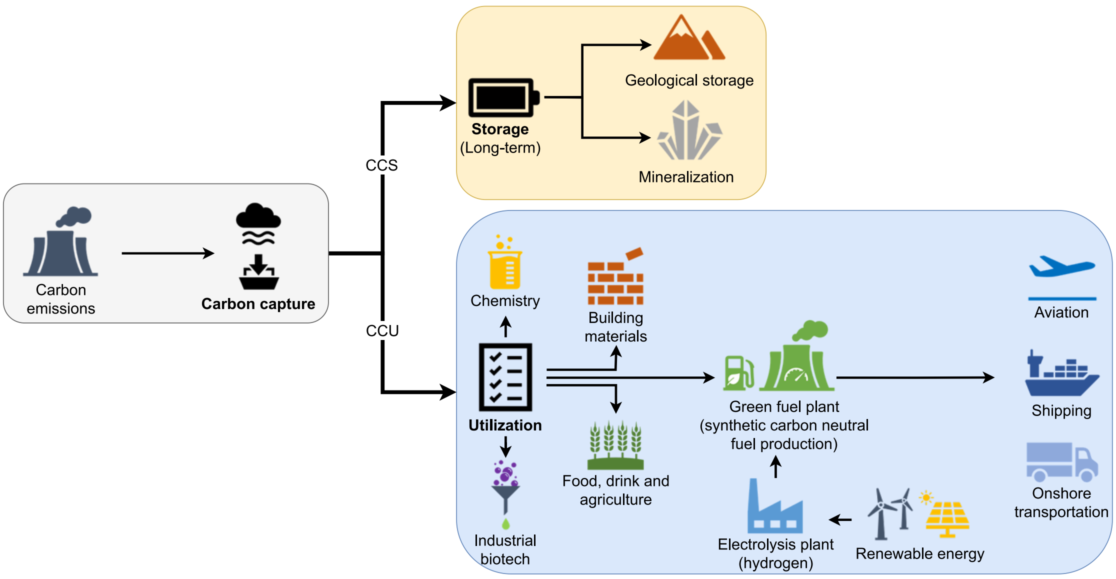

***Figure 2-6:** The chain of carbon capture, utilization, and storage.*

The CCUS chain is pivotal for reducing carbon dioxide emissions and achieving carbon neutrality in the economy. Projections for CCUS adoption are divided into three time frames: 2020-2030, 2030-2050, and 2050-2070. The initial phase (2020-2030) focuses on capturing emissions from existing power plants and factories, primarily through retrofit techniques, contributing to around 840 Mt of CO2 recovery by 2030. (IEA, CCUS in Clean Energy Transitions, 2020)

The second phase (2030-2050) anticipates accelerated CCUS deployment in industries like cement, steel, and chemicals, constituting one-third of global carbon capture growth. Hydrogen production from fossil fuels is also expected to play a substantial role, especially for energy and transportation needs. Shifting electricity generation toward natural gas-fired plants enhances renewable energy integration, such as connecting solar and wind power to methane production via electrolysis-generated hydrogen. Bioenergy with carbon capture and storage (BECCS) is projected to contribute significantly, accounting for about 15% of carbon capture growth. The cumulative recovery in this phase is projected to reach approximately 5000 Mt by 2050. (IEA, CCUS in Clean Energy Transitions, 2020)

In the final phase (2050-2070), carbon removal and utilization are set to accelerate, raising captured carbon by around 85% from 2050 levels. BECCS accounts for about 45% of this growth, while direct air capture (DAC) contributes roughly 15%. Additional carbon capture is achieved through regular CCS from fossil fuels and coal. This optimistic outcome aligns with sustainable development scenarios, relying on robust technological advancements and innovative systems. The total estimated carbon recovery in this phase is around 4300 Mt by 2070. Figure 2-7 illustrates the development of the total amount of carbon dioxide and the sources of recovery in the years 2020-2070. (IEA, CCUS in Clean Energy Transitions, 2020)

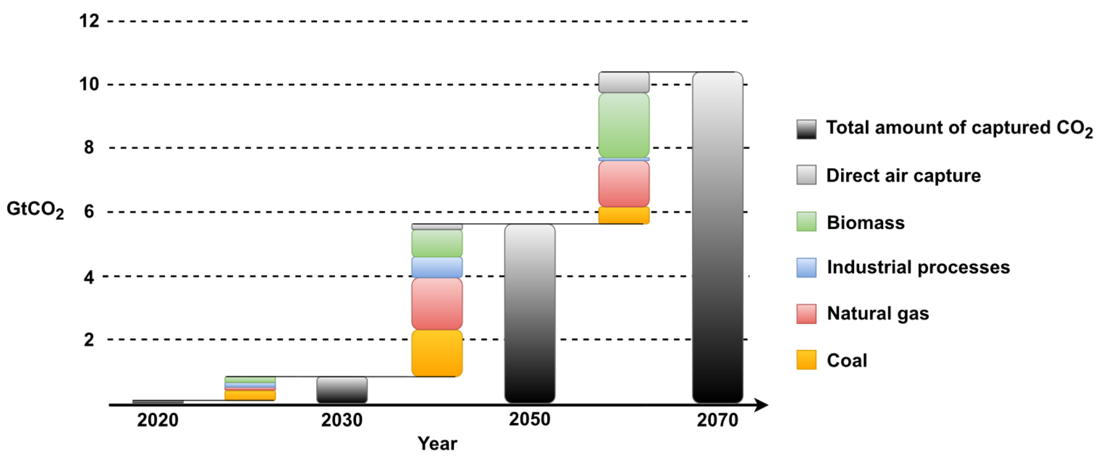

Figure 2-7: *The future outlook of carbon capture growth and sources. Based on source (IEA, CCUS in Clean Energy Transitions, 2020).*

2.2.2 CCUS and emissions trading

In the European Union, emissions trading refers to an arrangement in which facilities that generate harmful emissions are obliged to own a certain number of emission rights for each unit of emissions they produce. These emission rights, in turn, can be sold and bought by the facilities, which is called emissions trading. The underlying purpose of emissions trading is to limit and reduce the total amount of harmful emissions and steer production in the net negative direction. To achieve the underlying purpose of emissions trading as efficiently as possible, it is crucial how different technologies, and their utilization are taken into account within the scope of emissions trading. For this purpose, CCUS technologies offer new dimensions both through the storage and use of carbon dioxide. (Michaelowa, Shishlov, & Brescia, 2019)

For companies using CCUS technologies, emissions trading, such as carbon offsets, can be a significant part of the repayment and profitability of the investments made in them. Through CCUS implementation, companies utilizing this technology can offer enhanced services beyond carbon capture. For instance, they can provide additional processing capabilities for carbon dioxide, ensuring its permanent removal from the atmosphere in full compliance with regulatory directives. This can be done either by long-term storage or by converting it into products that utilize permanent chemical bonds. CCUS applications also offer alternatives for companies that do not have direct measures related to it themselves. Namely, these companies can buy the emission compensations they need from the companies that provide carbon dioxide reduction services. (Kaplan, Ramanna, & Roston, 2023)

2.3 Electricity network and markets in Finland

Most of the electricity used in Finland is transferred through the main grid. The electricity is transferred from production to consumption on public and fair terms. Fingrid is a transmission system operator (TSO) which is responsible for the main grid of Finland, and its purpose is to maintain and improve the grid and transmission connections to the neighboring countries based on the needs of the customers and society. (Fingrid, Electricity transmission and the use of the electricity system, 2023)

2.3.1 Electricity network

The electricity system in Finland consists of power plants, the main grid, high-voltage distribution networks, transformers, distribution networks, and electricity consumers, which is also roughly the general base model of global electricity networks (Electrical grid, 2023). The basic principle of the electrical grid is illustrated in Figure 2-8, but both the grid and its operation are evolving continually into a more complex system with new technologies, energy sources, and storage solutions. The electricity system of Finland is part of the Nordic electricity system, which also includes Norway, Sweden, and Eastern Denmark. In addition to the Nordic electricity system, direct current (DC) transmission links come from Estonia, which connects the Nordic system to the power system of the Baltic. Similarly, the system between Nordic countries is connected to Continental Europe via DC transmission links. Through this, Fingrid is also involved in ENTSO-E, the European association for the cooperation of TSO actors. (Fingrid, Electricity system of Finland, 2023)

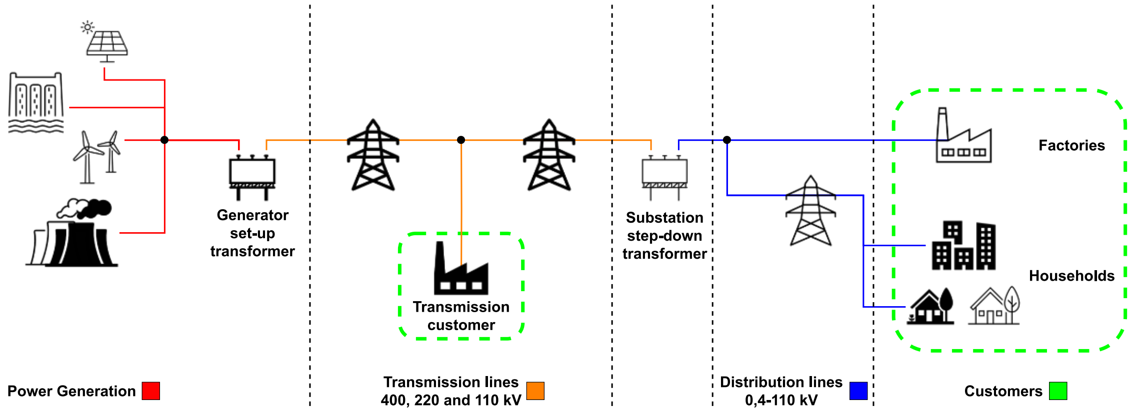

Figure 2-8: *Basic components of the electrical grid.*

As a transmission system operator, Fingrid is responsible for the technical functionality and reliability of the Finnish electricity system and takes care of the tasks that fall under the national balance responsibility and the national balance settlement in an appropriate, fair, and non-discriminatory way. TSO is also liable for maintaining the balance between the ongoing electricity production and consumption as well as for clearance of its own electricity balance and the electricity balances of the balancing coordinators in its area of responsibility. (Fingrid, Electricity system of Finland, 2023)

In order to maintain the balance of the electrical grid, TSO needs to have a well-designed balancing system that has immediate information and a good prediction of the changing state of the network. The distribution system operators (DSO) are responsible for planning and balancing their production and consumption in advance in their areas, but the balancing forecasts are always rough estimates, so it is ultimately the TSO's responsibility to take care that the required balance is achieved. (Fingrid, Maintenance of power balance, 2023)

The momentary balance of production and consumption is measured by the frequency of the electrical grid. The aim is to keep the frequency between the values 49,9 and 50,1

Hz. If the frequency of the grid exceeds the nominal value of 50 Hz, then production is greater than the expected consumption, and correspondingly, if the frequency is below 50 Hz, consumption has become greater than the planned production. In practice, Fingrid, as a TSO, takes care of the grid balance by activating regulation bids from the balancing power markets and by acquiring reserve capacity to support the system. The reserve capacity consists of the freely adjustable active power of the acquired production plants or consumption units, such as an electric power plant or a large factory participating in reserve operations. Simply put, Fingrid acquires different reserve products that react to changes in production and consumption balance at different time periods. These reserve products are, for example, Fast Frequency Reserve (FFR), Frequency Containment Reserve (FCR), and Frequency Restoration Reserve (FRR), which will be discussed in more detail later in this section. (Fingrid, Maintenance of power balance, 2023)

TSOs need to acquire reserve products to maintain the system's reliability. In the case of the main grid, operational reliability means the ability of the electrical system to withstand sudden disturbances or failures of network components while meeting the requirements set for the network. This means that power can be transferred from the generating units to consumers while the thermal or mechanical limits of the network components are not exceeded, the voltage level of the system will not cross the set boundaries, and the overall stability of the system is maintained. In other words, the power system needs to have the ability to balance production and consumption in real-time by managing variability, ramping constraints, and flexible loads so that an event like a large power plant or transmission line failure will not crash or significantly disturb the system. (Geocaris, 2022)

Maintaining operational reliability is constantly challenged by the increase of renewable energy sources in energy production because as the share of these forms of energy production increases, the traditional inertia from the rotating masses of large power plants connected to the electricity grid decreases (Razzhivin, Andreev, & Kievec, 2022). Generally, in physics, inertia means slowness and resistance to change. The inertia of the electrical network refers to the kinetic energy in the grid. This energy is tied up in machines in power plants and factories that run at the same frequency as the electric grid. In the case of the grid, inertia is usually a desired phenomenon, as it slows down and reduces the effects of disturbances on the network. If, for example, the frequency of the network is affected by a change either for reasons related to electricity consumption or production, inertia mitigates the upcoming real impact and its speed. The more inertia there is, the slower and smaller the changes in electricity consumption and production appear in the frequency. (Fernández-Guillamón, Gómez-Lázaro, Muljad, & Molina-García, 2019)

In the current situation, a lot of energy produced by renewable energy sources comes into the electrical grid, replacing the electricity production of traditional power plants with massive rotating turbines and generators. Wind and solar power are connected to the grid without a rotating mass. Even though wind power also has a rotating rotor, this does not appear in the same way as a rotating mass in the grid frequency, as with traditional power plants. This is because there is usually a frequency converter between the wind power plant and the electrical grid, through which the kinetic energy of the rotating mass is not automatically transferred to the grid. In traditional power plants, such as nuclear power plants, the amount of rotating mass is large and directly connected to the grid, thus increasing the inertia of the electrical grid. In addition to renewable energy sources, the amount of inertia that the grid has is also reduced in situations where a large quantity of electricity is transferred via DC links. (Fernández-Guillamón, Gómez-Lázaro, Muljad, & Molina-García, 2019)

One solution for situations of low inertia is to store the energy obtained from renewable energy sources and use the stored energy later as a reserve unit to balance the electrical grid. Storage is possible by converting so-called excess electrical energy, for example, into hydrogen through electrolysis. Hydrogen, which in this case presents energy carriers, works well as a subject for storage, and it can either be sold as such to the hydrogen market or be refined into another useful form, such as methane, and then sold to the energy market (Zwaan, Detz, Meulendijks, & Buskens, 2022). Respectively, the energy stored in the energy carriers could also be converted back into electrical energy, in which case the energy carriers would act as reserve energy units, which could facilitate the maintenance tasks of low inertia and network balance. (Razzhivin, Andreev, & Kievec, 2022)

Fingrid, as a TSO, promotes the operation of the electricity market by actively participating in the maintenance and development of the electricity market and by developing electricity transmission connections in a long-term and proactive manner. The development goal of the transmission network is the customers' future consumption and production needs, the promotion of the functionality and reliability of the electricity market in the Baltic Sea region, cost efficiency, and management of the grid aging. (Fingrid, Unified electricity market, 2023)

2.3.2 Electricity markets

In the electricity market, the price is formed based on the electricity produced by producers and used by consumers. Electricity network companies act as market enablers, as they physically connect the production and consumption of electricity through the grid. TSOs transfer electricity from power plants to DSOs and directly to large consumers, such as major factories. DSOs further distribute electricity to their customers. Finland is part of the Nordic electricity system and the European wholesale electricity market. The Nordic electricity system is divided into bidding areas according to the physical transmission capacity of the power system. For the Nordic countries, these bidding areas are divided in such a way that Finland as a whole is one area, while Sweden is divided into four, Norway into five, and Denmark into two areas. Within the bidding areas, the price of electricity is always uniform. The price differs between the bidding areas when the transmission capacity of the network limits the amount of energy that can be transferred between the bidding areas. (Fingrid, Unified electricity market, 2023)

Electricity is traded in various marketplaces, such as the electricity derivatives markets (financial markets), the day-ahead, the intraday, and the ancillary services (such as reserve markets). In addition to these, there is an imbalance settlement, which is carried out after the delivery of electricity. This settlement shows the actual supply of electricity between the operating parties in the electricity network and the resulting costs. Among the presented electricity market items, the day-ahead and intraday markets take place through the Nord Pool organization, which is one of Europe's energy markets and offers trading, clearing, settlement, and related services in 16 European countries. At the Finnish level, however, Fingrid is responsible for balancing energy and reserve markets and for imbalance settlement. Marketplaces and their trading periods are illustrated in Figure 2-9. (Fingrid, Johdanto sähkömarkkinoihin, 2023)

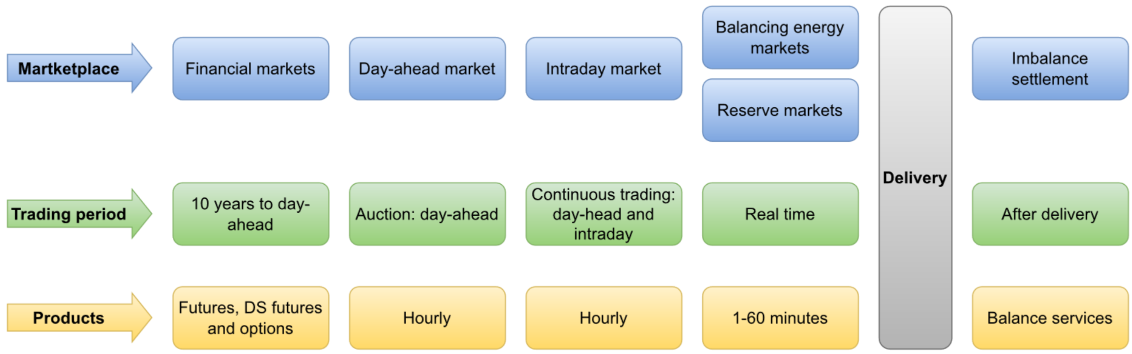

Figure 2-9: *Structure of the electricity markets. Based on source (Fingrid, Johdanto sähkömarkkinoihin, 2023).*

As shown in Figure 2-9, the longest trading period is in the financial markets. Derivative products related to the price of electricity, such as futures and options, are traded in the electricity derivatives market. The need for the electricity derivatives market arises from market participants' risk management against electricity price fluctuations. For example, an electricity producer can try to hedge against momentary changes in the price of electricity with the help of derivatives. It is also possible that a seller of electricity tries to seek protection against high electricity prices, as the seller's contracts with end customers in the retail market may be fixed prices. Electricity producers, sellers, or users looking for a trading partner for various derivative products on the exchanges can enter into bilateral agreements. Derivatives markets are mainly speculative in nature because the delivery does not include physical electricity. (Fingrid, Johdanto sähkömarkkinoihin, 2023)

In the day-ahead market, the next day's electricity is traded, and trading is done for each hour. Market participants closely monitor the course of the electricity market and plan and set their offer for the next day's electricity price by 1:00 p.m. (Finnish time) when the auction of the electricity exchanges closes. After this, the electricity exchanges form the price of electricity for each hour based on the purchase and sale offers made in the auction, as well as transmission capacities. The result of the auction is the same electricity price for all bidding areas if there are no bottlenecks in the transmission connections between the areas. If bottlenecks form, then prices differ between regions in proportion to the size of the bottlenecks. The electricity market's trading schedules are illustrated in more detail in Figure 2-10. (Fingrid, Johdanto sähkömarkkinoihin, 2023)

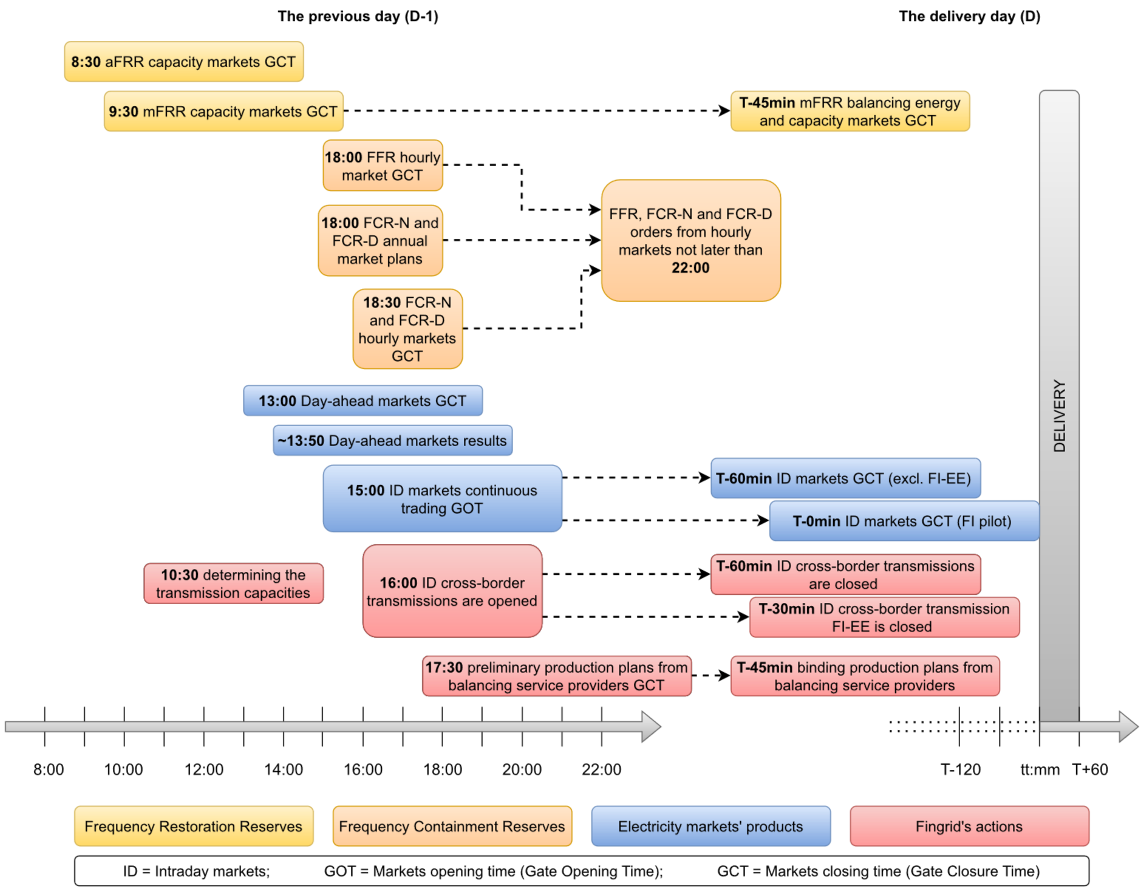

Figure 2-10: *Electricity market timeline. Based on source (Fingrid, Johdanto sähkömarkkinoihin, 2023).*

After the day-ahead market, the intraday market begins. In this market, the aim is to anticipate changes more accurately in consumption and production. Changes can occur, for example, in consumption decisions, weather conditions, and the operation of the production network. During the intraday market, all operators, therefore, have more information about their own production process situation, making it easier to outline and predict the required trades. Hence, these markets allow market participants to fine-tune their production and consumption plans closer to the moment of use. Intraday markets work on an hourly basis, but they can be traded continuously until the closing time. The closing times are currently zero minutes in internal Finnish trade, 30 minutes at the Estonian border, and 60 minutes at the Swedish border before the delivery hour. (Fingrid, Johdanto sähkömarkkinoihin, 2023)

The intraday market can be offered up to the gate closure time, but it no longer affects production or consumption changes that occur within the hour. During the delivery period, the balance between consumption and production is made using balancing energy and reserve markets. All Nordic TSO companies, including Fingrid, maintain both of these actions. TSO companies must constantly make sure that they have enough adjustable capacity to maintain electricity production and consumption balance. In this way, the companies can ensure the management of the national balance sheet responsibility. Ancillary service market parties' balancing service offers are only activated as needed, and the balancing offers can be submitted no later than 45 minutes before the delivery hour targeted by the offer. In addition to the balancing energy market, for example, Fingrid also maintains other reserve markets in Finland. These markets, in turn, consist of frequency containment reserves (FCR), automatic frequency restoration reserves (aFRR), and manual frequency restoration reserves (mFRR). Reserve markets' products and their requirements are presented in Table 2-1. (Fingrid, Fingrid, 2023)

Table 2-1: *Reserve market products and their requirements.*

	Remedial action	Frequency containment reserves			Frequency restoration reserves	
Reserve product	FFR	FCR-D upward	FCR-D downward	FCR-N	aFRR	mFRR
Full name	Fast Frequency Reserve	Upward Frequency Containment Reserve - Disturbance	Downward Frequency Containment Reserve - Disturbance	Frequency Containment Reserve - Normal	Automatic Frequency Restoration Reserve	Manual Frequency Restoration reserve
Regulation type	Upward	Upward	Downward	Symmetrical upward and downward	Upward and/or downward	Upward and/or downward
Maximum/Minimum bid size (MW)	10 / 1	10 / 1	10 / 1	5 / 0.1	50 / 1	50 / 1
Activation	Automatic activation for changes in frequency	Automatic linear activation within the frequency interval 49.50 - 49.90 Hz	Automatic linear activation within the frequency interval 50.10 - 50.50 Hz	Automatic linear activation within the frequency interval 49.90 - 50.10 Hz	Automatic activation for frequency deviations from 50.00 Hz	Manual activation when requested by Fingrid
Activation time	Three states for 100 %: -0.7 seconds at 49.50 Hz -1.0 seconds at 49.60 Hz -1.3 seconds at 49.70 Hz	50 % within 5 seconds and 100 % within 30 seconds	50 % within 5 seconds and 100 % within 30 seconds	100 % within 3 minutes	100 % within 5 minutes	100 % within 15 minutes
Endurance	30 seconds alternatively 5 seconds	At least 20 minutes	At least 20 minutes	1 hour (15 min in the future)	1 hour (15 min in the future)	1 hour (15 min in the future)

After the electricity delivery hours, an imbalance settlement is always made, where the difference between the offered and actual production and consumption of the balance responsible party operating in the electricity market is checked. Adjustment measures need to be made to the electricity system if the balance responsible party's plans do not match the actual amounts. In the imbalance settlement process, the market participants' balance deviation is clarified for each balance settlement period. As a result of the investigation, the costs of balancing can be distributed to those parties who are responsible for the need of balancing. Market participants with a balance deviation pay or receive money according to the magnitude, direction, and price of the balancing electricity shown in the imbalance statement. The price of balancing electricity acts as an incentive for all operators to always strive for balance in the market. (Fingrid, Balance services, 2023)

The electricity market and ancillary services presented above, which operate and are conducted through, for example, Nord Pool and Fingrid, are based on the general European electricity market standard, which is controlled and coordinated by ENTSO-E (European Network of Transmission System Operators for Electricity). ENTSO-E guides European companies to cooperate more seamlessly to implement the EU's energy policy and achieve energy and environmental goals. One of these main goals for ENTSO-E is, in addition to the European-wide functionality of markets and energy networks, to integrate renewable energy sources such as wind and solar power into the power system. Through these set goals, the organization aims to achieve the European Union's key energy policy ambitions of affordability, sustainability, and security of supply. ENTSO-E's long-term objective is to become the focal point for all transmission system operators and European grid-related technical, market, and policy issues linked directly to electricity system users, EU institutions, regulators, and national governments. (ENTSO-E, Market, 2023)

Even though the operation of the electricity market has been established according to the presented model, continuous development measures are also being taken. The aim of Fingrid is to get trading of the delivered electricity closer to the moment of delivery when forecasting the required production capacity is more accurate. For example, in intraday trading, three auction rounds will be implemented alongside the current continuous-time model. In this case, it is possible to create a value for cross-border transfer capacities in bottleneck situations. In 2023, the imbalance settlement period was reduced from one hour to fifteen minutes, after which the electricity exchange market trading and the day-ahead market will also be moved to a similar model. After the transition of the imbalance settlement period (22.5.2023), the intraday market can offer 15-minute products in the Finnish bidding area. The aim is to move the electricity exchange market and the day-ahead market to a 15-minute offer model in 2025. (Fingrid, Päivänsisäisten ja vuorokausimarkkinoiden kehityssuunta, 2023)

To guarantee the best possible functioning of the electricity market and electricity supply, Fingrid also has development projects regarding the flexibility of the electricity network. Fingrid's focus is on the flexible electricity market, where trading is done through the flexibility of the system's resources, which are part of the electrical system's management, for example, in terms of frequency, transfers, and voltage. Flexibility market projects are related to forecasting, visualization, information exchange, modelling, coordination, trading, and settlement of the need for flexibility, among other things. The functionalities produced by these projects are needed when transmission and distribution networks increasingly require market-based flexibility to support their electricity system and network infrastructure. (Fingrid, Flexibility market projects, 2023)

2.4 Green energy and a guarantee of origin

For the global economy to achieve the ever-tightening environmental goals set for it, all actors must understand and apply the restrictions created by the regulations in their operations. The energy conversion chain formed by green hydrogen and green energy carriers further refined from it, such as the methanol, methane, and ammonia studied in this work, has received a lot of interest and even government support (VM, 2023). However, the center of attention is the green and emission-free economy itself, which is why green energy production and its guarantee of origin are in an important position to achieve the right kind of economic profitability. (Rasoulinezhad & Taghizadeh-Hesary, 2022) This section introduces the definition and conditions of renewable energy production, its guarantee of origin, and the classification of green hydrogen that is essentially related to this topic.

2.4.1 Green energy

The starting point of the green economy is emission-free energy production, in which renewable energy sources play a significant role. As the name suggests, these energy sources are renewable and continuous natural processes. They can be divided into, for example, solar, wind, hydro, and geothermal power, as well as bioenergy (Peda.net, 2023). In general, renewable energy sources are feedstocks that are returned to the environment in a short time and do not decrease as a whole. However, the terms renewable and green energy sources are often used interchangeably, but not all renewable energy sources are collectively thought of as green. For instance, large hydropower plants can have significant effects on the environment, such as water life, fisheries, and land use. Therefore, green power is a subset of renewable energy sources representing sources and technologies that produce the greatest environmental benefits. A breakdown of energy sources is presented in Figure 2-11, where the sources are divided into conventional, renewable, and green power. (EPA, What Is Green Power?, 2023)

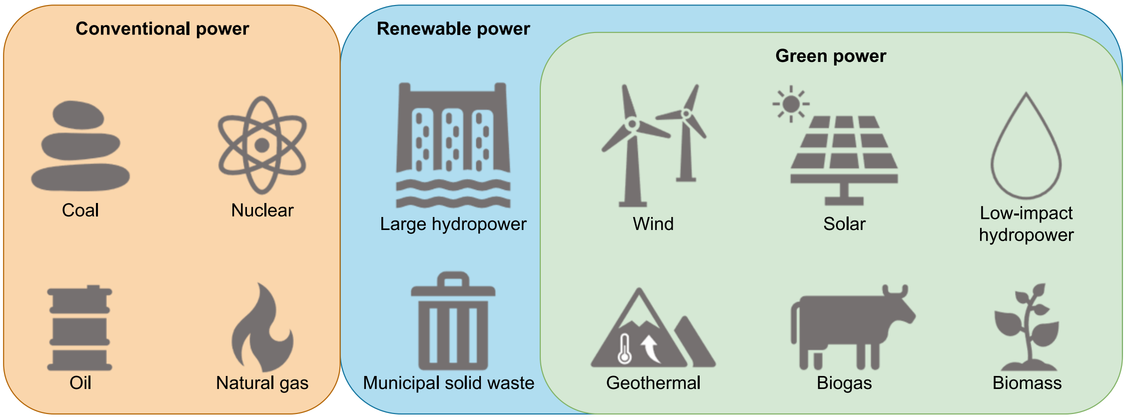

Figure 2-11: *Energy source classification. Based on source (EPA, What Is Green Power?, 2023).*

2.4.2 Power purchase agreement

In order for the energy-using industry and electricity consumers, in general, to be able to characterize themselves and their operations as green, the origin of the electricity used must be from renewable or green sources. Therefore, a power purchase agreement (PPA) is made for the electricity produced in the right way, with which it is possible to guarantee the origin of the electricity consumed. A PPA is often a long-term, for example, 10-20 years, electricity supply agreement between two parties, where the parties are simply the electricity producer and the electricity consumer or trader. Since PPA agreements are bilateral agreements, they are often diverse and usually customized to suit the situation and need. The terms of the contract are precisely defined in the PPA, such as negotiated prices, the amount of electricity to be delivered, accounting, and possible violation fees. Guaranteeing the origin of renewable or green electricity to the consumer is often mentioned when talking about PPA, but they are also useful for the electricity producer, as they reduce electricity-related price risks, especially for operators of plants with large investments and low operating costs (solar and wind power). (FWPA, 2019)

Due to the versatility of bilateral agreements, it can be difficult to define different types of power purchase agreements, but all agreements nevertheless share certain general features. PPAs can be divided into two main groups, which are physical and synthetic contracts. The first of these, i.e., physical contracts, can be further divided into three subsets, which are on-site, off-site, and sleeved PPAs. Common to all three is a fixed amount of electricity that is sold and supplied, and the only difference is the way the electricity is delivered. (NK, 2023)

In an on-site PPA, electricity is delivered directly, and the contract requires the physical proximity of production and consumption. This means that both production and consumption take place in the same area, for example, in the same facility. In this scenario, grid operators are involved only to the extent that residual electricity can be delivered to the grid. Another physical type of contract is the off-site model, where the supply of electricity is not as direct as it was in the case of the on-site model. In this contract, the delivery takes place via the electricity network, in which case the consumer is committed to using the amount of electricity determined by the PPA from the network. Since the model uses a public network, the transmission of electricity requires additional clarifications between the producer and the consumer related to the balance groups. However, this type of contract gives freedom and more flexibility for the location of both the producer and the consumer. The third subset of physical contracts, i.e., sleeved PPA, is simply an off-site PPA aimed at an energy service provider that acts as an electricity service intermediary from the producer to the consumer. The contract is concluded between the producer and the intermediary, which enables the provision of services such as management of balance groups, combining different electricity producers into a portfolio, delivery or sale of residual amounts of electricity, preparation of supply forecasts, marketing of green certificates and taking various risks (such as balancing energy costs). The term "sleeve" refers to the middleman's management fees and position between the producer and the final consumer, where the middleman takes care of matching the generator's production schedule to the consumer's schedule (so-called sleeving). (NK, 2023)

The second main group, i.e., synthetic PPAs, also known as virtual PPAs, separates the physical electricity flow from the financial flow. In this way, it is possible to create more flexibility in contractual arrangements. Similar to physical contracts, in the synthetic version, producers and consumers agree on the price of electricity, but it is not delivered directly to the consumer. Similar to the sleeved PPA, the produced electricity is transferred to the energy service provider, which in turn takes it as part of its balance group and trades with it. In this case, the consumer's energy supplier acquires exactly the input profile that the producer provides to the service provider on behalf of the consumer, i.e., the PPA partner. Therefore, procurement measures can be done, for example, on the spot market. The electricity supply profile acquired in the synthetic contract is supplemented by a so-called difference contract, with which the contract partners aim to compensate for the difference between the pre-agreed PPA price and the actual spot market price. Each contracting partner, therefore, has two payment streams, one with the corresponding energy service provider and the other with the PPA contract partner. However, the sum of these payment flows is the PPA price defined in the contract, in which case the procedure gives both parties the desired price guarantee. Without direct balance sheet connection and physical delivery between contracting parties, synthetic PPA is a simple and administratively advantageous method. Figure 2-12 shows how the PPA contract types are distributed between direct and indirect consumers. (NK, 2023)

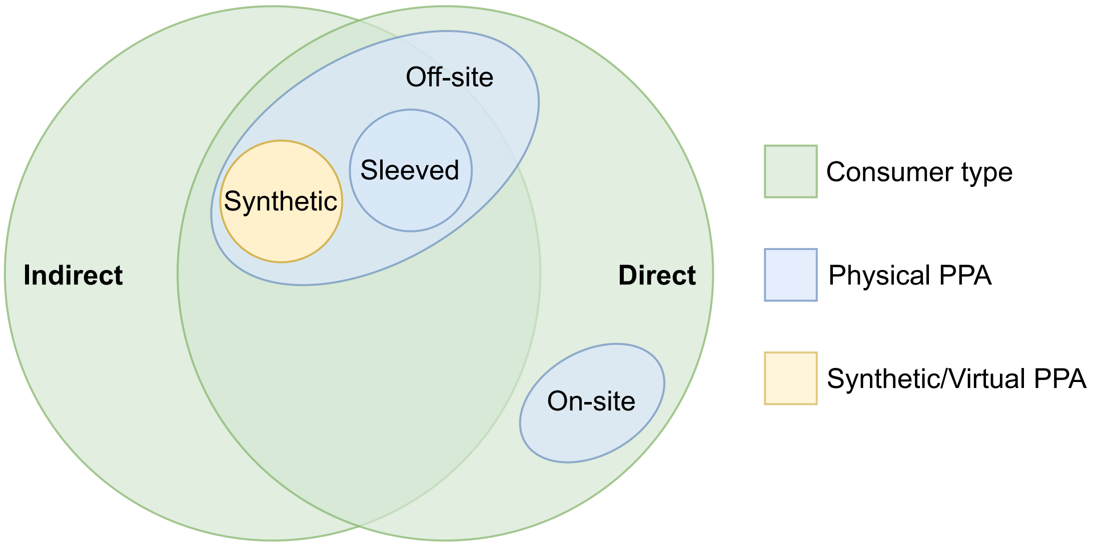

Figure 2-12: *Power purchase agreement types. Based on source (NK, 2023).*

2.4.3 Environmental classification of hydrogen production

PPAs, through which the availability of renewable and emission-free energy can be guaranteed, are an important part of the green economy and the associated green hydrogen. However, hydrogen can be produced in many ways, where the emissions and environmental load of the production process determine the quality of the hydrogen and, thus, the color code attached to it. Currently, there is a lot of talk about only green-produced hydrogen, but there are other low-emission or even zero-emission production methods for it too. There is still a little movement in the color coding of hydrogen, depending on the source. However, the coding seems to have settled on the six main colors in the most recent literature sources. The colors used are grey, blue, turquoise, purple, yellow, and green. (Ajanovic, Sayer, & Haas, 2022)

The gray color refers to production where hydrogen is produced from fossil fuels, such as natural gas, for example, using the steam reforming of natural gas (SMR) method. Similar to the production of gray hydrogen, blue hydrogen is also produced from fossil fuels, but CCUS technologies are added to it, which reduces the greenhouse gas (GHG) emissions of the process. Like the previous colors, fossil fuels are also used in the production of turquoise hydrogen, but the manufacturing process is pyrolysis, which has no carbon dioxide emissions at all, and the only by-product is solid carbon. Unlike the production methods presented so far, the manufacturing process of purple hydrogen is based on nuclear-powered electrolysis, which is also a very emission-free production option apart from nuclear waste. Yellow hydrogen, on the other hand, is produced simply by electrolysis, the power source of which is electricity obtained from the power grid, produced from various energy sources. Finally, green hydrogen, also called renewable hydrogen, is also produced by electrolysis but is powered by electricity from renewable energy sources. The six manufacturing styles of hydrogen and the color coding associated with them are further presented in Figure 2-13. (Ajanovic, Sayer, & Haas, 2022)

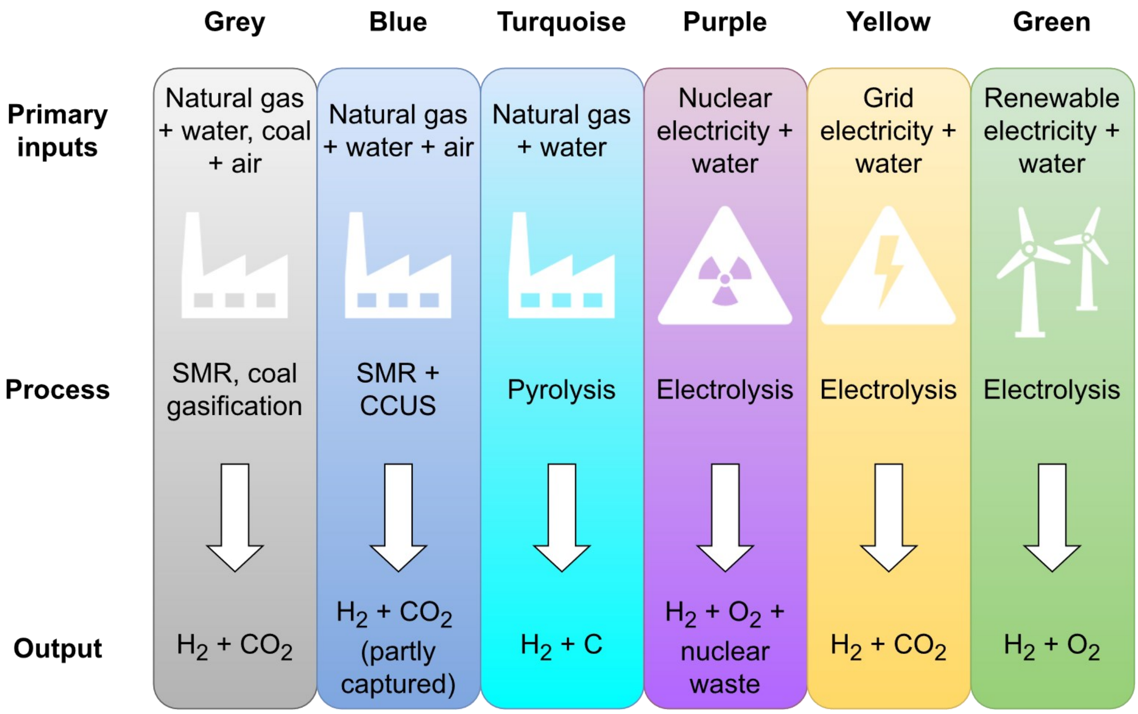

Figure 2-13: *Color coding of hydrogen. Based on source (Ajanovic, Sayer, & Haas, 2022).*

The Figure 2-13 illustrates well the distribution of hydrogen manufacturing methods according to its primary fuel input and end products. From an environmental point of view, the most popular methods are turquoise, purple, and green hydrogen production. Of these, the purple model is not preferred in European hydrogen strategies, but it is considered a possible alternative in other parts of the world, such as China and Russia. The turquoise hydrogen production model, on the other hand, has only gained interest in recent years, which is why pyrolysis has not yet been properly commercialized in terms of hydrogen production. However, pyrolysis is an emission-free form of hydrogen production, and the carbon produced as a by-product has its own market, which makes the production method attractive in terms of the cost structure. Despite the alternatives, the production of green hydrogen is an object of particular interest in the transition towards a more sustainable energy and transport system, as its production process and end products form a clean, clear, and simple energy transformation entity. (Ajanovic, Sayer, & Haas, 2022)

3. THE POWER-TO-HYDROGEN SYSTEM AND FURTHER PROCESSES

As weather-dependent energy increases, society's general need for electricity network flexibility also increases. Flexibility can be provided with P2X conversion and storage solutions, but the need for flexibility is not the only thing that draws companies to energy conversion chains. In addition to the possible network balancing tasks, P2X solutions can produce products made with green energy for the market, such as the hydrogen, methanol, methane, and ammonia studied in this thesis. Each of the presented energy carriers has its market incentives, and demand for them exists in, for example, different areas of industry, as shown in the previous chapter (IEA, The Future of Hydrogen, 2019).

This chapter presents the P2H2 version of the P2X model, where the surplus or low-cost renewable energy is converted into hydrogen using electrolysis technology. The chapter begins with an introduction to the studied hydrogen system, where the energy conversion process is studied as a whole. After this, attention is focused on the sub-processes of the system. The first to be introduced are typical electrolysis methods and their properties. Finally, the production of further processed products (methanol, methane, and ammonia) and their characteristics will be examined.

3.1 The examined energy conversion system

The investigated energy conversion chain consists of four sub-areas. These are energy production, conversion of energy into hydrogen, possible further processing of hydrogen, and sale of the end products, i.e., the hydrogen, methanol, methane, and ammonia studied in this work, to the market. In the system, the energy to be included in the chain must be produced from renewable sources, so when the energy is combined with the production of hydrogen by electrolysis, it can be called a P2H2 measure (Genovese, Schlüter, Scionti, Corigliano, & Fragiacomo, 2023). The electric power needed for electrolysis can be transferred either directly from renewable sources or from the power grid, enabled by the contract formed with the PPA partner (Ajanovic, Sayer, & Haas, 2022). In the P2H2 process, gaseous hydrogen is produced using water electrolysis, after which it is directed to consumption or further processing, sold to the customer, or stored for later demand, either in gaseous or liquid form. Water electrolysis techniques include, e.g. anion exchange membrane (AEM), alkaline water electrolysis (AWE), polymer electrolyte membrane (PEM), and solid oxide electrolyzer (SOE). (Park, 2021) If the hydrogen is directed for further processing, it can be used, for example, to produce the green methanol, methane, and ammonia mentioned above. Manufacturing processes of further refined products include, e.g., methanol synthesis, methane synthesis, and ammonia synthesis. The final products, including hydrogen, can still be stored at this stage before the final destination, which makes it possible to create buffers in case of fluctuations in demand or production. The described energy conversion chain from energy production to end users is shown in Figure 3-1. (Dias, Pochet, Contino, & Jeanmart, 2020)

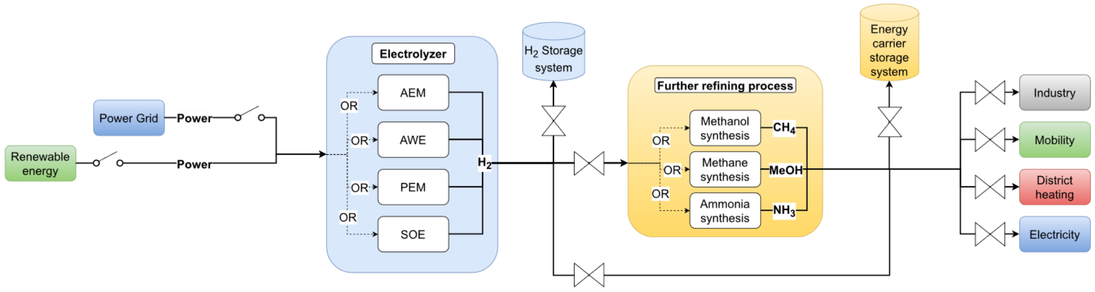

Figure 3-1: *Hydrogen-based energy conversion flowchart.*

The considered energy conversion chain can also be referred to by the terms power-to-gas, power-to-liquid, and power-to-heat, depending on which part of the chain is examined and which final products are focused on. When the object of examination is only hydrogen and methane gases, only the production and consumption of these gases are monitored. In this case, the technology can be referred to with the term P2G (Götz, et al., 2015). When, on the other hand, liquid fuels, such as liquid hydrogen and methanol, and their production are under review, the technology can then be referred to as P2L (Blanco, Nijs, Ruf, & Faaij, 2018). If the focus of attention is, for example, thermal energy generated as a by-product in the energy conversion process or intentionally produced, the term P2H can be used for the technology (Nastasi, Lo Basso, Garcia, Gumo, & de Santoli, 2018). In this work, however, the center of attention is hydrogen and the processes and markets revolving around it, so it is natural to generally refer to the technology with the term P2H2.

In addition to selling hydrogen in direct or further refined forms, it can be converted back into electrical energy. Hydrogen conversion into electricity occurs in a fuel cell, where the opposite reaction to electrolysis takes place. In the process, hydrogen reacts with oxygen through an electrochemical cell, producing electricity, water, and a small amount of heat. This technology enables the temporary storage of energy in hydrogen, which can be used, if necessary, for network balancing tasks in both electricity surplus and deficit situations. The conversion of electricity into hydrogen and then back into electricity is currently not the most attractive market niche, as the round-trip efficiency of this conversion chain is only around 30% at best. The biggest development target in this power-to-power process is the production of hydrogen and its conversion back into electricity. Improvements in these system areas can, however, lift the round-trip efficiency to 40% in the next decade. Connecting a power-to-power hydrogen system as part of the electrical grid is presented in Figure 3-2, which is a modified version of Figure 2-8. (Escamilla, Sánchez, & García-Rodríguez, 2022)

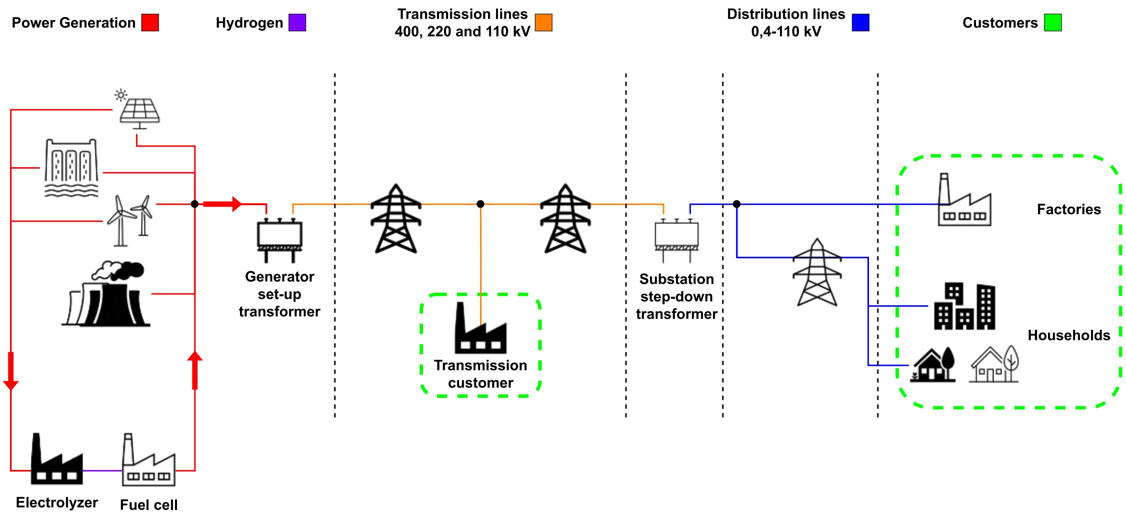

Figure 3-2: *Integration of power-to-power hydrogen system to the electricity network.*

The Figure 3-2 only illustrates the direct transfer of electricity from renewable energy sources to the electrolysis plant. However, electricity can also be transferred from the grid to the production of hydrogen, for example, with the help of the previously presented PPAs. In addition, the picture mainly focuses on the transmission of electrical energy, but the thermal energy generated in the power-to-power conversion chain can also be used in other processes or district heating, which can increase the profitability of the energy conversion solution in question (Olabi, Wilberforce, Sayed, Elsaid, & Abdelkareem, 2020).

3.2 Hydrogen production methods

Today, there are many different production methods for hydrogen, which are in different stages of development, and their economic and environmental costs differ significantly. Currently, hydrogen production is mainly based on fossil fuels, where production methods include, for example, natural gas steam reforming (SMR), partial oxidation of heavy hydrocarbons, and coal gasification. In addition to these, hydrogen can also be produced by biomass gasification, carbon dioxide-free methane pyrolysis, and water electrolysis. The last two methods use electric current as their power source, which can be produced by solar or wind power, enabling the creation of an emission-free energy transformation chain. Hydrogen production methods and their categorization are presented in Figure 3-3. (David, Ocampo-Martínez, & Sánchez-Peña, 2019)

The commercial production of hydrogen is mainly divided into four sources, which are natural gas, oil, coal, and water, which account for 48%, 30%, 18%, and 4% of global hydrogen production (Uddin, Nageshkar, & Asmatulu, 2020). About 96% of hydrogen production is, therefore, still based on fossil fuels, even though their environmental effects are generally unfavourable. In addition to environmental effects, efficiency and costs are also parameters used to compare different production methods. Along with the cost efficiency of fossil fuels, developing CCUS technologies supports conventional power sources. For example, carbon dioxide can be separated from natural gas with up to 95% efficiency (MTR, 2023). Even if CCUS technologies make it possible to produce hydrogen from fossil fuels almost or completely emission-free, the fuel in question is a diminishing natural resource. In addition, currently, hydrogen production based on renewable fuels is already emission-free, which continuously increases the demand and competitiveness of the technology. This work focuses on the production of hydrogen from renewable energy sources, i.e., electrolysis methods. (David, Ocampo-Martínez, & Sánchez-Peña, 2019)

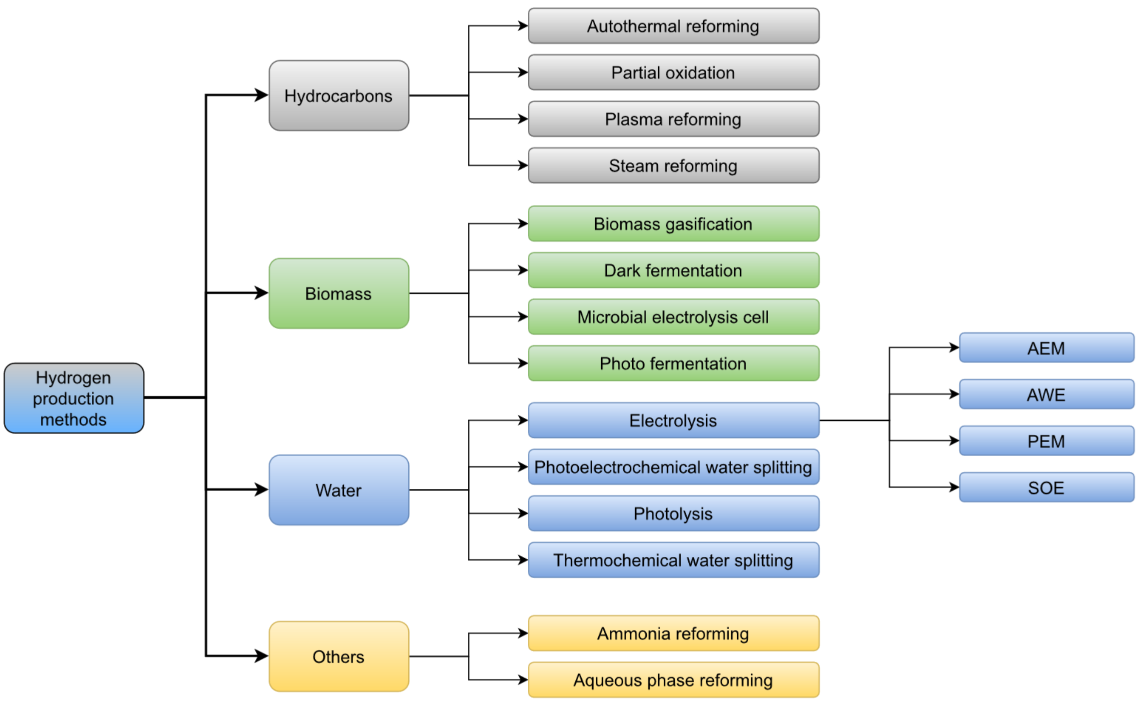

Figure 3-3: *Hydrogen production methods. Based on source (David, Ocampo-Martínez, & Sánchez-Peña, 2019).*

Carbon-free hydrogen production is best achieved by using electricity from renewable energy sources for water electrolysis, which is a process where water is split into hydrogen and oxygen. The reaction in question takes place in an electrolyzer, whose basic principle is built around the anode, the cathode, and the electrolyte that separates them from each other, similar to in fuel cells. There are many types of electrolyzers, which work in different ways due to the electrolyte materials used in them and the ions they conduct. Next, the four most used, potential, and researched electrolysis solutions are presented, which are alkaline water electrolyzer (AWE), anion exchange membrane (AEM), polymer electrolyte membrane (PEM), and solid oxide electrolyzer (SOE). Simplified versions of the cells of the presented electrolyzers are shown in Figure 3-4 (Miller, et al., 2020) (Ozturk & Dincer, 2021). (David, Ocampo-Martínez, & Sánchez-Peña, 2019)

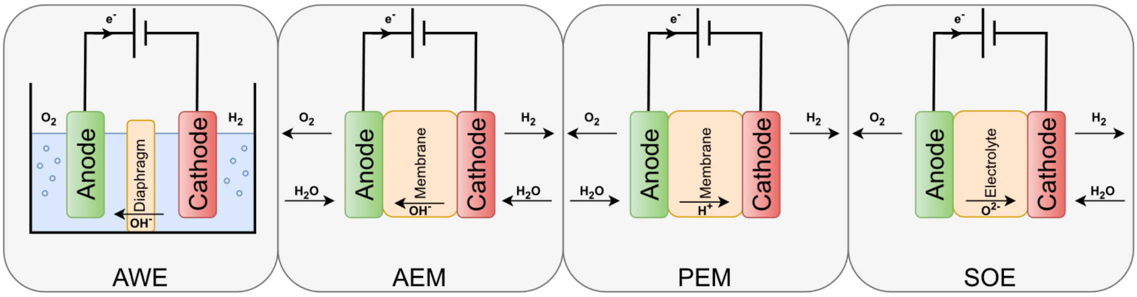

Figure 3-4: *Simplified cell structures of presented electrolyzers.*

3.2.1 Alkaline water electrolyzer

Alkaline water electrolysis (AWE) is the eldest, most mature, and commercially widespread hydrogen production method, and it’s still being researched and developed. Devices with this technology contain water and a liquid electrolyte solution such as potassium hydroxide or sodium hydroxide. When current is applied to the alkaline cell stack, the hydroxide ions move through the electrolyte solutions from the cathode to the anode of each cell. In this case, hydrogen gas is formed at the cathode, while oxygen gas is produced at the anode. The course of the reaction is shown in formulas (3.1), (3.2), and (3.3), which show the equations for the cathode, anode, and the whole process. (Brauns & Turek, 2020)

$$2H_2O + 2e^- \rightarrow H_2 + 2OH^- \tag{3.1}$$

$$2OH^- \rightarrow 0.5O_2 + H_2O + 2e^- \tag{3.2}$$

$$H_2O \rightarrow H_2 + 0.5O_2 \tag{3.3}$$

AWE electrolyzers are generally thought to have problems such as low current density and the inability to work with intermittent and fluctuating energy sources. However, these features are only part of the already outdated atmospheric electrolyzer technology, which was originally applied for continuous use. Modern and continuously developing pressurized AWEs can, on the other hand, achieve competitive performance and flexibility figures. With this newer technology, it is also possible to avoid the material availability problems that occurred with the older model. In general, however, AWE technology is not completely problem-free, as its operating temperature is limited by the structural stability of the diaphragm, which is why it is considered a low-temperature electrolysis technology. Therefore, the goal for the technology at the moment is to make it work at higher temperatures and improve the stability and conductivity of the diaphragm separators, which increases the cost-effectiveness of hydrogen production. (Ehlers, Feidenhans'l, Therkildsen, & Larrazábal, 2023) The main properties of the AWE electrolyzer are further presented in Table 3-1, where the corresponding values of all the techniques introduced in this work are compiled. The table is based on literature sources (El-Emam & Özcan, 2019), (Miller, et al., 2020), (Ozturk & Dincer, 2021), (Santoro, et al., 2022) and (Lopez, Ziar, Haverkort, Zeman, & Isabella, 2023) and presents the existing performance of each technology and lists some of their advantages and disadvantages.

3.2.2 Anion exchange membrane electrolyzer

Similar to the AWE electrolyzer, the anion exchange membrane (AEM) electrolyzer is a water-splitting technology, and it uses a semi-permeable membrane. The membrane conducts hydroxide ions, which is why the technology got its name from its anion exchange method. Compared to traditional alkaline electrolysis, which is not the previously presented pressurized version under development, the AEM electrolyzer combines its good features with the technology of the later presented PEM electrolyzer. (Li & Baek, 2021) In this way, the AEM method can make up for the shortcomings of AWE, whereby the electrolyzer works, e.g., in a dilute alkaline environment and with cost-effective materials. Furthermore, with the help of AEM, it is possible to produce cleaner hydrogen than with AWE in a safer and more scalable way. Despite its good properties, AEM technology is still in the development phase and needs more research to improve power efficiency, membrane stability, ion conductivity, stack costs, and catalyst integration. The reaction in AEM is presented in equations (3.4) and (3.5), which contain the reaction formulas for the cathode and anode. (Gul, Baldinelli, Farooqui, Bartocci, & Shamim, 2023)

$$4H_2O + 4e^- \rightarrow 2H_2 + 4OH^- \quad (3.4)$$

$$4OH^- \rightarrow O_2 + 2H_2O + 4e^- \quad (3.5)$$

Despite its novelty, AEM could play a decisive role in green hydrogen production. The technology is the youngest of the potential water electrolysis methods, and due to its continuous research and development, it is prone to major improvements in the near future. In order for the AEM method to be competitive with other technologies, it should work with a current density of more than 2 $\frac{A}{cm^2}$ and an operating voltage of less than 2 V. In addition, if it is possible to implement a higher operating temperature (80 °C) in the technology, it would improve the electrocatalytic activity, voltage efficiency, and electrical efficiency, which would significantly promote the profitability of the method. Similar to the other presented electrolysis technologies, the characteristics of the AEM method are summarized in Table 3-1. (Santoro, et al., 2022)

3.2.3 Polymer electrolyte membrane electrolyzer

As with AEM technology, polymer electrolyte membrane (PEM) was developed to solve the shortcomings of traditional AWE technology. In this way, it was possible to solve problems related to partial load, low current density, and low pressure. In the PEM method, water electrolysis takes place in a cell equipped with a solid polymer electrolyte (SPE). Comparable to other electrolyte techniques, SPE is responsible for the conduction of protons, the separation of product gases, and the electrical insulation of the electrodes. Unlike in AEM, in the cell of PEM, the exchange membrane transfers protons instead of anions. Alongside other electrolysis technologies, PEM is a highly potential electrolysis method due to its fast dynamic response times, large operating ranges, and high efficiency. In addition to these, the durability and environmental effects of its equipment guarantee very clean and efficient hydrogen production. Thus, PEM is already easily applicable as a median of energy conversion and storage technologies and can adapt to variable energy production from renewable energy sources. The reactions taking place in a PEM electrolyzer are presented in equations (3.6) and (3.7), which show the reaction formulas for the cathode and anode (Ozturk & Dincer, 2021). (Crespi, Guandalini, Mastropasqua, Campanari, & Brouwer, 2023)

$$2H^+ + 2e^- \rightarrow H_2 \tag{3.6}$$

$$2H_2O \rightarrow O_2 + 2H^+ + 2e^- \tag{3.7}$$

Although PEM electrolysis technology has a large number of positive features and is quite easily compatible with green hydrogen production, it is not a problem-free option either. One of the most significant challenges of the technology is the acidity of the system, which is why scarce, and expensive noble metals are added to electrocatalysts and coating layers. These materials alone add significantly to the capital cost of PEM devices. Currently, there are a few possible ways to solve the problem and limitations of PEM systems. These include, e.g., the greatest possible recycling rate of materials, the development of electrode surface coating technology, increasing production efficiency to achieve better cost efficiency, and the development of alternative materials. The development of more affordable alternatives to noble metals is an important and ongoing research target to guarantee the future success of PEM technology. The main features of the technology are again collected in Table 3-1. (Salehmin, Husaini, Goh, & Sulong, 2022)

3.2.4 Solid oxide electrolyzer

The last electrolysis method to be presented is the solid oxide electrolyzer (SOE), where a solid oxide or ceramic electrolyte is used in the water electrolysis process. The technology is currently an attractive hydrogen production model, as it produces very pure hydrogen, like PEM and AEM electrolyzers. In addition, SOE has high conversion efficiency and relatively low energy consumption, which makes it a cost-effective solution. In order for the solid oxide films contained in SOE to function properly, they must be operated at high temperatures, which are typically 500-1000 °C. According to the thermodynamical system properties, the need for electrical energy to electrolyze water in SOE generally decreases as the temperature rises (Wang, et al., 2021). Due to this, SOE electrolyzers are able to efficiently use the energy carried by the operating temperature, as a result of which the amount of electrical energy needed to produce hydrogen is lower than in comparable technologies. Similar to previous techniques, equations (3.8) and (3.9) show the reactions at the cathode and anode (Ozturk & Dincer, 2021). (Subotic & Hochenauer, 2022)

$$2H_2O + 2e^- \rightarrow H_2 + O^{2-} \tag{3.8}$$

$$O^{2-} \rightarrow 0.5O_2 + 2e^- \tag{3.9}$$

As with the previously presented electrolysis technologies, SOE also has major development targets. While high operating temperatures help achieve good voltage efficiency and low energy consumption, they cause longer start-up times, increased degradation rates, and mechanical and chemical compatibility problems. Other challenges are also caused by the effect of impurities, the service life of the electrodes, and the trade-offs related to the pressurization of the technology. Currently, research into the technology is mainly focused on stabilizing existing component materials, developing new and alternative materials, and lowering the operating temperature even below 500 °C. (Roy & Ethakota, 2022) The current main characteristics of SOE technology are collected in Table 3-1 in a similar way to AWE, AEM, and PEM methods.

Table 3-1: *Main characteristics of four electrolyzer technologies.*

Specifications	AWE	AEM	PEM	SOE
Cathodic Reaction	$H_2O + 2e^- \rightarrow H_2 + 2OH^-$	$4H_2O + 4e^- \rightarrow 2H_2 + 4OH^-$	$2H^+ + 2e^- \rightarrow H_2$	$H_2O + 2e^- \rightarrow H_2 + O^{2-}$
Anodic Reaction	$2OH^- \rightarrow H_2O + 0.5O_2 + 2e^-$	$4OH^- \rightarrow 2H_2O + O_2 + 4e^-$	$H_2O \rightarrow 2H^+ + 0.5O_2 + 2e^-$	$O^{2-} \rightarrow 0.5O_2 + 2e^-$
Electrolyte	NaOH/KOH (Liquid)	Anion exchange ionomer (e.g. AS-4)	Polymer (Solid)	Ceramic (Solid)
Operating Temperature(°C)	60-90	50-60	50-90	500-1000
Operating Pressure (bar)	2-10	1-30	15-60	<30
Charge Carrier	OH^-	OH^-	H^+	O_2^-
Cathode	Ni, Ni-Mo alloys	Ni, Ni alloys	Pt, Pt-Pd	Ni-YSZ
Anode	Ni, Ni-Co alloys	Ni, Fe, Co oxides	IrO_2, RuO_2	LSM-YSZ
Cell Voltage (V)	1.8-2.4	1.8-2.2	1.8-2.2	0.7-1.5
Current Density (A/cm^2)	0.2-0.4	0.2-1	0.6-2	0.3-1
Voltage Efficiency (%)	62-82	75-83	67-82	81-86
Hydrogen production rate (Nm^3/h)	<760	<1	<40	<40
Technology Status	Mature	R&D	Commercial	Demostration/Pilots
Hydrogen Purity	>99.8	>99.9	99.9	99.9
Lifetime of Stack (h)	<90000	<5000	<20000	<40000
Lifetime of System (year)	20-30	-	10-20	-
System Energy Consumption (kWh/Nm^3)	4.5-7	4.8-5.2	4.5-7.5	>3.7
Ramp up rate/ramp down rate (%/s)	0.3/0.3	0.47/10	10-50/40	-
Time from minimum to maximum load /maximum to minimum load (s)	333/333	213/10	10-2/3	-
Cold startup	>15min	-	<10min	>60min
Advantages	+Low capital cost +High stability +Mature technology +Long lifetime +No precious catalyst	+No caustic electrolyte +No Costly components +Fast ramp time +Compactness +High purity hydrogen	+High current density +Compactness +Rapid system response +Dynamic operating +High performance	+Low energy need +Low capital cost +High efficiency +Non-noble materials +Reversible operation as fuel cell
Disadvatages	-Corrosivity of electrolyte -Low current density -Dynamic slowness -Gas permeation	-Membrane degradation -Excessive catalyst loading -Durability -Maturity	-High cost of components -Noble metal catalyst -Durability -Acidic medium	-Sealing issues -Brittle ceramics -Unstable electrodes -Delamination of electrodes

3.3 Production of the further refined energy carriers

In the power-to-hydrogen energy conversion chain, the main focus is on the energy conversion process and storage of hydrogen. However, the chain can be extended by connecting to it further hydrogen refining processes, which in this work produce methanol, methane, and ammonia. In this way, the energy transformation chain becomes more comprehensive, more diverse, and more flexible in terms of markets. In addition, surplus energy can be used in a more efficient way because hydrogen, for example, is not yet suitable for traffic use as well as methanol, which allows the recovered energy to be channelled more easily for that purpose. (Dias, Pochet, Contino, & Jeanmart, 2020) This section examines the further refining processes of the conversion chain from hydrogen to methanol, methane, and ammonia, for which the technologies presented are methanol synthesis, methane synthesis, and ammonia synthesis. For each technology, the flow of the process, its conditions, current challenges, and development targets are reviewed.

3.3.1 Methanol synthesis

The first hydrogen further processing option to be examined is methanol synthesis. When the synthesis process is carried out as an extension of green hydrogen production, it can be referred to as green methanol or E-methanol production. In this case, carbon dioxide or carbon monoxide is made to react with green hydrogen to form methanol, which removes the expensive synthesis gas production part of the usual methanol production route (from fossil fuels). There are many types of reactors used for the synthesis process, such as adiabatic, continuous stirred-tank (CSTR), fluidized bed, and gas- and water-cooled fixed-bed reactors. Of these, adiabatic and gas-cooled reactors have fairly low to medium fixed costs, but the conversion and operating temperatures of CSTR reactors, for example, are lower. Fluidized bed reactors, on the other hand, are more efficient than fixed bed reactors in terms of methanol production rate. Consequently, each type of reactor has its own strengths, in which case the methanol production needs and conditions determine which reactor technology is applied. (Rafiee, 2020)

The hydrogen stream of the hydrogenation process of carbon dioxide and carbon monoxide in methanol synthesis can be produced by the electrolysis methods presented in the previous section, where the end products are hydrogen and oxygen gas. In order to maximize the positive environmental effects of the energy conversion chain, the carbon dioxide needed for the synthesis process can be produced with the CCUS technologies presented in Chapter 2. Thus, the obtained starting materials for the synthesis process generally work in the pressure range of 50-100 bar and in the temperature range of 200-300 °C. In the production of green methanol, the hydrogenation process requires catalysts whose main components are Cu and Zn, and their additives can include, e.g., Al, Zr, Cr, Si, B, and Ga. At the reaction level, methane can be produced from hydrogen and carbon dioxide in two ways, which are direct hydrogenation of carbon dioxide or reverse water-gas-shift (RWGS) followed by hydrogenation of carbon monoxide. The course of the reactions is shown in equations (3.10), (3.11), and (3.12), the first of which describes the direct reaction pathway and the latter two the indirect one. (Sollai, Porcu, Tola, Ferrara, & Pettinau, 2023)

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \tag{3.10}$$

$$CO + H_2O \leftrightarrow H_2 + CO_2 \tag{3.11}$$

$$CO + 2H_2 \leftrightarrow CH_3OH \tag{3.12}$$

After the hydrogenation of carbon dioxide or monoxide, the outlet flow is then condensed into a liquid product for methanol purification that takes place in the distillation column. The unreacted gas (mainly hydrogen and carbon monoxide) and the water produced as an end product are recycled back into the process to improve the conversion efficiency. Finally, methanol is stored in the liquid phase and sold to the demand destinations presented in Chapter 2. (Sollai, Porcu, Tola, Ferrara, & Pettinau, 2023) The most significant challenges in the production of green methanol so far are the availability of P2X technology and the scaling of low-emission electricity, which will be solved as the number of P2X technologies and renewable forms of energy production increases. (Mayer, 2022) The production of green methanol (and methane) is further illustrated in Figure 3-5.

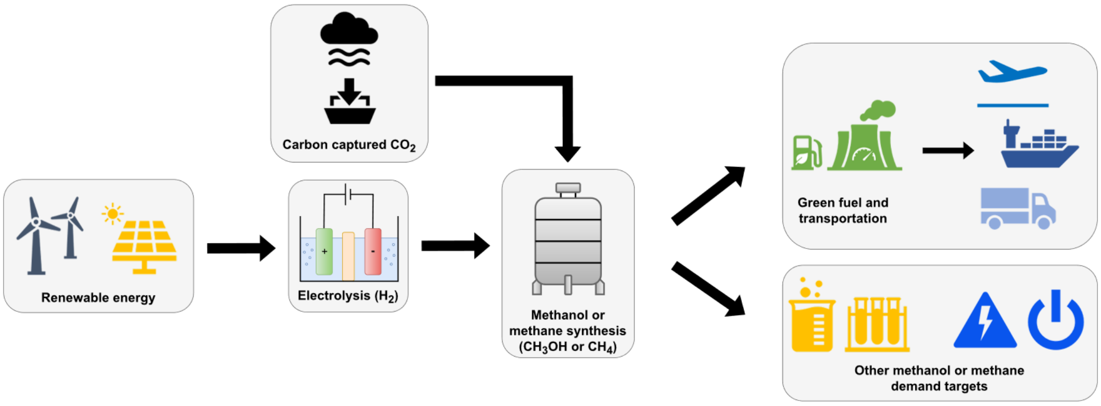

Figure 3-5: *Green methanol and methane production.*

3.3.2 Methane synthesis

The second examined processing target of hydrogen is the production of methane through methane synthesis, otherwise known as the Sabatier process. In the Sabatier process or reaction, methane is produced through hydrogen and carbon dioxide, i.e., similar to methanol synthesis. However, the reaction differs in terms of production conditions, used catalysts, and reaction products. The process conditions largely depend on the used catalysts and the reactor structure, but typically, the reactions are operated in the temperature range of 200–550 °C and between 1 and 100 bar. The catalysts, on the other hand, are based on Ni, Ru, Rh, and Co active phases, of which Ni is the most popular in terms of catalyst activity, selectivity, and costs. The course of the Sabatier reaction is described in equations (3.13), (3.14), and (3.15), the first two of which describe the two sub-steps of the reaction, while the last formula describes the entire process. (Tripodi, Conte, & Rossetti, 2020)

$$CO_2 + H_2 \leftrightarrow CO + H_2O \tag{3.13}$$

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O \tag{3.14}$$

$$CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O \tag{3.15}$$

Similar to methanol synthesis, many types of reactors can also be applied to methane synthesis. The simplest and most economical solution is an adiabatic reactor, which contains a certain number of adiabatic layers suitable for the situation. In order to achieve efficient operation of the reactor, it includes, in addition to adiabatic layers, an intermediate cooling mechanism. Other reactor options are, e.g., fluidized bed and fixed bed reactors, the first of which allows better temperature control but is more sensitive to an incomplete conversion process. In addition, fluidized bed reactors are generally challenging in terms of scalability. If the reaction speed of the process is to be maximized despite the costs, then fixed-bed reactors are the best option. (Tripodi, Conte, & Rossetti, 2020)

As in all the technological solutions presented in this work, the Sabatier process still has problems and areas for development despite its long existence. The most important subjects of process development and research are the stability of carbon dioxide and the deactivation of catalysts. Carbon dioxide is a linear and very stable molecule whose reduction to methane produces clear kinetic limitations and thus requires a relatively high energy input, catalysts with high stability and activity, and optimized reaction conditions. The deactivation of the catalysts, on the other hand, causes problems with the purity and speed of the reaction. Deactivation can be divided into two types: chemical and physical deactivation. In both cases, through the research and development of the reaction conditions, the impurities involved, and the materials used in it, it is possible to improve the costs generated in the life cycle of the process as well as the overall efficiency of the reaction. Green methane production can be illustrated alongside methanol production in Figure 3-5, as the process concepts are very similar. (Younas, et al., 2016)

3.3.3 Ammonia synthesis

The last hydrogen further processing method examined is ammonia synthesis. As in the previously presented processes, extending the green energy transformation chain from hydrogen to ammonia has also attracted a lot of interest. Ammonia has traditionally been produced using the Haber-Bosch method from fossil fuels, but the sustainable production of hydrogen through electrolysis makes it possible to update the Haber-Bosch technology to the production of green ammonia. The thermochemical Haber-Bosch process is by nature an energy-intensive process and is typically operated in a temperature range of 400-500 °C and a pressure range of 150-300 bar. However, alternative production methods have recently been developed for traditional hydrogen production technology, such as electrochemical ammonia production, nonthermal plasma (NTPL) technology, and nitrogenase-motivated peptide-functionalized electrochemical ammonia production. These ammonia production methods are divided into both low (100-400 °C) and high (400-750 °C) temperature ranges, where atmospheric pressure is sufficient for the process, depending on the catalyst. Among these alternative technologies, NTPL has received the most attention, as it allows operation at an operating temperature of 50 °C. (El-Shafie & Kambara, 2023)

For the synthesis of ammonia, similar to the previously presented synthesis processes, many types of reactors can be used, such as more traditional internal direct cooling and adiabatic direct cooling reactors (Khademi & Sabbaghi, 2017) as well as the newer type of double chamber, dialect barrier discharge plasma, and catalyst bed reactors (El-Shafie & Kambara, 2023). In turn, the catalysts used to guarantee the best performance of the reactors are generally Fe-, Ru-, Ni-, and Co-based materials, of which the best production rates are achieved with Ru-based catalysts. All the green ammonia production methods presented, despite their different intermediate stages and technologies, are based on the ammonia reaction scheme presented in equation (3.16). (El-Shafie & Kambara, 2023)

$$N_2 + 3H_2 \leftrightarrow 2NH_3 \tag{3.16}$$

Unlike previous methanol and methane production processes and the CCUS technologies applied to them, nitrogen molecules are needed in ammonia production instead of carbon dioxide. However, the nitrogen needed for ammonia production processes can be easily manufactured in two ways, which are pressure swing adsorption (PSA) and the cryogenic distillation process. The first of these is best suited for small-scale applications, while the latter works well in large-scale manufacturing situations. The entire production chain of green ammonia is illustrated in Figure 3-6. (El-Shafie & Kambara, 2023)

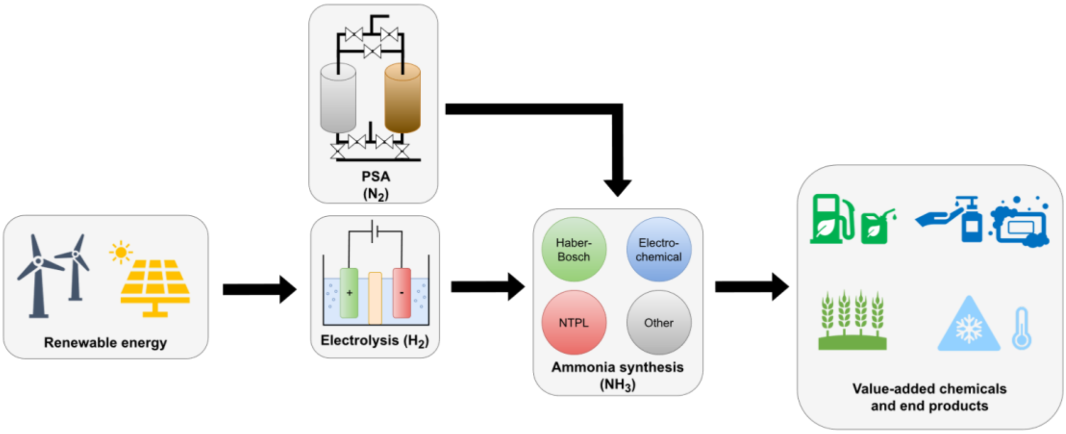

Figure 3-6: *Green ammonia production.*

Similar to the production methods of hydrogen and its further processing targets presented so far, development points can also be found in ammonia synthesis. Traditional problem areas have been, first of all, fossil fuels, which are slowly being phased out. But in addition to fossil fuels, high capital costs, production efficiency, optimization of the operating temperature and pressure of the process, achieving the right catalytic selectivity degree, and the scalability of the technology require attention. However, answers to these challenges are constantly being looked for, and the most potential results for the future can be found in the presented alternative ammonia production technologies. (El-Shafie & Kambara, 2023)

4. OPTIMIZATION WITH MIXED-INTEGER LINEAR PROGRAMMING

The number of previously presented energy conversion plants and companies has clearly grown in recent years, and more are constantly being planned. The most efficient, economically profitable, and competitive conversion technologies and facilities are continually being developed in order to achieve the best possible advantage and success. (IEA, Electrolysers, 2022) The stated goals are achieved with traditional competitive strategies, such as low costs for the company, differentiation of production or products, and increased customers' perceived value. When looking at energy conversion technologies and plants, a significant part of the costs is made up of resource management. With the right kind of resource management and optimization, even notable financial benefits can be achieved, which can directly influence both the competitive advantage and the company's own growth and development. (Liu & Liting, 2015)

In this thesis, the use of the components belonging to the P2H2 energy conversion process is optimized with the intended application, which was created with the optimization method suitable for the purpose. This chapter introduces optimization concepts related to the topic, starting with a general overview of optimization and modelling. After the overview, a theory applied to the subject called mixed-integer linear programming will be examined in a targeted manner. Finally, two studies on improving profitability are introduced, both of which utilize the presented mixed-integer linear programming method.

4.1 Optimization and modelling

Optimization tasks are based on a layout of problems, where the aim is to minimize or maximize a mathematical function of several variables with certain restrictions. The term optimization is generally used instead of minimization and maximization to describe the best possible achievable state formed by constraints and goals. A mathematical function intended for optimization, known as an objective function, is always formed from the investigated problem. The constructed objective functions can be very complex in structure and often have several variables. However, optimization tasks can also consist of a function of only a single variable, or, on the other hand, an entity formed by many objective functions. Depending on the nature of the optimization task, the variables of the generated model can be real numbers, integers, or even a combination of both. In addition to this, the optimization problem can be either constrained or unconstrained. In mathematical modelling, the constraint functions that may be formed next to the objective functions are always constructed according to three equation operators, which guide the optimization task in the desired or mandatory direction together with the objective function. These operators are equal to (=), less than or equal to (≤), or greater than or equal to (≥). (Sarker & Newton, 2007)

4.1.1 Mathematical model

A mathematical model, which can also be called a mathematical programming model, is generally built around the following basic framework:

$$\begin{aligned} & \mathit{Maximize\ or\ minimize}\ f(\bar{x}) \\ \mathit{Subject\ to}\quad & g_i(\bar{x}) \leq gb_i, \quad i = 1, \ldots, m \\ & h_j(\bar{x}) = hb_j, \quad j = 1, \ldots, p \\ & \bar{x} \geq 0 \end{aligned} \tag{4.1}$$

where the maximum or minimum value for the objective function $f(\bar{x})$ is searched in a manner controlled by the constraint functions g_i and h_j. The objective function can consist of either one variable *x* or a set of variables $\bar{x}$. The right-hand side of the constraint functions, i.e., gb_i and hb_j, are often known constants for deterministic problems, while the non-negativity constraint $\bar{x} \geq 0$ is necessary for many practical situations and solution approaches. However, the standard model in equation (4.1) may vary such that one or more variables $\bar{x}$ in the model have upper and lower bounds instead of a non-negativity constraint, and the model contains upper and lower bounds on $\bar{x}$ instead of any other constraint. Based on this, the general properties of the mathematical model can be described as follows:

- A limited number of resources is described in practical problems with a parameter (which are usually found on the right-hand side of the constraint equations).
- Resources are allocated to an activity or function (usually represented by a decision variable), such as producing and offering a service or product.
- There are several alternative methods for resource allocation.
- All activities that use resources create a return in relation to the set goal (affects the solution formed by the objective function).
- Resource allocation is usually limited by several constraints. (Sarker & Newton, 2007)

4.1.2 Defining optimization problem

Understanding mathematical modelling and its basic properties is an important starting point in optimization. Accordingly, when defining the optimization task and goal, it is also very crucial to identify and classify what kind of optimization problem it is. The classification of optimization problems can be divided into five levels, through which it is possible to determine the tools needed to solve the problem and, in general, whether the problem can be solved at all. Figure 4-1 shows the levels of classification of the problem and the possible combinations formed through it. (Sarker & Newton, 2007)

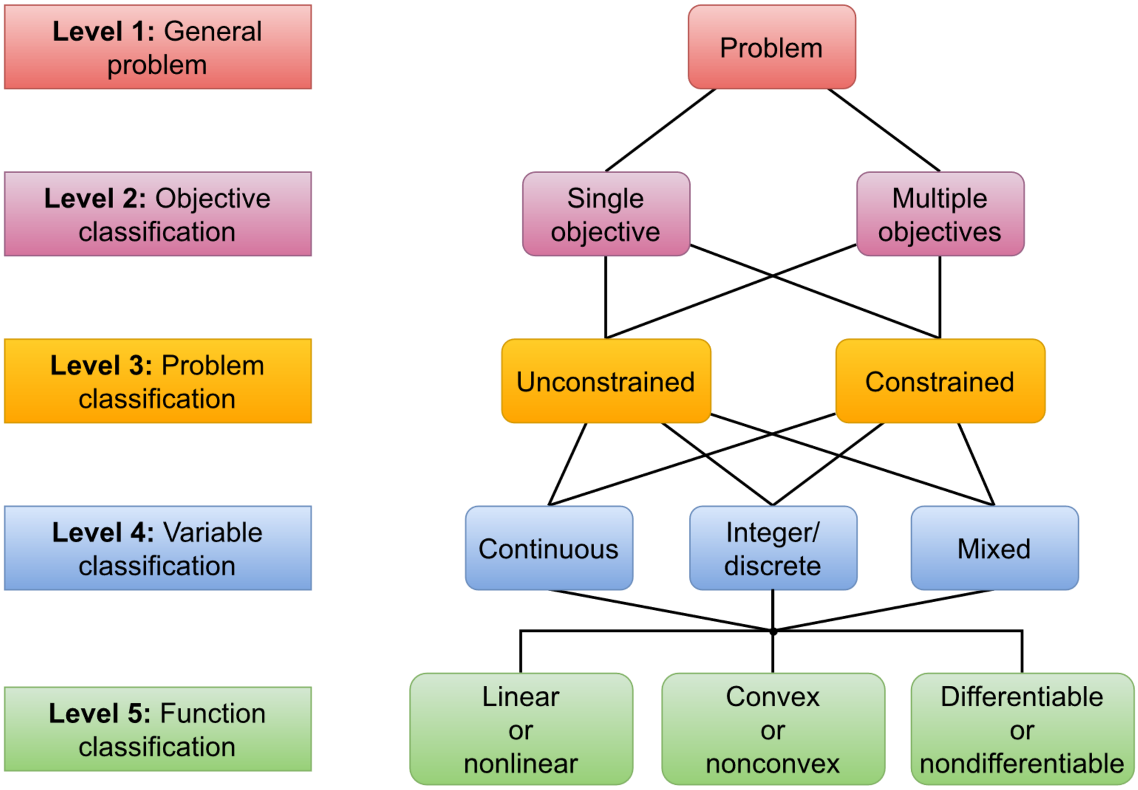

Figure 4-1: *Classification of optimization problems. Based on source (Sarker & Newton, 2007).*

As shown in the Figure 4-1, after defining the problem, it is identified whether there are one or more objectives. If there are several objectives, they might often be in conflict with each other and may, therefore, already cause problems for the optimization task. If problems or contradictions do not arise at this stage, tasks can usually be converted into a single-objective problem. After defining and editing the objective, it is identified whether the problem is constrained or unconstrained. It is generally believed that unconstrained optimization problems do not exist in the real world, as they are usually constrained by some factor or variable or both. However, unconstrained problems are very important, at least for research, as many optimization algorithms solve constrained problems by transforming them into unconstrained or sets of unconstrained problems. (Sarker & Newton, 2007)

After defining the constraints of the optimization problem, the type of variables is examined in the classification of the task. The types of variables can be clearly divided into real numbers, integers, or mixed integers, but many optimization practitioners still classify them as continuous, integer, discrete, or mixed. In problems of continuous variables, sequences of real numbers are usually sought. In turn, optimization problems of integer or discrete variables are generally called combinatorial problems, where the solution is sought from either a finite or an infinite set. (Sarker & Newton, 2007)

After the variable definition phase, the type of function that the optimization problem contains is finally identified. In this classification phase, the mathematical properties of the functions, which are significant from the point of view of the solution approach, are mainly examined. Objective or constraint functions can be either linear, nonlinear or in some cases both. If all the functions of the optimization problem are linear, the model created from the problem is called a linear optimization model or a linear model. If, however, one or more functions of the model have nonlinearities, the model is called a nonlinear model. Linear and nonlinear models have quite different solution approaches, of which linear models are more straightforward. Along with defining linearity, convexity is also considered an important property in classical optimization, as many optimization algorithms are based on the assumption that the function is convex. In addition to these, when classifying the optimization problem and its functions, it is still necessary to recognize its differentiability, according to which the solution approaches are divided into two large groups based on the continuity of the function. These groups are those with derivatives and those without derivatives. Thus, the result of the classification process can be, for example, a single-objective constrained problem with mixed variables and linear, convex, and differential functional properties. (Sarker & Newton, 2007)

In addition to the presented general problem classification, the optimization problem domain also takes into account function characteristics such as unimodality and multimodality, static and dynamic, and constraint characteristics such as soft and hard constraints. A function with only one peak and thus only one optimal solution is called an unimodal function, while a function with several peaks and thus local or global optima is called multimodal. Similarly, static and dynamism depend on the properties of a function, and if the properties change over time, it is called a dynamic function. Finally, soft and hard constraints are divided in such a way that hard constraints must be fulfilled in the final solution, while soft constraints can be violated with a certain punishment or under certain conditions. (Sarker & Newton, 2007)

4.2 Mixed-integer linear programming

A P2H2 energy conversion plant generally consists of many production-limiting and controlling factors, like process dimensions and related resources, such as equipment, fuels, available time horizon, and process control utilities. These often together create a broad platform for operational flexibility, through which significant advantages can be achieved with the proper planning of production schedules. Thus, the effective management of components has been generally the subject of research and attention for a long time, and through them, it is possible to influence the productivity of production and the resulting costs considerably. Mathematical programming, particularly mixed-integer linear programming (MILP), has become one of the most widely researched methods, especially in process scheduling and control problems, thanks to its accuracy, flexibility, and extensive modelling ability. MILP-based scheduling solutions are suitable from the simplest one-phase single-unit multi-product processes to the most common multi-function and product processes. Process scheduling problems are inherently combinatorial due to their many discrete decisions, such as assigning devices and scheduling tasks. In addition, these types of tasks belong to the group of nondeterministically polynomially complete (NP-complete) problems, which means that the solution time scales exponentially at worst as the size of the problem, i.e., the number of included devices, tasks, and goals, increases. MILP-based applications often work well for these problems and have generally achieved the desired results. (Floudas & Xiaoxia, 2005)

4.2.1 Linear programming

MILP is based on linear programming (LP) or, as it is called, linear optimization, where, as previously presented, the aim is to achieve the best possible result determined by constraints and objectives. In LP, to solve the objective function in the mathematical model, the requirements are represented only by linear relations and rules. In other words, LP is a technique for optimizing a linear objective function with linear equality and inequality constraints. However, the feasible region required by the LP technique is a convex polytope, which is a set defined as the intersection of finitely many half-spaces, each of which is specifically defined by linear inequalities. The objective function of such a set is a real-valued affine (linear) function defined for the formed polyhedron. The goal of the LP algorithm is to find a point on a convex polytope where the presented function has the smallest or largest value, if one can be found at all. Figure 4-2 shows a graphically simplified version of a linear optimization situation with two variables (V1 and V2) and six constraints (from C1 to C6). In this 2-dimensional example, the feasible region described in blue forms a polytope, from which the optimal point of the linear objective function is the intersection of the red line and the polytope. The red line describes the objective function, and the attached arrow indicates the direction determined by the optimization goal. (Vanderbei, 2008)

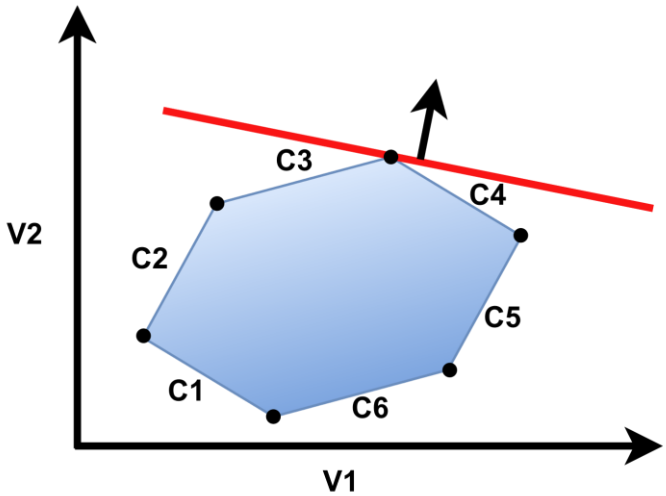

Figure 4-2: *A graphic representation of a polytope formed by two variables and six constraints, and an objective function.*

In addition to the features of linear programming presented above, the technique includes five basic assumptions, which are certainty, proportionality, additivity, divisibility, and nonnegativity. Based on these, the values of the parameters of the LP mathematical model must be known and constant, all functions (objective or constraint) must be proportional to the level of the activity (with consistent measurement units), the total result is the sum of the individual partial results, the decision variables could be only real or integer, and the variables can only have positive values. (Sarker & Newton, 2007)

4.2.2 From linear to mixed-integer linear programming

Linear programming can be further extended and specified to integer programming (IP). From the previously presented linear optimization assumptions, it can be defined that in the case of LP, the decision variables of the solution can be either non-negative fractional numbers or integer values. However, fractional values are not meaningful in all practical situations, as they are not suitable for some situations intended for production or business planning. For example, a car cannot be built only two-thirds, so a decision must be made whether it is more profitable to build the car completely or not to build it all. Thus, IP extension can be seen as linear programming with indivisibility requirements. However, integer programming can be further divided into three types of modeling subspecies, which are integer, binary integer, and mixed-integer linear. In the first of these, all the decision variables are integers. In the second they are binary, i.e., they either get the value one or zero. And in the last version some of the decision variables are integers, and some are real. (Sarker & Newton, 2007)

It is generally known that integer programming, and at the same time its subspecies mixed-integer linear programming, are extensions of the LP problem, which means that IP and MILP apply many concepts and techniques from ordinary LP when forming solution models. The most common solution approaches for IP models are based on complete enumeration, graphical method, rounding the noninteger solution, branch-and-bound, cutting plane, and branch-and-cut method. In MILP models, the branch-and-bound method has generally been found to be suitable for algorithms and an effective way to solve practical-sized problems that arise in the real world. For this reason, a large part of the available commercial IP packages is based on the branch-and-bound method. (Sarker & Newton, 2007) The method is used to solve combinatorial optimization problems that require exploring all possible permutations and combinations. Thus, it is an effective technique for solving crew scheduling, network flow problems, and production planning. In the method, the calculation system examines so-called branches or nodes under a particular subset of solutions, trying to find the best possible solution based on the given upper and lower boundary conditions (presented in equation (4.1)). The branch-and-bound method's solution search process is illustrated in Figure 4-3 with a simplified version of the state-space tree, where the green path describes the system's successful search path to the optimal solution. (Mitten, 1970)

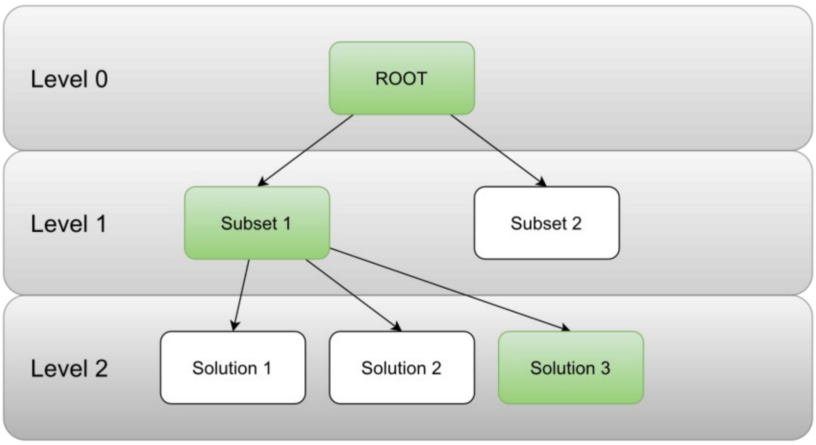

Figure 4-3: *State-space tree of the branch-and-bound method. Based on source (Mitten, 1970).*

However, it should be noted that not all IP and MILP problems can be solved with the presented method due to its computational complexity and the required computing capacities. Practical problems can still often be solved by approaching them with different methods and solver engines. There are numerous commercial software packages on the market for solving LP models that contain solvers, which in turn consist of one or more algorithms of a specific class or set of classes, such as simplex and interior point algorithms. Such software packages are, e.g., LINGO/LINDO, GAMS, OptiMax 2000, CPLEX and XPRESS, MINOS, Solver and Premium Solver, and many others. (Sarker & Newton, 2007)

4.3 Research done with mixed-integer linear programming

The MILP method is an effective way to model and plan the operation of systems and plants. It can be used to create a resource-efficient and scheduled layout for the problems presented in the previous section. MILP technology has also been used in many types of research, such as rationalizing the operation of a standard energy production plant and solving scheduling problems for equipment and features added to production plants. Next, two studies on the use of MILP are presented in relation to the use of renewable energy sources and the production planning of a chemical company. In the first of these, a stochastic MILP approach is used to study wind energy storage arbitrage in the day-ahead market. In the latter, the MILP model is used to plan the mid-term production of a chemical company.

4.3.1 Research article on the sale of wind energy

The first article (Gomes, Melicio, Mendes, & Pousinho, 2021) discusses a support information management system for a wind power producer with an energy storage system and participation in the day-ahead electricity market. The article highlights how energy storage has the effect of reducing the uncertainty of renewable energy production thanks to the more flexible energy usage time created by the storage. Due to the more flexible storage and usage time of the generated energy, the wind power producer has the opportunity to benefit from the arbitrage created in the electricity market. The article emphasizes that benefiting from arbitrage should be realized with the right kind of problem setting and the optimization model created for it. For this purpose, a stochastic approach is used, which is written as a mixed integer linear programming problem. In the research, the optimization is carried out for the operation control of the energy storage, i.e., its loading and unloading as determined by the electricity market and wind power production.

The goal of the optimization task presented in the article is to maximize the expected profit of the objective function. For this, the economic effects of the imbalance must be taken into account in the problem statement. In the optimization task, the real consequence of the uncertainty of market prices and the availability of wind power in terms of operating time must be anticipated. A bad assignment can, therefore, result in a loss of income. The formulation of the problem used in the research is based on a two-stage stochastic optimization task, where hourly prices and imbalances are the variables of the first and second stages. In addition to the objective function to be created, general constraints are defined for the stochastic MILP model, which affects energy offers, wind power and energy storage supply, and imbalance conditions. In addition to the general restrictions, only additional storage-related restrictions are created, which affect the capacity limits of the energy storage and the loading and unloading of the storage.

The research creates and compares results with three different scenarios, which are a non-coordinated electricity supply model, a deterministically coordinated model, and a stochastically coordinated model. The first two models were created by modifying the stochastic version. However, all models are based on the MILP method. The obtained results are quite close to each other and are ranked in terms of profitability: stochastic model, deterministic model, and non-coordinated model.

4.3.2 Research article on the mid-term production planning

The second article (Adrio, García-Villoria, Juanpera, & Pastor, 2023), on the other hand, examines the traditional production plan of a chemical company, which also uses an ad-hoc type of production control method. For the company, the research aims to find the optimal production method in conditions where the consumption of raw materials is not necessarily constant and depends on the manufactured quantity of one reference product (together, they form ad-hoc situations). In addition to these, the offered demand should be between the minimum and maximum values defined in the contract. The optimal production method for semi-finished and finished products is planned in such a way that the profit from the sale of the products is maximized, taking into account the resource costs. The work also compares different production scenarios, which provide more information about the possibilities of capacity expansion and alternative market positions.

For the MILP method used in the research, the profit-maximizing objective function and the constraint equations that determine and control the model's operation are defined. The article presents that the objective function consists of two parts, the first of which determines the profits of the production plan, such as the difference between the income from product sales and the costs of raw materials and other parts. In the second part of the equation, the weight and, thus, the priority of the soft constraints are determined. However, the article specifies that the first part of the objective function only defines the company's result, and the second part directs the optimization in the desired direction. In addition to the objective function, there are several constraint equations defined for the model, which is why they are divided into three groups. The first group of constraints examines inventory balance and the fulfillment of all available resources, production, and sales requirements. In the second group, on the other hand, restrictions are defined for elements that depend on production values. Finally, in the third group, special requirements defining the operation of the production processes of the investigated company are formed.

The results of the research show that through MILP-based optimization, it would be possible to enhance the productivity of processes and rationalize the sales volumes of products. The obtained growth is made possible by the reduction of the minimum demand, which leads to higher production flexibility and, thus, better results. Through the results produced by optimization, the chemical company is also able to assess which of its products are more significant in terms of the company's operations, which sub-processes run at full capacity and are, therefore, bottlenecks, and which sub-processes are underutilized. The company involved in the research is satisfied with the results produced by the optimization and modeling and recognizes the high value of the tool.

5. SETTINGS OF THE OPTIMIZED SYSTEM

Chapter 4 presented the use of optimization based on the MILP method in two studies. As in the presented studies, this work also uses MILP-based optimization to answer the thesis' research questions defined in Chapter 1. The optimization is carried out in this work with the Energy Optima 3 optimization tool, which is used to model the investigated system. Based on the modelling, the optimization tool forms the objective function and the necessary constraint equations, as presented in the last chapter. In addition to this, some special conditions are defined directly in the files used by the optimizer.

In this work, the optimization of the use of the P2H2 energy conversion plant is done in collaboration with a company called Woikoski Oy, which specializes in the gas industry and offers highly refined, high-quality gas products and expert services. The purpose of this chapter is to delimit the area of optimization work with the company and to present the parameters and assumptions of the system to be optimized. The chapter begins with an introduction to the optimization goals and continues from there to a more detailed definition of the system's configuration, such as the initial data and the constraints.

5.1 Configuration of the optimized system

The research object is the P2X hydrogen production plant (a P2H2 plant), the basic layout of which consists of three AWE-type electrolyzers, a hydrogen compressor unit, and a hydrogen storage. As presented in the work's research questions, the subject of research is to examine the effects of the three production scenarios through the profitability of using the facility. The three entities to be added to the basic layout are increasing the production capacity with one AWE electrolyzer, participating in the reserve electricity market with the production plant, and converting waste heat into district heat using a heat pump. The basic layout and the three entities needed for the research scenarios are presented in the system's principle picture 5-1.

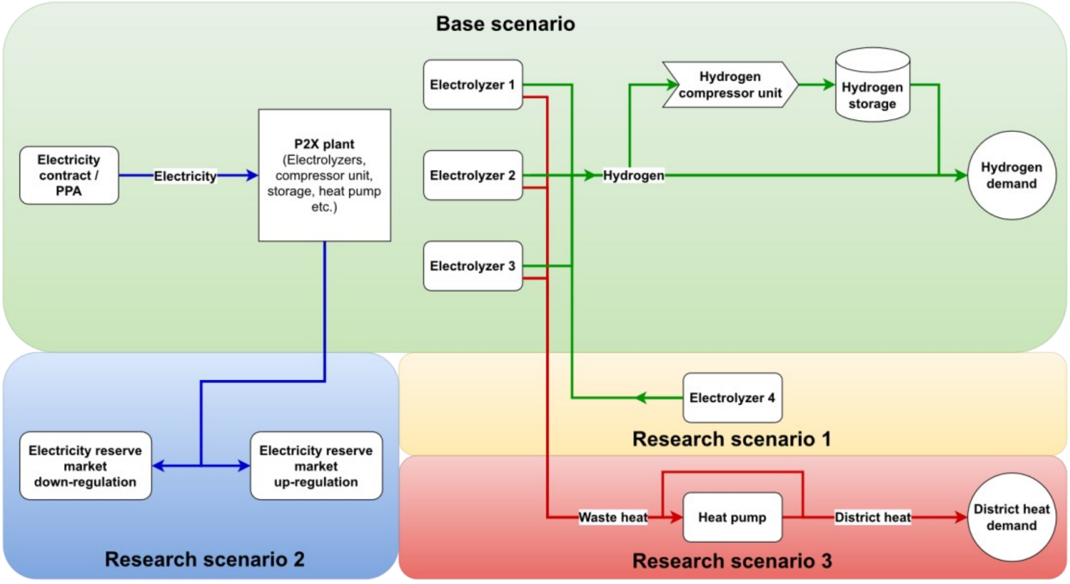

***Figure 5-1:** Principle picture of the base scenario and the added entities.*

The system shown in the Figure 5-1 is modelled in the EO3 optimization environment, where all components are parameterized and connected as shown above. The parameterization is implemented in such a way that the dimensions of the system to be modelled are established essentially according to the existing Woikoski Oy production facility, but some of the necessary initial data is also taken from the literature.

5.1.1 Initial data for the electrolyzers

First, in the base scenario, the properties of the electrolyzers present in the system are defined. The electrolyzers are of the same size and type, so all electrolysis units, even the one to be added in the first research scenario, are modelled in the same way. For optimization work, electrolyzers need their production size, ramp speeds both when driving up and down, and the production efficiency curve as input data. The size of the electrolyzers is 3 MW, which is the highest electric power that can be fed into one electrolysis unit. The maximum ramp speeds for the AWE-type electrolyzer are taken from the literature, i.e., from Table 3-1, where both up and down drives are limited to a maximum speed of 0.3 %/s. In the case of the electrolyzers defined in this work, this means that the modelled electrolyzers can be driven up or down by 0.009 MW/s. This means that shifting one running electrolyzer from minimum load to maximum load takes about 6 minutes. The last characteristic required for electrolyzers, i.e., the efficiency curve of their production, is also taken from the literature. MILP optimization uses linear equations, which is why the efficiency curve obtained from the source (Yanghong, Haoran, Hanghang, & Wei, 2023) is modified to the form shown in Figure 5-2.

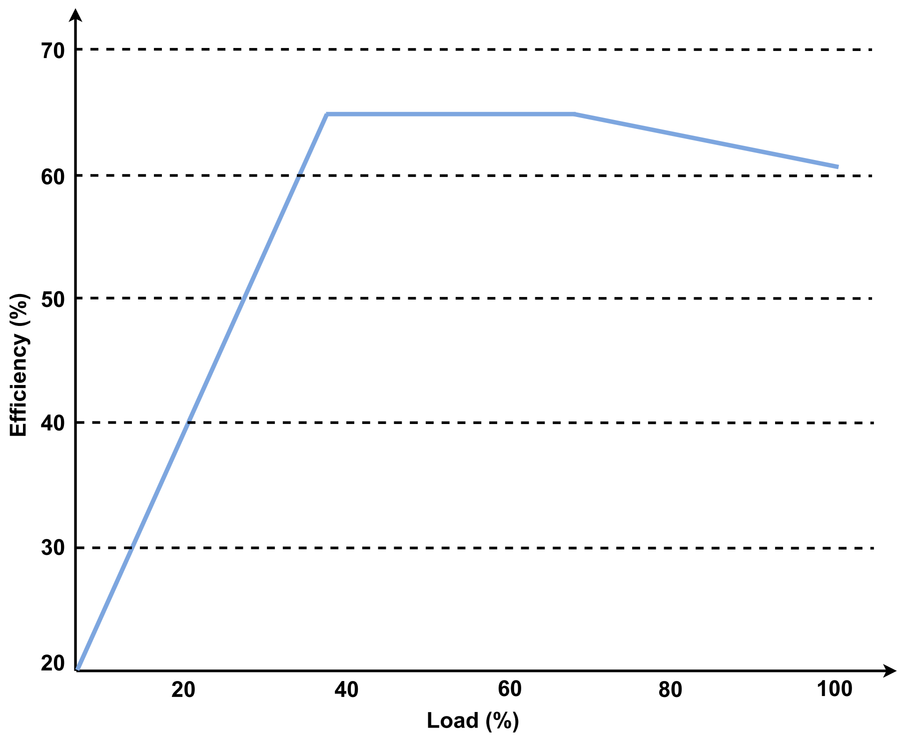

Figure 5-2: *The efficiency curve of the electrolyzer defined in sections.*

The source efficiency curve is for the 10 MW AWE electrolyzer. The three parts of the formed efficiency curve change in terms of the efficiency slope at points 35% and 70% of the maximum load. In this case, the areas of the curves for 3 MW electrolyzers are 0-1.05 MW, 1.05-2.1 MW, and 2.1-3 MW, whereby the efficiencies for the corresponding areas run linearly from 20%-65%, 65%, and 65%-61%. Thus, the maximum hydrogen production capacity determined by the efficiency curve with a power input of 9 MW (100% load) is approximately 5.49 MW.

5.1.2 Initial data for the hydrogen compressor and storage

The next system component in the base scenario to be defined is hydrogen storage, which essentially also includes hydrogen compression. Hydrogen is typically stored at pressures of 20-30 and 70 MPa, depending on the type of storage tanks (Barthelemy, Weber, & Barbier, 2017). In this work, we operate at a pressure of 70 MPa, so the density of hydrogen is 40 g/L. The size of the hydrogen storage considered in this work is 9600 Nm^3 (Normal Cubic Meter), which should be converted to megawatt hours for the optimization application. To determine the maximum energy content of the storage, the energy volumetric density of hydrogen under STP (Standard Temperature and Pressure) conditions is needed, which is about 0.0033 kWh/L. (Hassan, Ramadan, Saleh, & Hissel, 2021) With this information, it is possible to determine the storage size as 31680 kWh, which corresponds to 31.68 MWh. However, converting hydrogen to this density requires a notable amount of energy from the compressor, which, according to (Hassan, Ramadan, Saleh, & Hissel, 2021), is about 10% of the compressed energy content. The energy consumption of the storage is not taken into account in this work, so the consumption of the compressor determines the efficiency of the storage at 90%. In addition to this, the work also assumes that the pipelines involved in the transportation and transfer of hydrogen do not form restrictions and, therefore, bottlenecks for optimization. However, the limited capacity of the compressor is considered in this work, as the maximum flow determined for it is 1550 Nm^3/h, from which the maximum amount of hydrogen that can be compressed can be calculated using the energy volumetric density presented above. The maximum output of compressed hydrogen is approximately 5.115 MW. In addition to the compressor unit, a maximum limit is also set for the output of the storage so that the storage cannot be emptied immediately. The storage outflow limit is set at 6.3 MW.

5.1.3 Formation of the hydrogen demand

Next, in the base scenario, the hydrogen demand and price are viewed. The hydrogen demand model used in this work is not based on Woikoski's existing model and is generated as fluctuating demand series. In the actual demand and corresponding supply, there are seasonal fluctuations and factors limiting the operation of the plant, such as random breakdowns and annual maintenance, which are not considered in this work. The demand needed for the work is generated using a normal distribution, the mean of which is given as 4.2 MW. In this case, the mean is about three-quarters of the total hydrogen production capacity of three electrolyzers. The variance for this demand is set to 1 MW, which allows for a large enough variation for the series. The series generated in this way gives each moment of time its own demand value, which can vary greatly in a quick time frame. In order to smooth out this variation in demand, it is limited to occur every four hours so that the daily demand consists of six different sections. The behavior of hydrogen demand is illustrated in Figure 5-3, which shows the demand for a random four-day period.

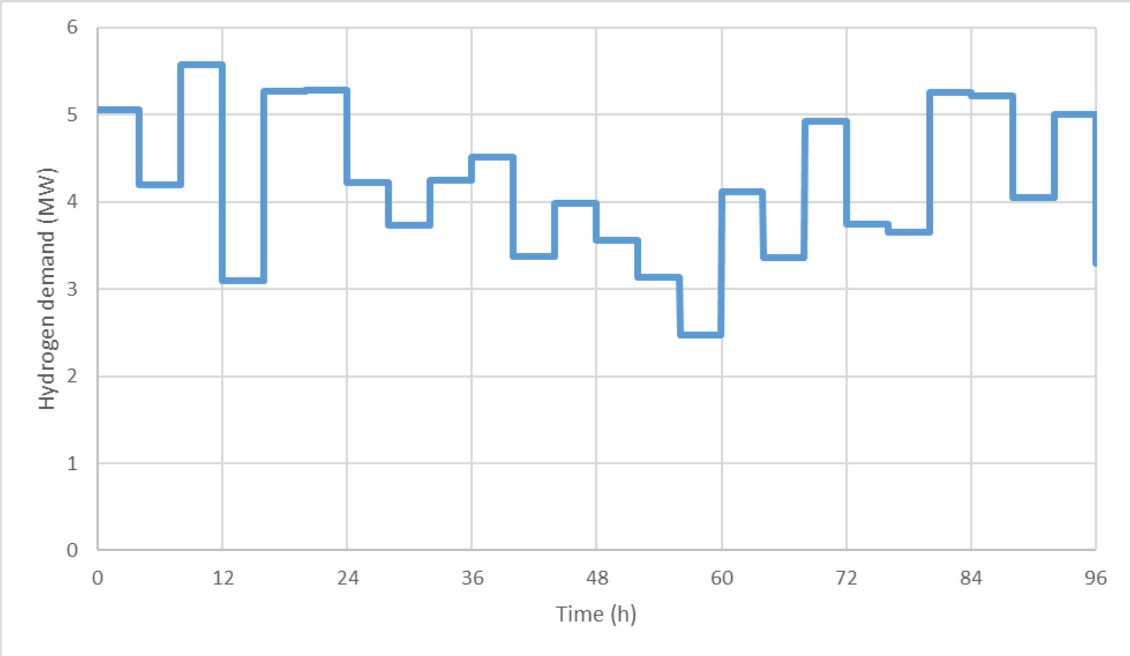

Figure 5-3: *Hydrogen demand for a random four-day period.*

The maximum and minimum values for the whole demand series formed in this way are 7.88 MW and 0.73 MW. It can be seen from the values that, first, the demand can, therefore, exceed the maximum hydrogen production of the electrolyzers, in which case the production must be supported by the buffer stock. In the demand series formed in this way, about 10% of hours exceed the actual production capacity, which emphasizes the importance of the buffer in balancing demand and supply. The second notable observation from the series is that the demand never goes to zero.

A price is also needed for hydrogen, which is paid by the customers of the P2H2 company. The price is determined based on the IEA's hydrogen report (IEA, Global Hydrogen Review, 2022), which shows that hydrogen produced from renewable energy sources with an electrolyzer will cost approximately 4.0-9.0 USD/kg (in 2021). In this work, it is assumed that customers pay the upper limit of the production cost for the hydrogen produced at the investigated plant, i.e., 9.0 USD/kg, which is 8.09 EUR/kg at the rate of 1.11 EUR/USD. According to the source (Yue, et al., 2021), the energy density of hydrogen is 33.33 kWh/kg, so the price of hydrogen is around 243 EUR/MWh and it is used as a constant price to be paid for hydrogen.

5.1.4 Power purchase agreement determination

The last area presented in the base scenario is electricity procurement. Many types of contracts can be formed for electricity procurement, a couple of examples of which are both fixed price contracts and contracts that behave according to consumption. In addition, these contracts can be tied around the procurement of green energy with the help of a PPA, as presented in section 2.4. In this work, the price of the input power to the system directly follows the realized hourly price of the day-ahead market. Figure 5-4 shows the moving average of the day-ahead electricity prices from the beginning of 2020 until the end of June 2023. In the figure, the data is based on prices examined at the hourly level. The day-ahead prices used in the figure have been exported from (ENTSO-E, Day-ahead Prices, 2023). The moving average is formed according to a week, i.e., 168 hours, so that the overall behavior of the price of electricity can be easily demonstrated.

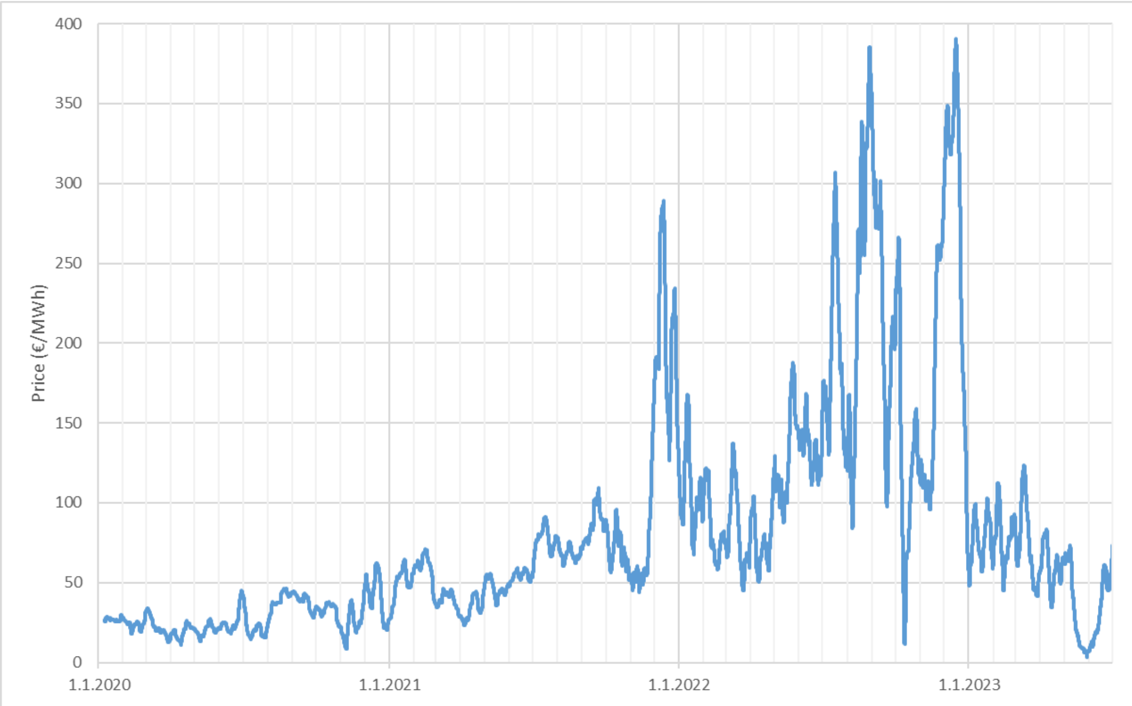

Figure 5-4: *Week-weighted moving average of the day-ahead electricity prices 2020-2023.*

The Figure 5-4 shows how the price of electricity rose slightly from 2020 to 2021 but made its biggest fluctuation and increase in 2022 as a result of the situation in Ukraine, due to which EU-level electricity production could not fully meet demand (STRF, 2023). The year 2023, on the other hand, has been significantly more moderate in terms of electricity prices than 2022 and roughly corresponds to the level of 2021 in terms of prices. The situation in the electricity market has calmed down, and in addition, the Olkiluoto 3 nuclear power plant was able to start regular electricity production on April 16, 2023, which has a noticeable downward effect on electricity prices in Finland (EPV, 2023).

For the research questions of this work, the years 2021 and 2022 will be used from the presented time frame, as it is to the advantage of the research to use whole years when the operation of the plant is affected by the seasonal variation of both electricity prices and the price and temperature of district heating, which will be presented later. Of the years used, 2021 roughly represents 2023 in terms of electricity prices (assuming that the end of the year corresponds to the beginning), while 2022 represents a more exceptional year in terms of the global situation and electricity prices. In this case, it is possible to see how the profitability of the studied scenarios manifests themselves with respect to very different years.

Next, all the initial data and parameters required for the research scenarios are presented. The increase in production capacity examined in the first research scenario does not require additional information, i.e., as previously stated, the fourth electrolyzer is identical to the existing electrolyzers and thus uses the same initial data and parameters. Therefore, the initial data is supplemented only with the information required by research scenarios two and three.

5.1.5 Initial data for the electricity reserve markets

The second research scenario examines the possibilities of the electricity reserve market, in which the presented hydrogen production plant would participate. Table 2-1, presented in Chapter 2, describes the functional and operational capabilities required by different reserve market products. In terms of these requirements, the essential characteristics of a hydrogen production facility are the production input power capacity and its ramp speeds (seen in Table 3-1). In the plant studied in this work, the input power is 3 MW per electrolyzer (9 MW in total), and the ramp speeds are respectively 0.009 MW/s (0.027 MW/s in total), as previously presented. Among the reserve products, the FFR and FCR-D types clearly require faster ramp speeds than the studied system contains, but the requirements of the FCR-N, aFRR, and mFRR products are promising. The minimum limits of these products are, respectively, 0.1 MW in three minutes, 1 MW in five minutes, and 1 MW in fifteen minutes. Within the given time limits, one AWE electrolyzer can, with its ramp speed, provide 1.62 MW, 2.7 MW, and 8.1 MW in the corresponding order (if the 3 MW capacity limit per electrolyzer used in the work is not considered). Therefore, it can be stated that the system would be able to participate in the examined markets. However, due to the scope of the work, only aFRR and mFRR products from these options are selected as the target of the study.

For the optimization work, the up and down regulation prices of the aFRR and mFRR products, as well as the activated quantities, are needed as input data. However, it should be noted from the data that in the case of the aFRR reserve market, the aFRR up and down regulation price is only for capacity reservations, on top of which the mFFR regulation price is also paid for the realized aFRR energy demand. The data for the information above has been exported in hourly format from the source (Fingrid, Search data, 2023). The upward and downward capacity and regulation prices are shown in Figure 5-5, and the activated regulation quantities are shown in Figure 5-6. Both graphs are formed similarly to Figure 5-4, i.e., using the moving average.

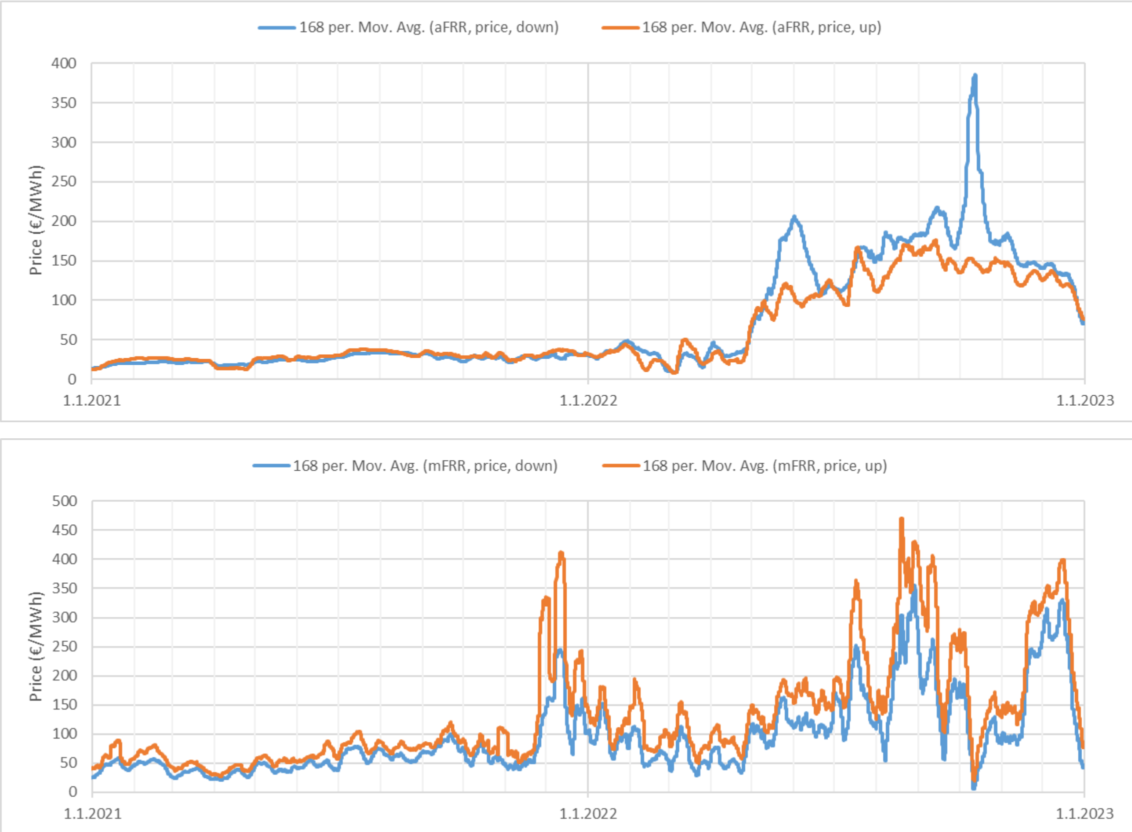

Figure 5-5: *Week-weighted moving average of the aFRR and mFRR regulation prices 2021-2022.*

The Figure 5-5 shows how the aFRR up and down regulation capacity prices behave fairly evenly throughout 2021, but in the end of the spring of 2022, they start to grow considerably. In mFRR prices, in addition to 2022, a clear price spike can already be seen at the end of 2021, which was also reflected in the day-ahead prices but not in aFRR capacity prices. Similar, equally clear, year-specific differences are not discernible in Figure 5-6 of the activated regulation quantities.

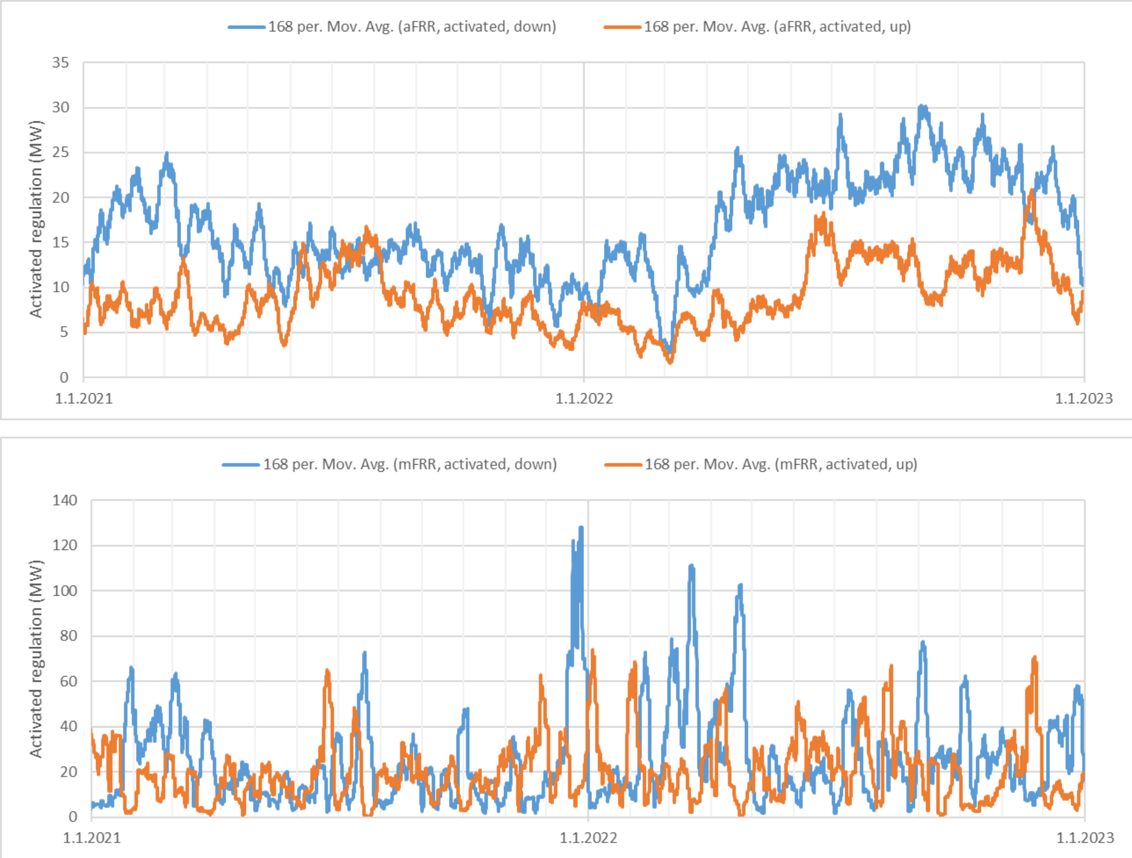

Figure 5-6: *Week-weighted moving average of the aFRR and mFRR activated regulation quantities 2021-2022.*

The Figure 5-6 shows that the activated aFRR megawatts in 2022 are, on average, higher than in 2021, but the difference is not as clear as in the prices shown above. mFRR adjustments, on the other hand, differ even less between years than in the case of aFRR. However, when looked more closely, it can be seen from mFRR activations that they have been higher on average in 2022, but at the same time, as in the situation of aFRR, the difference is not nearly at the same level as it was for the prices.

5.1.6 The initial data for the heat pump

Finally, the initial data necessary for the third research scenario, i.e., the production and demand for district heat generated from waste heat, will be presented. Most of the waste heat is generated in electrolyzers, where it is possible to collect it and lead it either directly or via an additional heat pump to the district heating network. According to Table 3-1, AWE-type electrolyzers operate at 60-90 °C, so for example, when running the electrolyzer at exactly 90 °C, the waste heat obtained is equal or lower than this. In this work, the waste heat temperature to be obtained is assumed to be a constant 80 °C. The purpose of the heat pump added to the system is to raise the temperature of the waste heat to the value determined by the district heating network's need. The electrical power needed to increase the heat pump's temperature is proportional to the pump's efficiency, which is commonly referred to as the COP (Coefficient of Performance). The COP value is determined as the ratio of the energy coming out of the system and the work done by the system (equation (5.1)), where the work done is dependent on the input and output temperatures. (Akmal & Fox, 2016) Therefore, according to the previous source, equation (5.2), which depends directly on the temperature difference, can be formed from the results of experiments carried out with equation (5.1). In this work, a simplified linear version of equation (5.2), i.e., equation (5.3), is used to determine the power required by the heat pump. The referred equations are:

$$COP = \frac{Q}{W} \tag{5.1}$$

$$COP = 0.0008x^2 - 0.138x + 7.4545 \tag{5.2}$$

$$COP = -0.138x + 7.4545\,, \tag{5.3}$$

where the variable *Q* is the output energy of the heat pump, *W* is the work done by the pump and *x* is the temperature difference between the outgoing and incoming liquid.

5.1.7 Formation of the district heat temperature need

The temperature difference shown in equations (5.2) and (5.3) is determined solely by the temperature demand of the district heating network when the waste heat temperature of the electrolyzers is constant. Therefore, to determine the electrical power required by the heat pump, the temperature demand of the district heating network for the considered period is needed. The need for the network can be calculated using the equation (Energiateollisuus, 2020):

$$T_{DH} = \begin{cases} 115 + (t_u - t_x) \cdot \dfrac{45}{8 - t_u}, & t_x \leq 8 \\ 70\,, & t_x > 8 \end{cases}, \tag{5.4}$$

where T_{DH} is the temperature demand of the district heating network, t_u is the dimensioning temperature of the locality and t_x is the outdoor temperature.

Equation (5.4) requires information on the dimensioning temperature of the locality and the outdoor temperatures of the review period to work. Dimensioning temperature for Kokkola (P2H2 plant location) is -29 °C according to the source (FINLEX, 2017). The outdoor temperatures of Kokkola, on the other hand, are obtained from the source

(Ilmatieteenlaitos, 2023) and are presented together with the temperature demand of the district heating in Figure 5.7.

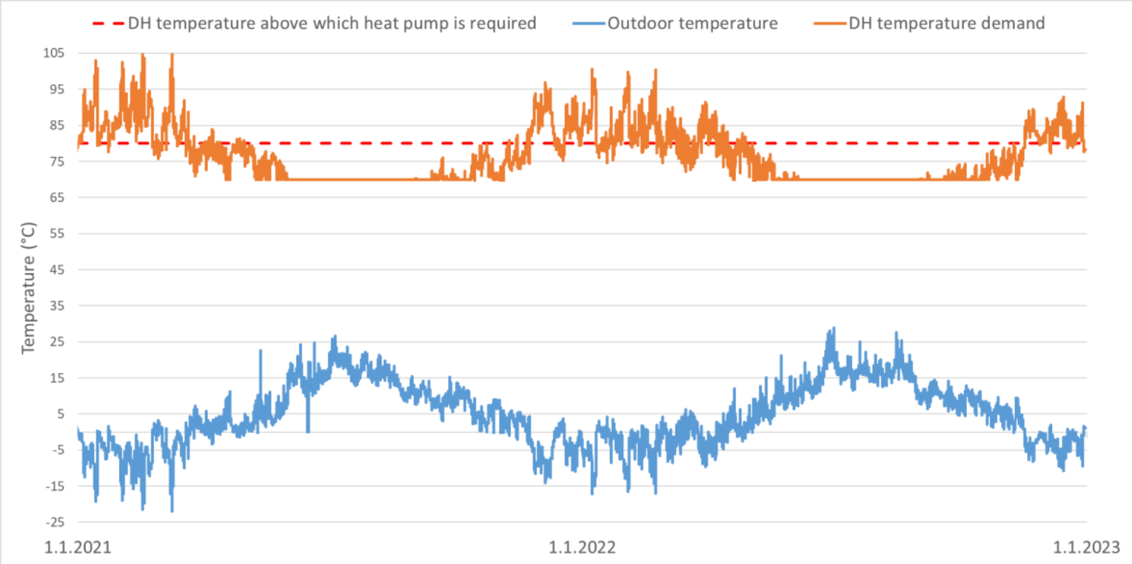

Figure 5-7: *District heating and outdoor temperatures 2021-2022.*

The Figure 5-7 shows how the temperature demand of the district heating network follows the outdoor temperature and levels off to a standard value of 70 °C in summer. In the period under review, the temperature behavior is roughly the same from year to year and from season to season. The figure also illustrates the need for a heat pump with the red dashed line. The temperature demand of district heating above the dashed line can only be met with the help of a heat pump.

5.1.8 Pricing of district heat sold to an energy company

The last input required for the work is the price to be paid for the produced district heat. The price paid for district heat is the result of a negotiation between two parties (the heat producer and the owner of the district heating network). The price series generated for this work has been formed with Tampereen Energia Oy as an indicative estimate of what it could be. In this work, the district heating network does not set limits on the output of the district heat produced by the P2H2 plant but only determines the temperature of the produced district heat. The P2H2 plant can, therefore, produce district heating when it is profitable and possible for it. The price series used in the work is formed according to a simple seasonal model, and it is shown in Figure 5-8.

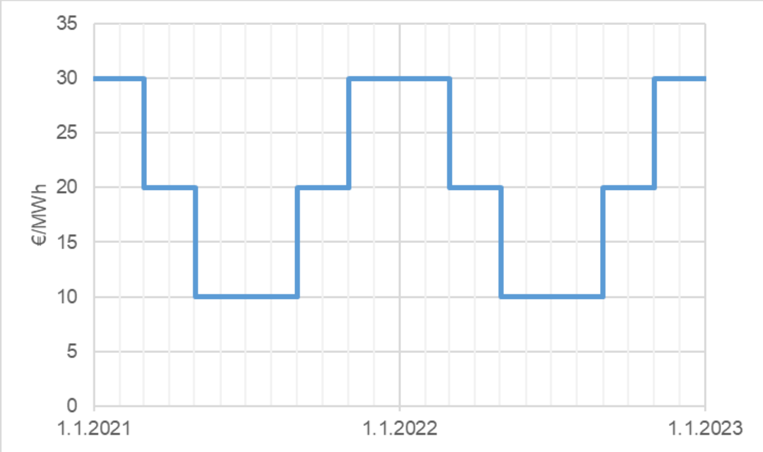

Figure 5-8: *Used district heat price 2021-2022.*

The series shown in the Figure 5-8 is formed according to winter, intermediate, and summer season pricing, where the price per megawatt hour is fixed at €30 in the winter season, €20 in the intermediate season, and €10 in the summer season. The winter seasons are defined as months 1, 2, 11, and 12, the intermediate seasons are months 3, 4, 9, and 10, and the summer season is months 5, 6, 7, and 8.

5.2 Definition of the system model constraints

Results for the research questions of the work are produced with the EO3 optimization application, which uses the initial data presented in the previous section. However, the optimization application treats input data such as electricity prices and realized reserve market offers as reliable information and, therefore, does not treat them as predictions that would contain uncertainty. In this work, the optimizations are created with historical data, in which case all information is certain, and the results generated without restrictions would then be ideal because there would be no surprising changes for the optimizer. In a situation where the optimizations would be carried out into the future, such as the end of 2023, the profitability results would be clearly weaker compared to the results given with historical data due to unexpected factors and wrong predictions. Consequently, some level of ideality in this work is accepted for simplicity, but for research scenarios two and three, limitations and conditions are created to ensure more realistic participation in the reserve markets and the proper type of system operation.

5.2.1 General constraints

The base operation of the system and the operation regarding research scenario one are not given conditions supplementing the optimization's own limitations, i.e., the system is allowed to use electricity day-ahead prices and hydrogen demand as reliable information. However, specifications that guide the optimizer are created in the system for the operation of the electrolyzers, such as shutdown and start-up costs. The costs are set at €100 for both events. Research scenarios two and three, on the other hand, require more complex limitations. Concerning research scenario two, without limitations, the optimizer would plan plant's operation in such a way that all reserve markets would be participated with all free or freed capacity at every possible moment in time, which does not correspond to reality. With regard to the production of district heat, the system must be defined under which conditions waste heat is directed directly to the district heating network and when it requires the assistance of a heat pump.

5.2.2 Constraints for the electricity reserve market

For research scenario two, both initial data and functional constraints are made into the system. Initial data restrictions aim to influence how many aFRR capacity markets are participated in and how many regulation offers from the aFRR and mFRR markets are realized. This restriction is intended to somewhat model the uncertainty present in the market, according to which it is not always reasonable to offer capacity or the offered capacity is not needed by the TSO. Functional constraints, on the other hand, ensure that the system has the capacity to participate in the offered marketplaces.

In the restrictions made on behalf of initial data, it is assumed that 10% of all hours can be offered to the aFRR market (for both upward and downward capacity). After this, the system checks whether there is a need for capacity for the examined hour. If there is a capacity need, the system checks whether the capacity also needs activation, on the basis of which the system knows at which hours the production plant could be involved in a regulation event. However, the operation of the system is simplified a bit so that it considers offers only when there is a need for both capacity and activation. Unlike in the aFRR product, mFRR only pays for realized regulation hours, and no capacity reservations are made for them in advance. Consequently, the realized mFRR offers are limited in the same way as in the case of aFRR, i.e., 10% of the hours are determined to be marketable, after which the system checks whether there is a need for the offered hour and, if so, the offer is accepted. Figure 5.9 demonstrates one result of the presented restriction with the amount of possible participation for aFRR down-regulations compared to all aFRR down-regulations.

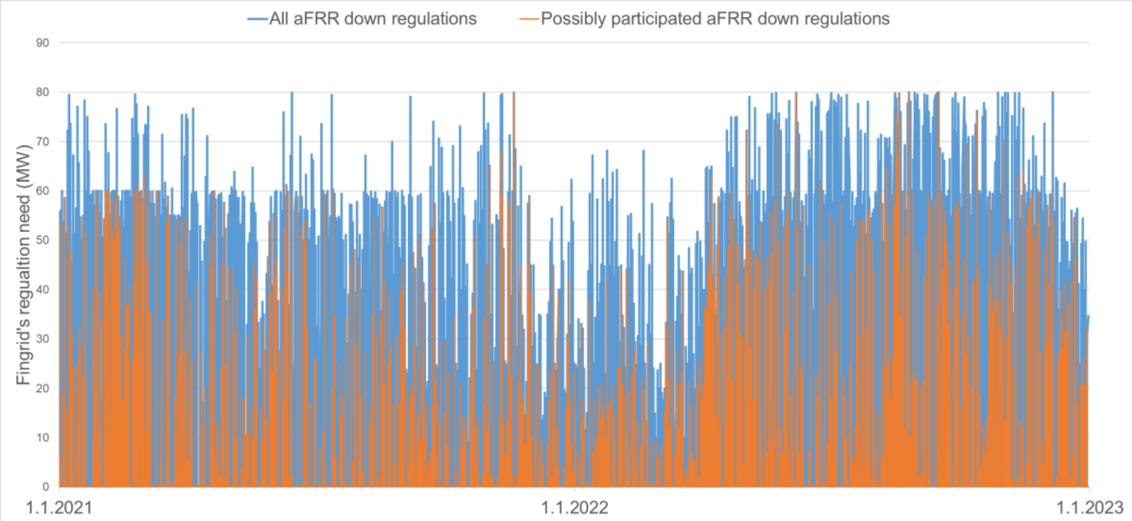

Figure 5-9: *All aFRR and possibly participated aFRR down-regulations.*

In the Figure 5-9, the orange lines represent situations where aFRR down-regulations could be participated in. In the case of the figure, these events cover about 9.6% of all aFRR down-regulation hours and about 6.3% of all hours. When looking at the graph, it should be noticed that due to the thickness of the blue and orange lines, it seems that they cover more than they actually do. In addition, it is good to remember that the blue lines still represent the initial data to be entered into the system, which is reflected in the size category of the regulation needs (y-axis).

The production facility's participation in the reserve market is also controlled by functional limitations affecting the offered capacity in addition to the above-mentioned scheduling limitations. First of all, it is specified in the system that the up regulation offered to the reserve market and the electric power used by the system is, at most, the maximum input power of three electrolyzers, i.e., 9 MW. In this case, when increasing the frequency of the electric grid, the power released to the grid is not used by the electrolyzers. Correspondingly, down-regulation is also limited. The system can increase its production (down-regulation event) by a maximum of three electrolyzers, i.e., 9 MW.

Another functional constraint is built to limit overlapping aFRR and mFRR regulation events. It is specified in the system that it cannot participate in up-regulation and down-regulation events in the same hour. The restriction is implemented for the reason that without it, the system could trade aFRR and mFRR products between down and up regulation offers because the system works on an hourly level, where down and up-regulation events can occur at the same time.

Finally, functional constraints are created according to Table 2-1, where the lower limit is determined as 1 MW for both aFRR and mFRR products. However, aFRR participation also has a maximum limit of 2.7 MW according to the capabilities of the system. The maximum limit is determined based on the operational capability of the AWE electrolyzer presented earlier and the aFRR time requirement, according to which 2.7 MW can always be provided if the production level allows it.

5.2.3 Constraints for the operation of the heat pump

Unlike research scenario two, only two functional conditions are specified for research scenario three. According to the first of these, when the temperature requirement of the district heating is 80 °C or below, the waste heat can also be directed to the district heating network via the bypass valve so that the heat pump can be turned off if necessary. Another functional condition is the same as with electrolyzers, i.e., the shutdown and start-up cost set for the heat pump. The cost is chosen to be the same €100 as for electrolyzers, and its purpose in both cases is mainly to guide the optimization and to symbolize the costs generated in connection with the units' shutdowns and start-ups.

6. THE RESULTS OF THE OPTIMIZED PRODUCTION SCENARIOS

In the previous chapter, the system to be researched and optimized in the work was parameterized, and the initial data and limitations for the operation were determined. In this chapter, the results produced by the research scenarios will be presented and analysed. The chapter examines each optimization scenario separately and presents the effects of each scenario on the system usage. The optimizations are run with the initial data of the years 2021 and 2022 when the clearly different behaviour of electricity prices affects the operation and the resulting costs of the investigated plant. All optimizations are performed with a time span of one year and a resolution of one hour.

The chapter begins by presenting the basic optimization scenario, where the base production capacity is set to work in the most cost-effective way possible, as guided by day-ahead electricity prices and hydrogen demand. Next, the effects of the capacity increase by one electrolyzer will be studied and presented. After this, the effects of participating in the reserve electricity market are investigated and presented. Hereafter, the influence of the district heat formed from the waste heat by-product of the P2H2 energy conversion is examined and shown. Finally, the monthly net profit distribution of all scenarios is presented and analysed.

6.1 P2H2 plant base operation

Through the basic operation scenario of the hydrogen production plant, the production profit achieved by the optimization system for the years 2021 and 2022 is presented. The base scenario serves as a reference for the studied research scenarios. The object of comparison is the profit generated from the use of the plant, which in the base scenario is affected by the price of electricity, the demand for hydrogen, and the degree of use of electrolyzers and storage. The behaviour of these components is presented in Figure 6-1, where the review period is the first seven days of 2021.

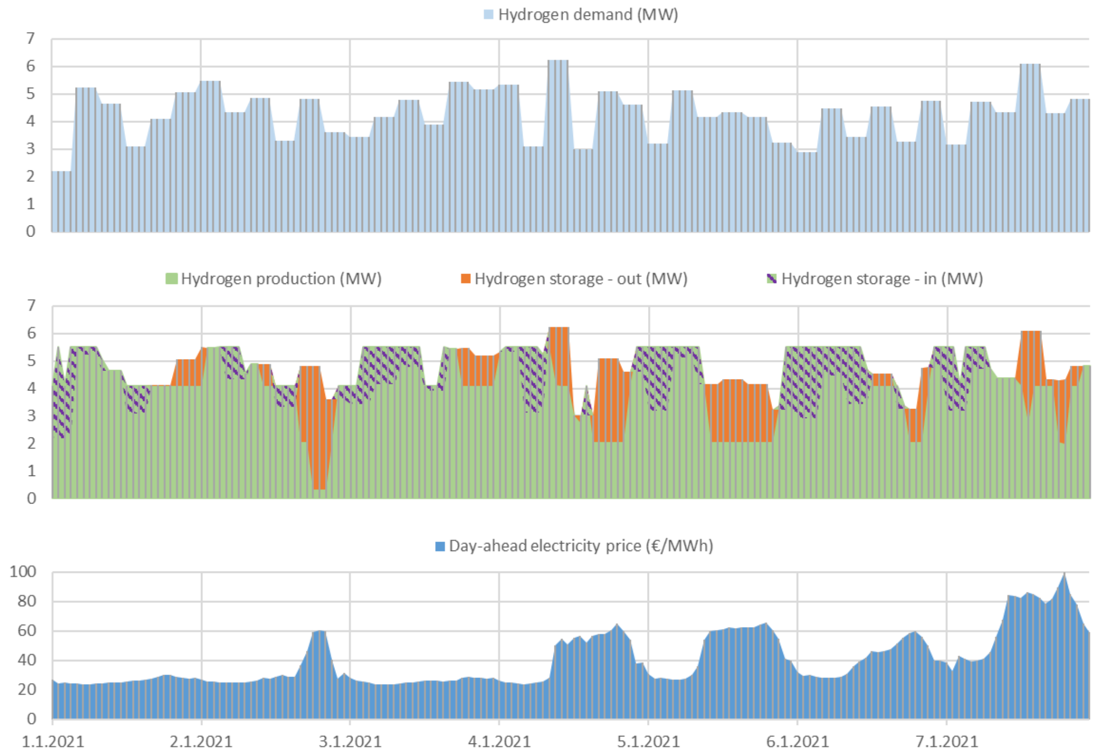

***Figure 6-1:** The main components of the profit of the P2H2 plant's hourly base operation in the first seven days of 2021.*

The Figure 6-1 shows how hydrogen production directly follows electricity prices and hydrogen demand. Based on these, optimizer determines the most reasonable hydrogen production time and the utilization rate of the storage. In general, the optimizer tends to unload storage during periods of high electricity prices. For example, on January 2, 2021, the cost of electricity has high peak, which is why the electrolyzers are directed to minimum production, and the demand for hydrogen is met mainly from storage. The optimizer does not turn off the electrolyzers at this point, as this would otherwise result in shutdown and start-up costs, in which case, according to the optimizer, the most reasonable production method in terms of costs is to keep them running. Unlike in the case of storage use, it can be noted from optimized production that hydrogen storage is generally filled at low electricity prices or before periods when electricity prices are expected to be high. In addition, it can be seen from the figure that storage also plays a significant role when the demand occasionally rises above the maximum capacity limit of the electrolyzers (5.49 MW). Such a situation is, for example, on January 4, 2021, when the demand for hydrogen is 6.23 MW, and the production of hydrogen is 4.10 MW, in which case the rest of the demand is handled through storage. The situation also shows how the optimizer decides to produce hydrogen with better efficiency (according to Figure 5-2) and higher storage utilization because the price of electricity is high at the time.

The figure also shows how the price of electricity follows the time of day, which is a typical phenomenon related to the balance of electricity demand and production. For example, the 4th, 5th, and 6th of January (Monday, Tuesday, and Wednesday) closely follow the pattern where electricity is more expensive during the day than at night. In this period, it is also noticeable how the optimizer plans the utilization rate of the storage in such a way that it is filled at night and used during the day, in which case hydrogen delivery can be guaranteed as cost-effectively as possible.

In terms of the research questions, it is essential to look at the value of the cost function of the optimization, which expresses the revenues generated by the plant. For the year 2021, the optimizer was able to generate a profit of approximately 5.25 million euros based on the given initial data and assumptions. For perspective, that year's average hourly electricity price was around €72. Correspondingly, for the year 2022, the optimizer was able to generate about 1.29 million euros as profit, while the average hourly electricity price was around €154. Between the years, electricity prices roughly doubled, and the income dropped to about a quarter of the 2021 result. Thus, the years represent very different productive periods.

6.2 P2H2 plant with increased production capacity

In the first research scenario, the effect of increasing capacity on the profitability of the operation of the investigated facility is considered. As presented in Chapter 5, the capacity increase is implemented with one AWE electrolyzer, which is identical to the existing units. In this optimization scenario, the demand for hydrogen is not increased, even though the increase in capacity would make it possible. Figure 6-2 shows, similar to Figure 6-1, the demand for hydrogen, the price of electricity, and the use of electrolyzers and storage in the first seven days of 2021.

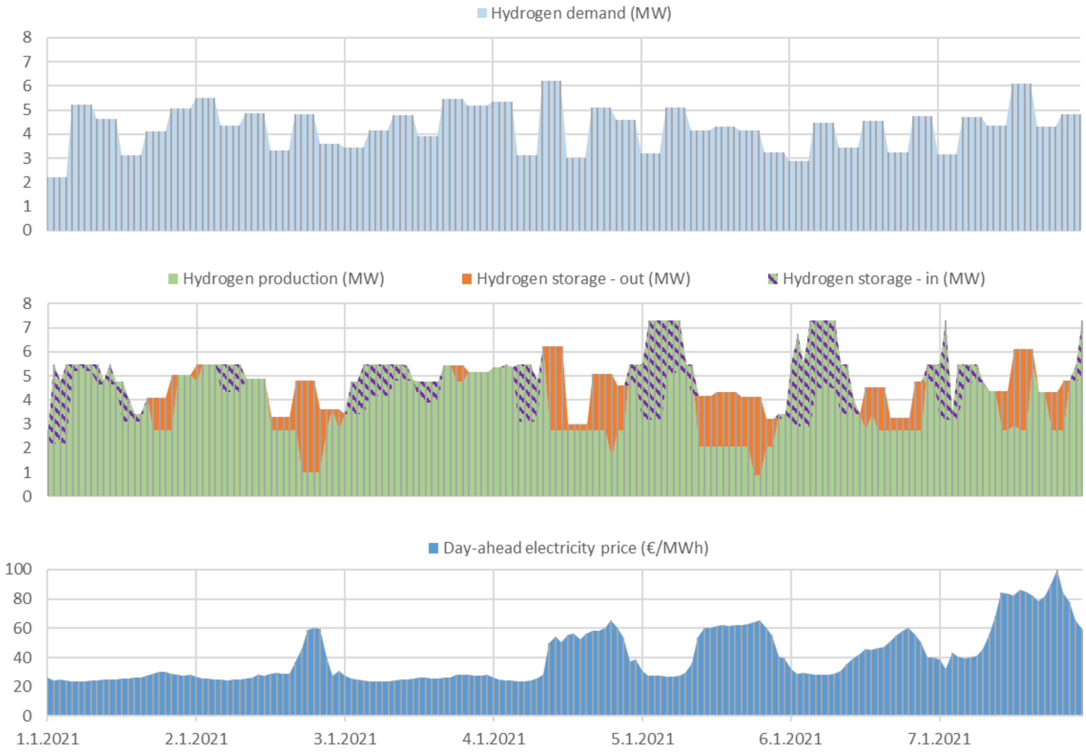

Figure 6-2: *The main components of the profit of the P2H2 plant's hourly capacity scenario in the first seven days of 2021.*

Based on the Figure 6-2, it can be seen that in this scenario, the storage can be loaded more often because, in addition to the production used for the demand for hydrogen, there is now more production capacity regarding the storage fill-up. Consequently, hydrogen production and storage use can be implemented more cost-effectively on, for example, the 5th and 6th of January. In addition to this, hydrogen production can be realized more profitably by running the electrolysis units in better efficiency ranges, as shown in Figure 5-2.

Due to the increased capacity, the revenue of the hydrogen production plant reached approximately 5.48 million euros in 2021 (previously €5.25 mill.), i.e., the revenue increased by about 4% with this production modification. Correspondingly, the revenue for 2022 was around 1.90 million euros (previously €1.29 mill.), which was an increase of around 48%. The biggest difference in this scenario comes from the difference between the night and day electricity prices in 2021 and 2022. The average daytime electricity price (between 10 am and 6 pm) in 2021 was around €87, while in 2022 it was around €186. The corresponding figures for electricity night-time prices (between 10 pm and 6 am) were around €52 and €108. Therefore, in 2021, the differences between the average day and night electricity prices were about €35, and in 2022 about €77. Thus, with a larger production capacity, the flexible hydrogen production enabled by the storage and efficiency ranges of the electrolyzers can be better utilized.

6.3 P2H2 plant with participation in the reserve market

The second research scenario examines the effects of participating in the electricity reserve market on the profitability of using the P2H2 plant. As presented in Chapter 5, the production plant can participate in the FCR-N, aFRR, and mFRR reserve markets, but in this work, only the participation in the last two markets is investigated. Figure 6-3 shows again through the first seven days of 2021 how the optimizer plans production when there is also the possibility of participating in the reserve market.

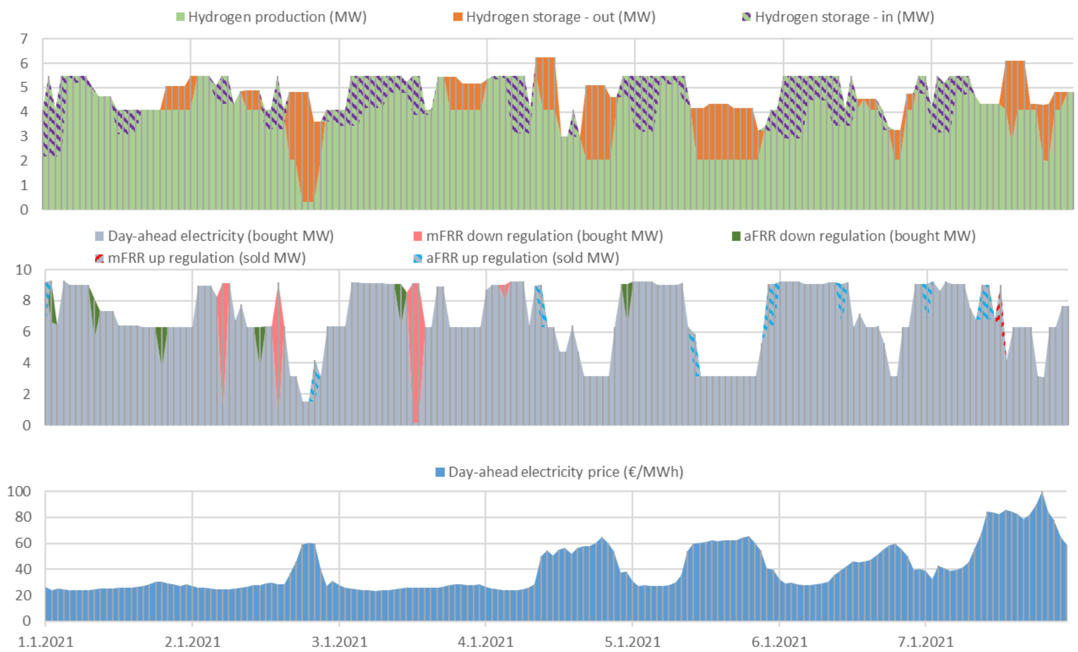

Figure 6-3: *The main components of the profit of the P2H2 plant's hourly reserve scenario in the first seven days of 2021.*

When interpreting the Figure 6-3, it should be noted that the optimization application knows, based on the initial data, at which points it has the opportunity to participate in the reserve market, as presented in Chapter 5. The optimizer seems to plan the hydrogen production in almost the same way as in the base scenario but sometimes uses up-and-down regulation products. These participations in the reserve market also affect the production of hydrogen and its storage, as can be seen, for example, from 2 January 2021 at 2 p.m. In this case, the facility participates in the grid's down regulation operation by increasing its own production and placing part of the excess production in storage. The middle section of the Figure demonstrates how the optimizer buys electricity sometimes from the Day-ahead market (grey area) and sometimes through aFRR (green area) or mFRR (light red area) down-regulation products. In addition, sometimes the optimizer sells part of the purchased Day-ahead electricity through aFRR (blue dash pattern) and mFRR (red dash pattern) up-regulation products back into the market, i.e., as in reality, leaves part of the purchased electricity unused and receives compensation for it.

As a result of participating in the reserve electricity market, the revenue of the P2H2 hydrogen production facility was approximately 5.45 million euros in 2021 (previously €5.25 mill.), i.e., compared to the base scenario, the facility's revenue increased by approximately 4%. Correspondingly, in 2022, the revenue generated for the production facility was approximately 2.01 million euros (previously €1.29 mill.), which means approximately a 56% increase in revenue compared to the base scenario. However, both of the obtained results are mainly indicative, as the uncertainty typical of the market cannot be fully modelled in the optimization based on historical data. This is especially emphasized in 2022 when, in the electricity market, alongside the high day-ahead prices, the prices of regulated electricity were also high. For example, in 2021, the average hourly price of mFRR down-regulation was around €61 (Day-ahead equivalent €72), so the profit per hour with this reserve product was around €11 on average. The corresponding indicators in 2022 were around €127 (Day-ahead €154) and around €27. Therefore, in 2022, participating in the reserve market had a greater weight in the optimization, in which case the yield obtained is not only double but significantly larger. In addition to mFRR products, the capacity prices of aFRR products also increased. For example, the average hourly capacity price of aFRR down-regulation increased from €25 to €120. In addition to this, it should also be noted that in aFRR products, in addition to the capacity price, the mFRR price is also paid for activations. Therefore, it can be concluded from the results that clear returns are also available in the reserve market. In terms of income, it should be noted that participating in the market does not require similar investments, such as increasing the production capacity or starting the production of district heating. Mainly, automation system applications' modifications are required.

6.4 P2H2 plant with district heat production

In the third and last research scenario, the effects of the sale of district heat generated from waste heat on the profitability of using the P2H2 plant are investigated. As presented in Chapter 5, a heat pump is added to the system. Through the heat pump, the sufficient temperature for the district heating network and the sale of district heat can be guaranteed all year round whenever the plant is running and the waste heat is generated. Figure 6-4 shows again through the first seven days of 2021 how the optimizer plans production when the system can also receive income from the sale of district heat.

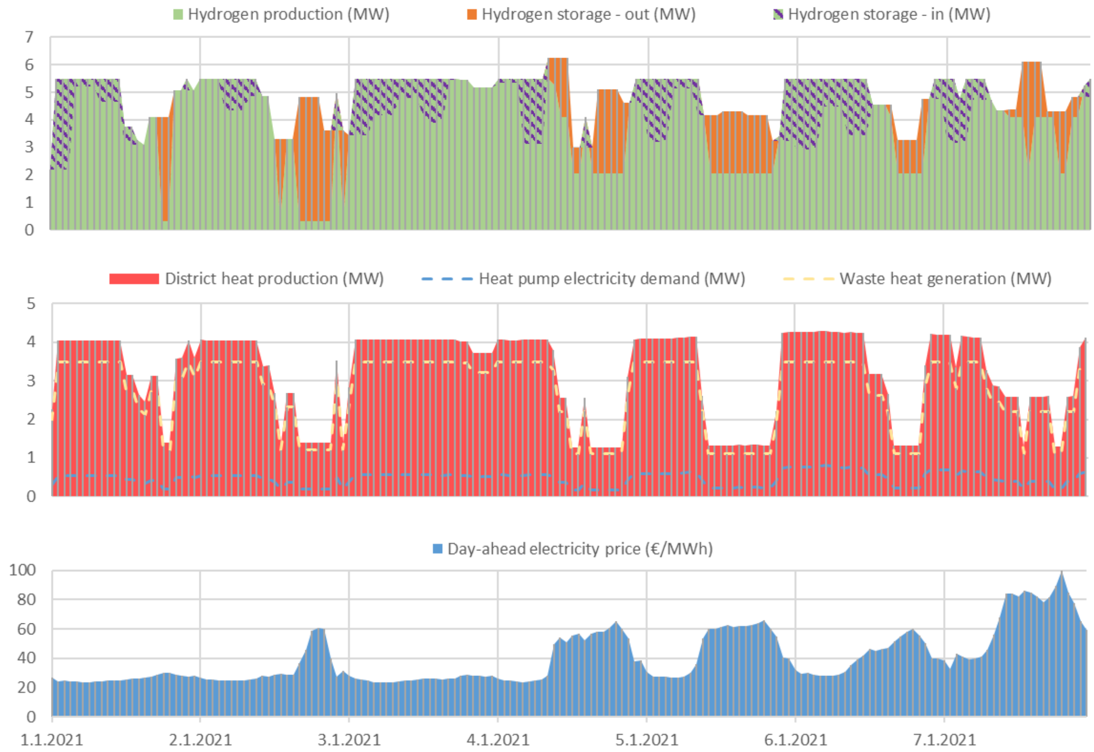

Figure 6-4: *The main components of the profit of the P2H2 plant's hourly district heat scenario in the first seven days of 2021.*

The Figure 6-4 illustrates well how the market made possible by district heating affects the hydrogen production model, which now consists of more uniform blocks than in the base scenario. In this situation, it makes sense to run the plant at maximum power more than before because the additional income from district heating is greater than the additional cost caused by the decrease in production efficiency. In this production model, hydrogen storage is still unloaded at high electricity prices, while filling takes place at low prices. Consequently, the production of district heat and the yield obtained from it smooth out the general operation of the plant. The production of district heat, on the other hand, naturally occurs along with the production of hydrogen, which can be seen from the correlation between the production of district heat (red area) and the formation of waste heat (yellow dashed line). The electrical power taken by the heat pump is marked with a blue dashed line, and it also shows that no district heating is produced in the considered season without the pump and that the power taken by the pump, therefore, directly follows district heat production.

The use of the heat pump was mainly timed for the intermediate and winter seasons when the waste heat did not meet the temperature demand of the district heating. However, the heat pump was also used in the summer season at times when the price of electricity was favourable. In this case, the district heat produced is fed and mixed into the district heating network with a higher flow, so it does not raise the temperature of the network. During the winter seasons, especially in 2022, the heat pump also had periods when it was not used, and district heating was therefore not produced. During these periods, the price of electricity was simply high enough to make district heat production unprofitable, even if it was generated from waste heat.

As a result of participating in the sale of district heating, the P2H2 production facility's revenue in 2021 was approximately 5.64 million euros (previously €5.25 mill.), which means that compared to the basic operating model, the facility's revenue increased by approximately 8%. Correspondingly, in 2022, the production facility increased its revenue by 22%, when the revenue received was approximately 1.57 million euros (previously €1.29 mill.). Thus, starting the production of district heating clearly brought additional income despite the difference in years. The higher percentage return obtained from 2022 can be explained by the fact that, based on the assumptions made, the district heat can be produced and sold when it is profitable because no quota amounts have been set for its demand (unlike hydrogen). In addition to this, inexpensive hydrogen production moments, when the situation cannot be compensated with storage, district heat production can prove to be an alternative that lowers the established costs. Therefore, meeting the demand for hydrogen in both 2021 and 2022 is more profitable compared to the base scenario due to the plant's increased efficiency as a result of the utilization of waste heat.

6.5 The monthly income structures of the scenarios

In the previous sections, the structure of the production plan formed by the optimizations, scenario-specific properties, and key figures created for the year were presented. In this section, the monthly income and cost structure of all the studied scenarios and their behaviour are examined. Table 6-1 shows the distribution of the net profit of each scenario by component, and the figures presented in it are in thousands of euros. Table 6-1 is formed from a more detailed table found in the appendix. In both tables, the start-up and shut-down costs of the electrolyzers and the heat pump are included in the cost of purchased electricity due to their marginal size and the clarity of the table. When interpreting the tables, it is good to note that the down-regulation products of the electricity reserve market are marked as costs because, in the modelled system, down-regulation electricity is purchased. Down-regulation electricity is, however, only purchased if it is cheaper than day-ahead electricity. Thus, the yield obtained is formed by the difference between the prices in question.

***Table 6-1:** The monthly income structures of the scenarios in thousands of euros, which is based on hourly optimizations.*

	Base scenario		Scenario 1 (Capacity)		Scenario 2 (Electricity reserve market)					Scenario 3 (District heating)		
Month	Hydrogen sales	Day-ahead electricity purchase	Hydrogen sales	Day-ahead electricity purchase	Hydrogen sales	Up regulation sales	Down regulation purchase	Day-ahead electricity purchase	Net electricity cost	Hydrogen sales	District heat sales	Day-ahead electricity purchase
1	780	243	780	235	780	12	10	232	230	780	69	260
2	697	231	697	224	697	10	10	218	218	697	62	249
3	757	167	757	162	757	11	6	161	156	757	43	175
4	737	155	737	150	737	11	6	152	147	737	40	159
5	740	197	740	187	740	12	5	193	186	740	19	197
6	764	252	764	234	764	13	5	246	238	764	19	253
7	765	365	765	347	765	27	12	360	345	765	18	364
8	761	314	761	302	761	22	9	311	298	761	19	314
9	740	396	740	377	740	16	6	400	390	740	36	396
10	744	255	744	231	744	20	7	248	235	744	40	257
11	747	346	747	307	747	29	10	352	333	747	59	349
12	759	822	759	757	759	64	36	794	766	759	48	846
Total profit 2021	5248 (base)		5478 (+4%)		5449 (+4%)					5644 (+8%)		
1	742	443	742	422	742	26	18	433	425	742	58	465
2	689	311	689	287	689	9	6	296	293	689	58	329
3	769	348	769	319	769	23	9	325	311	769	41	364
4	737	318	737	300	737	34	11	316	293	737	38	330
5	758	550	758	501	758	52	13	549	510	758	19	554
6	716	534	716	486	716	67	8	560	501	716	18	540
7	753	786	753	718	753	72	9	754	691	753	19	791
8	757	1031	757	913	757	128	29	1044	945	757	20	1042
9	730	833	730	722	730	95	12	793	710	730	37	844
10	769	493	769	455	769	50	-14	471	407	769	42	496
11	721	817	721	770	721	85	18	808	741	721	40	826
12	713	1104	713	1060	713	70	21	1071	1022	713	27	1116
Total profit 2022	1286 (base)		1901 (+48%)		2005 (+56%)					1574 (+22%)		

The Table 6-1 shows that the electricity purchased for production is at a significantly different level in 2021 and 2022, while the sale of hydrogen remains the same. When viewed on a monthly basis, the purchased electricity goes directly according to the day-ahead price of electricity shown in Figure 5-4. In scenarios 2 and 3, it is possible to influence the costs of electricity by scheduling production and participation on the electricity reserve market. This can be seen in both scenarios as a lower electricity purchase (in scenario 2, net electricity cost). In scenario 2, the benefit from the electricity reserve market is included under net electricity cost for comparability. In scenario 3, electricity is also used to operate the heat pump, in which case the advantage achieved is not directly visible in the purchased electricity. However, the income generated from the sale of district heating is a clear additional income, which was greater than the increased electricity procurement. This is also reflected in the total profit.

The income structure of scenario 1 is almost similar to the base scenario, with the difference that there are fewer costs sunk into the purchase of electricity. In scenarios 2 and 3, on the other hand, the income structure changes clearly due to participation in new markets. The electricity reserve market exhibits largely the same phenomena as the day-ahead market. From the table, this can be seen from the fact that during high and low electricity day-ahead prices, the trade on the reserve market is also at a similar level. One anomalous situation in Table 6-1 occurred in October 2022. In this case, the negative cost of down-regulation products is due to the aFRR market, where the price is determined by the sum of the down-regulation electricity to be purchased and the capacity reservation to be paid. In this instance, due to the low down-regulation price, the price paid for participating in the capacity reservation event turns the cost into profit. The sale of district heating, on the other hand, behaves in its own way and is linked to the outside temperature and seasonal district heating sales price in addition to electricity prices. This can be seen from the high yield obtained in the winter and the correspondingly low yield obtained in the summer. The effect of the price of electricity can also be seen, for example, in the winter of 2022, when the use of the heat pump was expensive and, therefore, the yield obtained was comparatively lower than in the previous year.

Each of the studied scenarios improves the profitability of using the facility. In 2021, the most additional income came from the sale of district heating, while the additional production capacity and participation in the electricity reserve market were equally profitable. In 2022, the importance of each addition to the facility was emphasized. In this case, participation in the reserve market brought the most additional income, then capacity increase, and lastly, the sale of district heating.

7. CONCLUSIONS

The purpose of the work was to carry out a profitability study of the Power-to-Hydrogen (P2H2) production plant. The study examined the effects of three different production scenarios on the plant's profits. The scenarios were increased production capacity, participation in the electricity reserve market, and the selling of district heat generated from waste heat. To support the understanding of the operation of the production facility, the work also carried out a comprehensive literature review of the Power-to-X (P2X) concept. Through the literature review, an effort was made to study the markets that drive the industry forward, as well as entities belonging to the industry. The examined entities were divided into two parts, which were the P2X operating field and its more limited entity, the P2H2 model. In addition to these, the work reviewed the basics of optimization with mixed-integer linear programming (MILP) and introduced two studies that utilized MILP-based optimization in a similar way as in this work.

The profitability study of the P2H2 production facility was conducted for Valmet Automation Oy in cooperation with Energy Opticon AB, Woikoski Oy, and Tampereen Energia Oy. The research was carried out with the Energy Optima 3 (EO3) optimization application from Energy Opticon AB. The optimization application served as a research platform on which the examined P2H2 production plant was modelled and with which the presented research questions were answered. Woikoski Oy helped with the modelling of the hydrogen production plant by providing important initial data for the research as well as plant and production dimensions. Tampereen Energia Oy, on the other hand, assisted in determining the price of the district heating purchased by an energy company. Some of the initial information was also taken from the literature.

For the research, a variety of initial data was needed for the P2H2 production plant and its operations, which were divided into three areas. The first of these was the P2H2 plant, where information was needed for the alkaline (AWE) electrolyzers, hydrogen compressor, hydrogen storage, hydrogen demand, and the power purchase agreement. The second area consisted of the information needed for the reserve market, which in turn concerned the automatic frequency restoration reserve (aFRR) and the manual frequency restoration reserve (mFRR) regulation products. The last area consisted of the initial data needed for the heat pump and district heating demand.

The research was executed with year-long production optimizations with an hourly resolution, which were meant to describe long-term profits, and which are affected by the year's fluctuations, such as electricity prices and the required district heating. The optimizations were executed for the years 2021 and 2022, the first of which represents a relatively steady period in terms of day-ahead electricity prices. The year 2022, on the other hand, was exceptionally variable regarding the electricity prices, which made it possible to compare the profitability of the production plant between very different years. The research results obtained for the years are presented in Table 7-1. The presented revenues have been calculated based on the sale of hydrogen, electricity reserve markets, and district heating, and the purchase of electricity used for the plant's use. When looking at the results of this work, it is good to note that the forecasts used by the optimizer for electricity purchase, hydrogen demand, and district heat sales do not contain uncertainties, which are nevertheless part of real production planning. These uncertainties include, for example, electricity prices deviating from forecasts and unexpected fluctuations in demand for hydrogen and district heating.

The base scenario of the P2H2 production plant was used as a reference point for the research scenarios, the production planning of which was also implemented with the EO3 optimization tool. As can be seen from the results in Table 7-1, the profit of the production plant is at a very different level in 2021 and 2022. The only difference between the years is the day-ahead electricity price, which serves as the plant's power purchase agreement in this work. The average hourly price of electricity was slightly more than double in 2022, which is why the yield obtained was also clearly lower. In general, the difference between night and day electricity prices is quite large and in 2021 it was around €35, while in 2022 it was exceptional as it was around €77.

The effect of the first research scenario, i.e., increasing the production capacity, was clear, especially in 2022. As in the other scenarios studied, the only change to the basic layout was the added feature. Thus, although the production capacity was increased in this scenario by one electrolysis unit, the demand for hydrogen did not change. However, with a larger production capacity, hydrogen can be produced in a better efficiency range of the electrolyzers, and the available storage can be filled more efficiently during times of lower electricity prices. In this case, the difference between night and day electricity prices is also emphasized. In 2022, with exceptionally high and fluctuating electricity prices, the flexible use of storage and production will make a significant difference in the resulting costs, as seen from the results.

In the second studied scenario, where the production facility participated in the electricity reserve market (aFRR and mFRR products), the returns obtained are similar to the first scenario, highly dependent on the year. The additional profit gained in 2021, which describes a normal year, was very moderate, but in 2022, it was possible to benefit from very high regulation prices in the electricity market. In contrast to the other studied scenarios, participating in the reserve market would not require large investments and, therefore, careful planning of payback periods. Thus, participating in the reserve market could be characterized as a strategic project with a lower entry threshold than others because only automation system modifications are required.

In the last research scenario, i.e., district heating generated from waste heat, the yields compared to the basic operation were more even between the reviewed years than in the other research scenarios. When running a hydrogen production plant, a relatively large amount of waste heat is generated. The best efficiency of the used AWE electrolyzers (when running mid-load) was only about 65%, which means that about a third of the electrical power used was converted into heat. Therefore, the waste heat recovered and processed according to the need (district heat demand) increases the overall efficiency of the production facility. The waste heat converted and sold as district heat is not directly able to benefit from the electricity market situation in the same way as the two previous scenarios. However, through the improved efficiency of the plant, the district heat sales affect the production planning and the revenues, the positive effect of which can be seen in the results of Table 7-1.

Table 7-1: *The profitability of the studied research scenarios and average hourly day-ahead electricity price per year.*

	Profit per year (million EUR)		
	2021	**2022**	**Main benefit**
Base scenario	5.25	1.29	-
Research scenario 1 (Capacity)	5.48 (+4%)	1.90 (+48%)	Brings flexibility to the plant's operation
Research scenario 2 (Reserve market)	5.45 (+4%)	2.01 (+56%)	Is a low-threshold investment
Research scenario 3 (District heat)	5.64 (+8%)	1.57 (+22%)	Improves plant's overall efficiency
Average hourly day-ahead electricity price per year (€/MWh)	72	154	-
Average difference between day and night electricity prices per year (€/MWh)	35	77	-

Based on the results, it can be stated that each presented scenario would increase the income generated from the use of the production facility. Each scenario is an advantageous and profitable investment in its own way when the production is planned with optimization and the process is controlled accordingly. Increasing production capacity brings flexibility to the plant's use, participating in the reserve market is a low-threshold investment, and selling district heat improves the plant's overall efficiency.

The research done and the tools used provided useful information about running the plant and its components, such as the meaning of the power purchase agreement and the possibilities of the three studied scenarios for the production plant. However, along with the research, limitations must be made, and the objects to be researched must be pruned. In this work, the importance of hydrogen storage in production planning was emphasized, and the variation of its size could be a lucrative subject for further research. In addition to varying the size of the storage, the inclusion of methanol, methane, and ammonia production, as well as CCUS technologies as part of the optimization model, would open up many new and topical further research targets. Other relevant research subjects could also be the study of the investments required for the scenarios and the related payback periods, the analysis of the increase in hydrogen demand made possible by the growth in production capacity, and the analysis of the effects of various district heating sales contracts.

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APPENDIX:

The comprehensive table of the monthly net income distributions of the scenarios, which is based on hourly optimizations

	Base scenario			Scenario 1 (Capacity)			Scenario 2 (Electricity reserve market)								Scenario 3 (District heating)			
Month	Hydrogen sales	Day-ahead electricity purchase	Profit	Hydrogen sales	Day-ahead electricity purchase	Profit	Hydrogen sales	mFRR up regulation sales	aFRR up regulation sales	mFRR down regulation purchase	aFRR down regulation purchase	Day-ahead electricity purchase	Net electricity cost	Profit	Hydrogen sales	District heat sales	Day-ahead electricity purchase	Profit
1	780	243	537	780	235	545	780	2	10	8	2	232	230	550	780	69	260	589
2	697	231	466	697	224	473	697	4	6	9	1	218	218	479	697	62	249	510
3	757	167	590	757	162	595	757	3	8	6	0	161	156	601	757	43	175	625
4	737	155	582	737	150	587	737	5	6	5	1	152	147	590	737	40	159	618
5	740	197	543	740	187	553	740	4	8	4	1	193	186	554	740	19	197	562
6	764	252	512	764	234	530	764	4	9	4	1	246	238	526	764	19	253	530
7	765	365	400	765	347	418	765	9	18	10	2	360	345	420	765	18	364	419
8	761	314	447	761	302	459	761	9	13	7	2	311	298	463	761	19	314	466
9	740	396	344	740	377	363	740	4	12	2	4	400	390	350	740	36	396	380
10	744	255	489	744	231	513	744	8	12	3	4	248	235	509	744	40	257	527
11	747	346	401	747	307	440	747	10	19	6	4	352	333	414	747	59	349	457
12	759	822	-63	759	757	2	759	46	18	22	14	794	766	-7	759	48	846	-39
Total 2021	8991	3743	**5248**	8991	3513	**5478**	8991	108	139	86	36	3667	3542	**5449**	8991	472	3819	**5644**
1	742	443	299	742	422	320	742	12	14	11	7	433	425	317	742	58	465	335
2	689	311	378	689	287	402	689	3	6	4	2	296	293	396	689	58	329	418
3	769	348	421	769	319	450	769	8	15	5	4	325	311	458	769	41	364	446
4	737	318	419	737	300	437	737	22	12	7	4	316	293	444	737	38	330	445
5	758	550	208	758	501	257	758	20	32	8	5	549	510	248	758	19	554	223
6	716	534	182	716	486	230	716	41	26	4	4	560	501	215	716	18	540	194
7	753	786	-33	753	718	35	753	36	36	13	-4	754	691	62	753	19	791	-19
8	757	1031	-274	757	913	-156	757	60	68	25	4	1044	945	-188	757	20	1042	-265
9	730	833	-103	730	722	8	730	52	43	24	-12	793	710	20	730	37	844	-77
10	769	493	276	769	455	314	769	16	34	10	-24	471	407	362	769	42	496	315
11	721	817	-96	721	770	-49	721	40	45	16	2	808	741	-20	721	40	826	-65
12	713	1104	-391	713	1060	-347	713	36	34	10	11	1071	1022	-309	713	27	1116	-376
Total 2022	8854	7568	**1286**	8854	6953	**1901**	8854	346	365	137	3	7420	6849	**2005**	8854	417	7697	**1574**