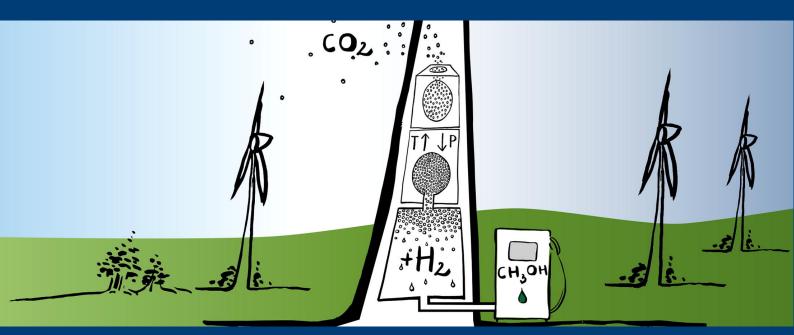
The role of power-to-methanol technologies in the energy mix

# K. Afzali

Investigation of the impact of stimulating power-to-methanol technologies on reliability of the Dutch power grid and CO<sub>2</sub> reduction





# The role of power-to-methanol technologies in the energy mix

by

# K. Afzali

Master thesis submitted to Delft University of Technology, in partial fulfillment of the requirements for the degree of Master of science in Complex Systems Engineering and Management, Faculty Technology, Policy and Management to be defended publicly on Thursday August 24, 2020 at 11:00 AM. Student number: 4902130 Project duration: February 10, 2020 - August 24, 2020 Thesis committee: Dr. ir. L. Stougie, TU Delft, supervisor Dr. A. F. Correljé, TU Delft, chair Ir. G. Dahm RoyalHaskoningDHV RoyalHaskoningDHV Ir. P. Katakwar,

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## Preface

In front of you lies my thesis which I fulfilled as a partial requirement to obtain my Masters degree in Complex Systems Engineering and Management. This research is conducted in order to explore the possible future impacts of deploying power-to-methanol technologies. The research was carried out in collaboration with Royal HaskoningDHV as a graduation internship, from February to August, 2020.

Introducing a new technology into the market, especially a technology which has an impact on a large scale, always comes with uncertainty and risk. Regarding power-to-methanol technologies, the production scale is normally high and hence, the power demands are high. In case power-to-methanol technologies are widely deployed, it has considerable implications for the power grid, the investors in renewable power supply and other large power consumers. Besides electricity, other building blocks like hydrogen production and CO<sub>2</sub> supply should be stacked in order to realize the technology. All these steps are entangled with the availability of infrastructure. On top of the technical system, several actors have stake and are making decisions in this context. These actors have various and occasionally conflicting interests and powers. The dynamic ecosystem that is created from the interdependence of actors and technologies evolves into the future states of the system. The tools and methods I acquired in the CoSEM program helped me to a great extent to capture the complexities involved in this highly complex, socio-technical problem.

I am honored and pleased to work with amazing, experienced and friendly colleagues in RoyalHaskoningDHV. During a period that we were all required to stay home, I missed the experience of working in an office but the many insightful and eye-opening discussions I had with the experts in-house fulfilled my goal to do a professional work. I would like to specially thank Piyush Katakwar for all his sincere support from the very beginning of the project to the very end of my journey as a graduate intern. I express my gratitude to Gertjan Dahm for providing his inputs, monitoring my progress and guiding my thoughts with his experience.

I should thank Lydia Stougie, my supervisor, for her eye-for-detail and her contribution in defining the right problem. I am thankful for her patience when I shifted my scope several times and for the freedom she gave me in formulating my research. I thank Aad Correljé for chairing the graduation committee and for pushing me to unravel the theoretical background of interview results.

Finally, I thank my family and my friends for their continuous support and positive vibes when I was tired, disappointed or demotivated.

I hope you enjoy the insights this report brings to you.

K. Afzali Delft, August 2020

### Executive summary

The government of the Netherlands has long been supporting development of renewable power production in order to meet carbon reduction goals set in the "klimaatakkoord". High penetration of renewable power production is beneficial for decarbonization of the power system, though might have a negative impact on the reliability of the power grid. Renewable power production varies not only on a day-to-day basis but also seasonally. Large-scale storage systems complement renewable power production by compensating volatility of renewables. Power-to-methanol technology is a category of Power-to-X technologies that can be used to store electrical energy into chemical molecules. Power-to-methanol technologies make use of power-tohydrogen (water electrolysis) as the first step to store electrical energy in a chemical medium. Methanol has a potential to be used as an alternative low-carbon fuel in the transport sector. In this way, decarbonization goals of the transport sector can be met easier.

While energy storage in a substance like methanol can allow decarbonization of other sectors, the question of whether the power grid remains reliable after large scale deployment of power-to-methanol technologies, is not comprehensively answered. Furthermore, there is a debate about the role that power-to-methanol technologies and the technologies alike can play in the course of decarbonization. In fact, little is known about the system level impact of power-to-methanol deployment in the future.

This research addresses the above mentioned gaps in the understanding of power-to-methanol technologies gies. The main question answered in this research is: *How does deploying power-to-methanol technologies influence the power grid's reliability and CO<sub>2</sub> emission reduction in the Netherlands until 2050?* To answer this research question, first the drivers for and barriers to deployment of power-to-methanol technologies are identified from literature review and expert interviews. As the next step, the impact these factors can have on the reliability of power grid and CO<sub>2</sub> emission reduction is studied using a quantitative model. The primary sector demanding the methanol as an alternative low-carbon fuel is assumed to be the shipping sector. An agent-based model is developed to link and combine technical and social aspects of the problem. The model outcomes are explored using two sets of experiments. These two experiments simulate two hypothetical cases: "flexible grid" experiments in which the power grid is assumed to have several flexibility options, e.g. batteries and demand response, and "low flexibility grid" experiments in which the grid cannot easily adapt to high levels of renewable power production. For a flexible grid, as more renewable power supply is realized, the surplus hours increase moderately. For a grid with low flexibility, however, surplus hours increase greatly when more renewable power is realized.

In general, it can be concluded that deploying power-to-methanol technologies has a considerable influence on power grid's reliability. Results of all experiments show that the yearly balance of demand and supply of renewables oscillates sharply, which indicates bad conditions for the reliability of power grid. The faster the growth rate of renewable power production, the sharper and more frequent the variations become. The desirable state for the power grid is to have a rather constant balance close to zero. Without any power-tohydrogen and power-to-methanol technology being realized, grid balance will rise proportional to the rise in renewable power production capacity. These technologies do have an effect in containing the growth of grid balance, though they cannot be considered as the only flexibility solutions for the power grid. Another aspect studied in the experiments is CO<sub>2</sub> reduction. Results show that deploying power-to-methanol technologies could contribute to achieving climate goals. The sequence of events is roughly similar in all experiments. Up until 2027 when the carbon capture utilization and storage (CCUS) network is realized, no CO<sub>2</sub> reduction is observed. From 2027 onward, industries begin to capture their emissions. Within a couple of years, the capacity of the CCUS network is fully utilized while some industries have not yet (fully) captured their emission. The CCUS network remains full unless CO<sub>2</sub> is extracted from the network for utilization in powerto-methanol process. As a result, before power-to-methanol becomes attractive for investors, CO<sub>2</sub> reduction has an upper bound equal to the capacity of CCUS network. Power-to-methanol technologies begin to pay off only around 2040. When power-to-methanol technologies are widely deployed, there is a three-fold impact on CO<sub>2</sub> reduction. First and foremost, power-to-methanol process creates a demand for CO<sub>2</sub> and hence, more industries will capture their emissions. Second, it funds green hydrogen production. The green hydrogen can be directed to the industry to substitute gray hydrogen and hence, save CO2 emissions from hydrogen production in the industry. Last but not least, in some cases more methanol is produced than demanded as fuel. Therefore, green methanol can flow to the chemical industry to replace normal methanol which is produced in a carbon-emitting process. Considering fulfillment of carbon reduction goals, in some circumstances it is possible to achieve carbon reduction goals only by deploying power-to-methanol technologies. However, power-to-methanol technologies are not helping with the 2030 reduction goals.

To put it in a nutshell, deployment of power-to-methanol technologies can help to contain renewable energy grid balance and hence improve power grid's reliability to some extent, but it cannot be considered as the only alternative to make the power grid reliable. On the other hand, power-to-methanol technologies can greatly help in meeting carbon reduction goals in the industry. It is important to note this research is one piece of the puzzle to clarify the steps that should be taken for a smooth and effective energy transition. This research can be replicated to study the role of other Power-to-X options. The comparison of studies on different Power-to-X options is more conclusive of the decision to be made by respective actors. Furthermore, this research focuses on the production side, whereas the demand side is an equally powerful lever of the development. Future research can include the dynamics of demand side, too. Finally, market models for green hydrogen and methanol can provide new insight into the economic aspects of the development.

# Glossary

**CAPEX** Capital Expenditure on an investment.

- **CCS** Carbon Capture and Storage.
- CCU Carbon Capture and Utilization.
- CCUS Carbon Capture, Utilization and Storage.
- E-fuel Product of Power-to-X process which can be used as a fuel.

Green methanol The product of power-to-methanol process when renewable power is used.

Green hydrogen The product of power-to-hydrogen proccess when renewable power is used.

NPV Net Present Value.

- **OPEX** Operational Expenses of a technology.
- Power-to-X Process which uses electrical power to synthesize a chemical substance X.
- PtM Power-to-Methanol.

PtX Power-to-X.

**RE grid balance** The amount of renewable energy available for power production deducted by energy produced by conventional power plants.

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# 1

### Introduction

This chapter provides the background information for the report.

#### 1.1. Need for energy storage

Penetration levels of renewable energy sources are gradually increasing worldwide in an attempt to transition to a more sustainable energy mix (Habib, Sou, Hafeez, & Arshad, 2018; Hadjipaschalis, Poullikkas, & Efthimiou, 2009). Renewable power is uncontrollable and is highly volatile throughout the year. Some days no wind blows and some days are stormy, sometimes sun shines the whole day and sometimes there is no sunshine for weeks in a row. In contrast to renewable power, conventional power production (based on fossilfuel) is controllable and predictable. Controllability of conventional power plants aids the system operator to balance demand and supply and maintain power grid's reliability. Whenever needed, the system operator can ramp up or ramp down the conventional power plant units in order to meet the demand. Although conventional power plants were playing a major role in the power system in the past decades, the Dutch government aims to gradually phase out coal and gas power plants in light of the climate agenda.

Phasing out conventional power plants results in a higher "renewable penetration level", i.e. ratio of renewables to the total power production. Volatility of renewables at high penetration levels causes problems such as periods of power shortage as well as periods of oversupply, and close-to-zero prices that reduce the return on investments (Habib et al., 2018; Tremel, 2018). At high penetration levels, if there is a lack of supply the grid runs a risk of unmet demand. The grid is then considered as "unreliable" from the perspective of consumers. If there is oversupply, however, "curtailment" of renewables is the option for system operator. Curtailment refers to the situation in which renewable power production units are asked to maintain zero power output even though plenty of renewable energy is available. Curtailment of renewable power generation units as a method to manage renewable power supply is not the best way to utilize the investments in renewable power supply. From a system perspective, curtailment is a lost opportunity.

Unless there is a way to flatten the renewable supply curve, the power system relies on conventional power plants to maintain security of supply. As a result, complete phase out of conventional power plants would seriously affect security of supply and the grid stability. One way to flatten the curve is to plan for large scale storage systems, which can store energy when there is more generation than demand, and utilize the energy when there is a lack of supply.

#### 1.2. E-fuels as energy storage medium

One storage method is to store the energy of electrons into a chemical form (Decker, Schorn, Samsun, Peters, & Stolten, 2019). This could be done through Power-to-X (PtX) processes. The "X", i.e. the output of PtX process, can be a fuel, in which case it is called "E-fuel" or electrofuel. E-fuels could be combusted later to generate electricity or be employed in another application, e.g. transportation (Bellotti, Sorce, Rivarolo, & Magistri, 2019). In this way, the synergies between power sector and other sectors will be exploited and the segregated energy system of today can be integrated (Connolly, Lund, & Mathiesen, 2016). Studies suggest that among all storage techniques, the largest storage capacity, the lowest discharge rate and lowest storage costs could be achieved by E-fuels (Bargiacchi, Antonelli, & Desideri, 2019; Connolly et al., 2016).

Besides the main use of E-fuels as seasonal energy storage (FCH JU, 2019), the produced E-fuel can be used for other purposes. It can be reconverted to electricity in combined heat and power units, where the heat is also utilized for district heating (Connolly et al., 2016). Aviation and maritime sectors are also potential users of E-fuels as low or zero carbon alternatives (Blanco, Nijs, Ruf, & Faaij, 2018; Schemme, Samsun, Peters, & Stolten, 2017). Finally, most of the E-fuels, such as methanol and ammonia, can serve other industries as feedstock (Bellotti et al., 2019; Räuchle, Plass, Wernicke, & Bertau, 2016). By supplying E-fuels to other sectors, the renewable energy is directed to the sectors that are facing difficulty for electrification.

#### 1.3. Green hydrogen and organic E-fuels

Hydrogen produced from water electrolysis is a substance that can store electrical energy. If the power comes from renewables, it is called "green hydrogen". The current process for hydrogen production is steam methane reforming (SMR) which emits  $CO_2$  in the air. The product is hence called "gray hydrogen". Hydrogen has a high energy value. Combustion of unit mass hydrogen releases 2.5 times as much energy as is released from combustion of natural gas. Hydrogen can be reconverted to electricity using fuel cells. Furthermore, hydrogen can potentially be used as transport fuel and for domestic heating Blanco et al. (2018). It allows integration of power sector with heating and transport.

Hydrogen economy, however, faces two major barriers. First of all, production and transportation of hydrogen requires expensive infrastructure. As a result, individual investors are reluctant to invest. Besides, end user technologies for the use of hydrogen for transport and heating are only in demonstration phase. Finally, upfront costs of electrolysers are high as well as operation and maintenance costs. Even though a well-though regulatory framework can trigger the developments, regulation in EU have not been successful in this regard yet (Blanco et al., 2018).

Hydrogen can be converted to other substances, producing hydrogen-based E-fuels, that allows storing the energy of green hydrogen in another form. According to Bargiacchi et al. (2019), the most promising hydrogen-based E-fuels are methane, methanol and ammonia. These chemicals are widely used in the industry and have well-established markets. Meanwhile, new demand is created by initiatives in transportation -e.g. in the shipping sector- to replace conventional fuels with low-carbon alternatives such as methanol. Methanol and ammonia can be easily used in internal combustion and diesel engines with some modifications of combustion technology (Grinberg Dana, Elishav, Bardow, Shter, & Grader, 2016). In essence, E-fuels penetrate the barrier green hydrogen faces with respect to end user technologies.

Methanol is a widely used chemical and a promising fuel for heavy duty transportation. Recently in the

Netherlands, a consortium of leading international maritime companies have joined forces in the Green Maritime Methanol project to study "green methanol" as an alternative bunker fuel. Green methanol refers to the product of CO<sub>2</sub> hydrogenation process using green hydrogen. In contrast to conventional method of methanol production from natural gas, green methanol production shows a potential to contribute to CO<sub>2</sub> reduction (Bargiacchi et al., 2019). Compared to ammonia and methane, methanol transportation is easier because it is liquid at room temperature. The extra, energy consuming step of liquefaction which should be taken for hydrogen, ammonia and methane transport, is not necessary for methanol. Furthermore, methanol is a widely used feedstock for the chemicals industry, for example in the production process of ethylene and acetic acid (Bellotti et al., 2019; Räuchle et al., 2016). Finally, the industrial process to produce methanol is mature and is utilized in large-scale (Schnuelle et al., 2019; Tremel, 2018).

Given the potential of green methanol to serve as energy storage medium, its potential to couple power and transport sectors and the promise of helping with CO<sub>2</sub> reduction, this research focuses on the role of green methanol and Power-to-Methanol (PtM) technologies in the energy system.

#### 1.4. System level effects of power-to-methanol

In general, E-fuel production creates a variable load on the electricity grid. The production can start when there is excess energy available and stops when there is lack of supply. For methanol in particular, there is a possibility to use it as transport fuel or as feedstock in the industry. In this way, it enables coupling of sectors. Since different sectors have different energy demand profiles, sector coupling increases power demand flexibility (Connolly et al., 2016). Using power-to-methanol technologies, renewable energy is stored in times of abundance and diverted to other sectors. The adverse effects of renewable oversupply can thus be limited. Moreover, power-to-methanol can have an influence on  $CO_2$  emissions from the energy system. Studies have argued that production of methane and methanol can potentially contribute to meeting carbon abatement goals (Bargiacchi et al., 2019; Decker et al., 2019; Koytsoumpa, Bergins, & Kakaras, 2018). In addition, study shows that ambitious levels of  $CO_2$  reduction is not achieved without E-fuels in the energy mix (Bellocchi et al., 2019). In fact as explained in section 1.1, if energy storage technologies such as E-fuel production are not available, conventional power plants cannot be abandoned. Therefore, carbon abatement in the power sector cannot go beyond a certain limit if the focus is only on renewable power generation and not on storage.

Power-to-methanol technologies, however, are not beneficial to deal with shortage of renewable supply. Although methanol can be reconverted to electricity using fuel cell or in power plants (Grinberg Dana et al., 2016), the round-trip efficiency (i.e. the ratio of released energy to the energy consumed for storage) is limited by the efficiency of re-conversion step (McDonagh, Wall, Deane, & Murphy, 2019). Moreover, the influence of a large-scale deployment of these technologies on critical infrastructures such as the power grid might rebound: the grid will be exposed to extra load from power-to-methanol. As a result, green methanol production which was, once, contemplated to resolve curtailment issue, might be harmful to the grid in another way. On the other hand, the need for  $CO_2$  raises a concern in terms of transition speed: green methanol production maintains the demand for  $CO_2$  as a feed and finances the continuous operation of  $CO_2$  rich processes. This results in a lock-in state and makes substitution for sustainable processes difficult (Decker et al., 2019), unless direct-air-capture methods become economically feasible. Finally, if green methanol is used in other sectors, such as in transportation, the problem is that the fuel is combusted and  $CO_2$  is released in the atmosphere again.

#### 1.5. Knowledge gap

The positive effects of power-to-methanol presented in section 1.4 will not be achieved unless power-tomethanol technologies reach a sufficient scale in production capacity. As any solution in the context of energy transition, scale up of power-to-methanol technologies is a joint effort among different actors and can result from massive investments in technologies and infrastructures. The coordinated move of actors is shaped by proper regulatory framework and support mechanisms. However, as with any new technology, the future perspective for power-to-methanol technologies is blurred. This lack of insight affects the private sector considering production or consumption of green methanol. It also hits public authorities in terms of decision making about the required regulations or supports.

There are many uncertainties regarding the future of energy system including power-to-methanol technologies. As a result, decisions are postponed to a later time and development is stagnated. Meanwhile, the policy makers are not sure if E-fuel production must be stimulated or not. There seems to be a lack of insight about the potential pathways that the energy system might take in the future if green methanol production is largely deployed. In this research, the knowledge gap regarding the influence of power-to-methanol technologies on the power grid and on  $CO_2$  reduction is addressed. Other influences that deployment of power-to-methanol technologies can have on the energy system are not discussed in this research, due to time limitations.

#### 1.6. Report outline

The rest of this document is organized as follows: In chapter 2, the research setup is presented, including the research questions, research methods and the scope. Chapter 3 presents the system description based on the scientific literature and business reports. In chapter 4, interviews are analyzed to identify drivers of power-to-methanol technologies. In chapter 5, the elements of the model is elaborated upon, with an explanation of assumptions, inputs, outputs and model logic. In chapter 6, the results of simulations are presented. First of all, important drivers of power-to-methanol technologies are identified using the model. Furthermore, the dynamical behavior of grid balance and CO<sub>2</sub> reduction is simulated and presented. In chapter 7, conclusions are drawn and are discussed. Finally, recommendations are made for academy and business.

# 2

### **Research setup**

In this chapter, the research objective, research questions and research approaches are outlined. Furthermore, the research methods, data analysis methods and the limitations of the approach are discussed. Finally, the scope of the project and the key performance indicators are specified and the research flow is presented.

#### 2.1. Research objective and social relevance

The main objective of this research is to explore the range of dynamics in the power grid's reliability and  $CO_2$  emission reduction in the Netherlands, should power-to-methanol technologies be deployed. This exploration informs policy making for power-to-methanol, providing a comprehensive insight into the possible future states of the energy system when power-to-methanol technologies gain importance. Furthermore, the results of this study will facilitate decision making for the system operator when she considers promoting different flexibility options. Considering the private sector, actors are willing to have an overview of the role power-to-methanol technologies for a potentially new market. This research is a building block in the series of researches on hydrogen and Power-to-X options, which provide crucial understanding to public and private decision making tables. It will establish correlation between various socio-technical aspects of deployment of power-to-methanol technology, and provide analyses on the impact of these technologies on the power grid reliability and  $CO_2$  reduction.

#### 2.2. Research questions

Like discussed in section 1.5, there is a lack of knowledge about the potential pathways that the energy system might take if power-to-methanol technologies are deployed in a large scale. Two aspects of the energy system are taken as the focus in this research: power grid reliability and CO<sub>2</sub> emission reduction. Based on the knowledge gap, the main question for this research is *How does deploying power-to-methanol technologies influence the power grid's reliability and CO<sub>2</sub> emission reduction in the Netherlands until 2050?* 

To investigate the main research question, the following subquestions are formulated:

• SRQ1 What are the major drivers of and barriers to deployment of power-to-methanol technologies?

- *SRQ2* Which socio-technical parameters have the largest influence on the power grid's reliability and CO<sub>2</sub> emission reduction?
- *SRQ3* What is the impact of deploying power-to-methanol technologies on power grid's reliability until 2050?
- *SRQ4* What is the impact of deploying power-to-methanol technologies on CO<sub>2</sub> emission reduction until 2050?

#### 2.3. Research approach

The aforementioned problem involves various actors with heterogeneous perspectives. Furthermore, developments happen in a bottom-up manner: no actor can steer the developments. Finally, the technical systems of interest have not been demonstrated yet. This means, much is unknown and uncertain about the path of developments. Exploration of the possible future scenarios seems necessary. Therefore, an Exploratory Modeling and Analysis (EMA) approach is a suitable for this research. This section provides a rationale for this choice.

#### 2.3.1. Exploratory Modeling and Analysis

Exploratory Modeling and Analysis (EMA) is a method developed by Bankes (Bankes, 1993) at the RAND Corporation. Bankes contrasts EMA with consolidative modeling: EMA makes use of computational experiments with a system that has uncertainties in parameters, structures and methods, while consolidative model is based on known facts and historical behavior of the model (Bankes, 1993). Consolidative models are used to make predictions about the future of a system. However, predictions can utterly go wrong if the system is highly uncertain in the parameters or the structure (Kwakkel & Pruyt, 2013). Socio-technical systems are often highly uncertain and complex. Therefore, forecasting the behavior of these systems is inherently limited due to the adaptive, chaotic nature of them (Porter et al., 2004). EMA allows for exploration of a wide range of possible dynamics that might occur to a complex system.

#### 2.3.2. Future-oriented Technology Analysis

Whenever a new technology emerges, many questions arise about the role it will play in the society and the impact it might have in the economy. Future-oriented technology analysis (FTA) is the umbrella term referring to all systematic processes to answer the questions with respect to a new technology (Porter et al., 2004). An example of FTA is *technology foresight*, which corresponds to the endeavor to identify future developments of a certain technology and its interactions with the society and the economy (Porter et al., 2004). Technology foresight requires a system level analysis and exploration.

#### 2.3.3. Exploratory Modeling for technology foresight

Technology foresight investigation is one among several FTA problems and is distinctive in that it is performed *prior* to any large-scale demonstration of the technology and very early in the course of its development. Hence, there is no historical information about the system that could be used for model validation. The interactions of society with the technology and with other compartments of the system are not recorded yet, and there is little to no data available that could be used for model validation. One can say that the models are always incomplete for this type of problems. The strength of the EMA approach, however, is that even if strict validation of the model is not possible, it can reveal new aspects of a complex and uncertain problem (Kwakkel & Pruyt, 2013). Therefore, EMA is a suitable method to perform technology foresight analysis. The main research question of this thesis calls for a technology foresight investigation, hence an EMA approach is taken in this research.

As explained by (Kwakkel & Pruyt, 2013), the process of technology foresight is as follows: the existing information about a new technology is incorporated in a model and the unknown aspects are taken as uncertainty. Then for each uncertain aspect (e.g. price, adoption rate, etc.) the researcher makes guesses and derives plausible scenarios. Experiments are conducted with the model in each of these scenarios and insights are gained about the behavior of the system in case the guesses for each scenario are correct. Rather than aiming at "optimizing a complex system with a certain goal to accomplish" (Kwakkel & Pruyt, 2013), EMA excels in stimulating out of the box thinking. With the EMA approach, one can "address *beyond what if* questions" (Kwakkel & Pruyt, 2013) such as "under what circumstances would a certain technology be widely adopted?" and "what is the range of plausible future dynamic developments of a phenomenon of interest?".

#### 2.4. Research methods

As discussed in section 2.3, the research question for this research is an example of technology foresight, i.e. a category of FTA. Agent-based modeling is listed in Porter et al. (2004), as one of the methods suitable for FTA. In this research, agent-based modeling is used to derive technology foresight. This section explains the agent-based modeling method in detail. A number of unstructured interviews with experts are also conducted to help with the construction of the model and validation of the results.

#### 2.4.1. Agent-based modeling

An agent-based model is a model of a system represented as a collection of autonomous entities called agents. These agents often follow simple interaction rules with each other and with their environment. While mathematical models of system might fail to capture some dynamics, an agent-based model can exhibit complex behavior patterns (Bonabeau, 2002). Agent-based modeling can account for learning of agents which results in emerging, unexpected patterns of behavior (van Dam, Nikolic, & Lukszo, 2013). It is demonstrated that agent based models are promising tools to understand complex adaptive systems such as infrastructures (van Dam et al., 2013).

Given the exploratory nature of the problem, an agent-based model could provide valuable insights into the complexities involved (Lye, Tan, & Cheong, 2012). An agent-based model is a computer simulation that is used to explore relationships among inputs and outputs of the system, e.g. CO<sub>2</sub> emission, tax level or total costs. In the context of EMA research approach, the agent-based model is used to experiment with the system. Agent-based models are powerful in identifying emergent behaviors, which is defined as "novel and coherent structures, patterns and properties that arise through interaction of multiple distributed elements" in Wilensky and Rand (2015). Therefore, it is a suitable method to explore future scenarios in a highly uncertain environment.

In the agent-based modeling approach, very simple rules hold at individual level. The many actors involved in the system force a bottom-up development. Therefore at the system level, patterns of behavior emerge that are not easy to contemplate. These patterns might be seen in real world. Then, with an agentbased simulation, one can understand the mechanisms that generate those patterns, project what might happen later, and suggest on actions to take in order to enable/avoid certain patterns. Agent-based model could be used to perform an EMA study and experiment with a large-scale, dynamic system to understand the range of possible behaviors it might develop. More details about the agents involved in this model can be found in chapter 5.

#### 2.4.2. Unstructured interviews

The technical system for methanol production can have different configurations. Furthermore, green methanol production is only one among many concurrent efforts for energy transition. It is crucial to understand the potential and positioning of green methanol production among those solutions. Besides, the results of any quantitative model should be validated to be practically valuable. Expert opinion can essentially answer these concerns. By conducting unstructured interviews, firstly the drivers for and barriers to deployment of power-to-methanol technologies are identified (answer to subquestion 1). Secondly, the quantitative model is conceptualized. Finally, the results and logic of the model is validated triangulation of methods is realized that leads to better understanding of the problem. The data collected from interviews are analyzed by a deductive thematic analysis. The themes are: strategies of actors, current and short-term moves of actors, influence of regulations and prospect on the future of energy transition.

#### 2.4.3. Limitations of the two methods

Agent-based modeling is a promising tool to model complex adaptive systems, though computational limitations cause difficulties in capturing system dynamics in different time scales (Chappin et al., 2017). For example, reliability of the grid should be maintained at the minute scale, while CO<sub>2</sub> emissions and development trends are best captured at a yearly time scale. This leads to huge amounts of data and difficulty in verification of the results and in drawing conclusions. In order to eliminate this limitation, a new measure of grid reliability is defined on a yearly basis.

Interviews are useful to elicit expert perspectives, though there is a high chance of bias due to limited number of respondents. It is difficult to generalize outcomes of the interviews. In order to overcome this limitation, the results of interviews are evaluated using the literature. It should be noted, however, that the conclusions from interviews should be enriched with further research.

#### 2.5. Data analysis methods

This research combines quantitative data with qualitative data. This section explains how the data is analyzed.

#### 2.5.1. Thematic analysis of interviews

The interviews are conducted in order to answer the first subquestion, to be used for model conceptualization and for model validation. These were unstructured interviews with predefined themes. The themes and the reason to include each theme are listed below.

- Facts and current state of affairs: The current state of affairs based on the view of interviewees shows the context of developments. An example could be the challenges that the power grid is facing.
- **Strategies of actors**: Each actor has or should have a certain approach with respect to the technical system under his/her control. Actors approach are implemented in the model as agent behavior rules. This category includes, for example, investment strategies in hydrogen production.

- **Current and short-term moves of actors**: The current state of affairs in the system defines the initial conditions of the simulation. This theme includes, for example, current initiatives to produce green hydrogen.
- **Regulations**: Regulations create a framework in which actors can take decisions. Regulatory framework can also influence strategies of actors. A clear example is the subsidy scheme and the influences investment decisions.
- **Prospect of the future of energy transition**: The solution that power-to-methanol technologies offer is one among many solutions to facilitate energy transition. Expert opinion is useful to understand how these solutions compare and combine to realize the transition. An example is the position that green hydrogen production will take in the future as compared to E-fuels.

These themes are used to conduct interviews and organize the data. In chapter 4 a detailed overview of findings from the interviews is presented. List of interviewees and statements can also be found in appendix C.

#### 2.5.2. Data visualization of model outputs

The developed model is capable of simulating the behavior of the system under exploration (depicted in Figure 2.1) for every year in the period between 2020 to 2050. The agent-based model provide loads of data. The main use of this data is to find patterns and structures in them. Therefore, first the correlation of model outputs with each other and the correlation of outputs with inputs are calculated. Next, for pairs with high correlation, the patterns of mutual correlation are visualized on suitable plots. These plots are made using a python script.

#### 2.6. Scope

The proposed research questions cover a broad scope that does not fit into the time frame of this thesis. Therefore, important choices and assumptions were made with respect to the scope. Three of these choices, namely the demand for methanol, the geographical scope of the project and the involved actors are discussed in this section. For model development, more specific assumptions were made that are further discussed in chapter 5. For ease of reference, all assumptions are listed in appendix A. Figure 2.1 illustrates an overview of the scope. All the technical systems (such as electrolyser), infrastructures (such as Carbon Capture, Utilization and Storage (CCUS) pipelines) and actors shape a system of interest. For convenience, it is called "the system" in the rest of the document.

#### 2.6.1. Demand for methanol

One of the main factors that can initiate E-fuel production is the demand for methanol. If there is no new demand for methanol, one can doubt whether a new method of methanol production can play a role in the market. At the time this research was conducted, shipping was one of the main sectors expected to raise the demand for methanol as a low-carbon alternative to bunker fuels. Therefore, it is assumed that green methanol production firstly serves the shipping demand. If supply exceeds this demand, it replaces conventional methanol in other applications.

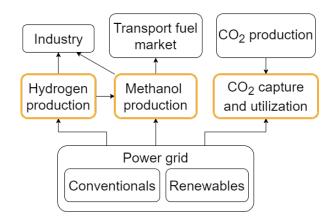


Figure 2.1: Scope of the research. Boxes with orange borderline refer to the subsystems which create dynamics of the system.

#### 2.6.2. Geographical scope

The geographical scope of this project is the national power grid of the Netherlands. In order to keep the research manageable within the available time frame, import and export of E-fuels are not taken into account. It is assumed that the produced E-fuels are supplied to the national market. Furthermore, it is assumed that the climate goals force no new fossil fuel power plant from 2020 onward Finally, it is assumed that the power grid expansion goes along with the demand and supply, i.e. the transmission system operator has proper plans to accommodate on the grid the new supplies and demands created by the developments of E-fuel production. The final choice is made in order to limit the complexities of grid development.

#### 2.6.3. Actors

In a development pathway which power-to-methanol technologies are going to be deployed and utilized, choices of several actors contribute to the state of the system. These actors are either involved with different stages of the green methanol supply chain, or have stakes in the whole system development.

In this research, investors in all technical systems immediately related to the supply chain of green methanol are involved in the development. Investors in green hydrogen production (electrolysers), carbon capture and green methanol production are engaged with the system within the scope of this project. These actors are considered as autonomous entities who make decisions based on their own preferences. Furthermore, the possibility to form consortia is neglected in this research, due to the complexity of modeling collective behavior of autonomous actors. Future work must include this aspect in order to provide more pragmatic conclusions.

The dynamics created by some actors are neglected in this research. These actors include the investors in renewable power plants, the Transmission System Operator (TSO) and the government. The choice to leave out renewable power plant owners is based on the assumption that regulations have provided a relatively stable incentive for new investments in renewable power generation. By dropping the TSO, its role is omitted from the model. Therefore, whatever happens in the power grid shows the worst-case scenario because in real life TSO would play a governance and compensation role for the grid. Finally, the political processes that lead to government actions are beyond the scope of this project, hence the omission of government.

#### 2.7. Key Performance Indicators

The main performance indicators to investigate are grid reliability and  $CO_2$  emissions. It is important to note, however, that the grid reliability can be measured by various variables. The scope of measuring  $CO_2$  emissions is of importance, too. This section discusses a more precise definition of Key Performance Indicators (KPI's) in this research.

#### 2.7.1. Grid reliability

Grid reliability is an indication of the power grid's ability to satisfy the needs of grid customers. When the penetration of renewable power plants especially wind power plants increases, the power grid faces reliability issues arising from dependence on environmental factors (Yoon, Suh, & Jung, 2020). One basic cause of low reliability for the power grid is grid unbalance. If the total supply available to the grid is less than the demand, part of the load cannot be met. If the supply is more than demand, part of power generation will be curtailed. Most of the times, renewable power plants are the cause of oversupply and will be curtailed. The accumulated value of grid balance in a year can be estimated by the equation:

$$GB = E_{RES} + E_{Conv.} - D.$$
(2.1)

In this equation,  $E_{RES}$  is the amount of electrical energy available from renewable energy sources *before* curtailment,  $E_{Conv.}$  is the amount of electrical energy dispatched from conventional power plants and D is the total yearly energy demand.

When the yearly grid balance is positive, it means *surplus power* could have been available to the power grid. This surplus is predominantly coming from renewable sources because they are not controllable. The amount of surplus power in a year is roughly equal to the value of yearly grid balance. Specifically, there is a number of *surplus hours* throughout the year which the renewable supply exceeds the amount necessary to meet the demand. The surplus power is thus equal to:

$$GB = P_{RES}T_{RES} , \qquad (2.2)$$

in which  $P_{RES}$  is the installed capacity of renewable power plants and  $T_{RES}$  is the number of surplus hours. This surplus power should ideally be satisfying the demand in times of renewable power shortage. Furthermore, in light of climate goals, the system operator wants as little energy to be dispatched from conventional power plants as possible. Therefore, the optimal condition for the power grid is to have  $E_{RES} - D$  close to zero. In order to measure how close is the power grid to meeting climate goals, the new term "Renewable Energy (RE) grid balance" is defined as:

$$GB_{RE} = GB - E_{Conv.} , \qquad (2.3)$$

which is equal to  $E_{RES} - D$  (look at equation 2.1). The optimal value of  $GB_{RES}$  is zero. Revisiting the concept of grid reliability, The amount of renewable energy available for power production deducted by energy produced by conventional power plants (RE grid balance) indicates grid reliability at the highest level of aggregation. It is measured on a yearly basis. If RE grid balance is positive, it means the grid is able to meet the yearly demand solely from renewable power. If the balance is negative it indicates a need for conventional power plants. This means the decarbonization of power sector has not been fulfilled yet. If the grid balance is predicted to be positive or negative for extended periods of time, system operator will balance it by export/import or by calling on strategic reserves.

#### 2.7.2. CO<sub>2</sub> reduction

If power-to-methanol technologies are implemented,  $CO_2$  emissions change at different parts of the energy system. In this research, the emission reduction that happens at the production side is considered. The total  $CO_2$  reduction consists of:

- **Industrial capture**: Industries capture CO<sub>2</sub> and hence, cut on their emissions. Furthermore, the captured CO<sub>2</sub> is utilized later, which frees up capacity in the pipelines to handle more captured CO<sub>2</sub>.
- **Renewable power**: Introduction of more renewable power in the power grid, pushes the conventional power plants out of merit. Therefore, for instance, a wind turbine is supplying electricity instead of a coal plant.
- **Green hydrogen**: Currently, a large share of the hydrogen used in the industry is produced as gray hydrogen. However, if more green hydrogen is produced than demanded for green methanol production, the industry can use green hydrogen instead of gray hydrogen.
- **Green methanol**: Currently, methanol used in the industry is produced by steam methane reforming (SMR) process. However, if more green methanol is produced than demanded in the shipping sector, the industry takes up the remaining green methanol instead of conventional methanol.

#### 2.8. Research flow diagram

In this section, the sequence of research questions is explained and the corresponding methods are explained. The research flow diagram, showing research steps and methods, is depicted in Figure 2.2. In this diagram, white boxes contain research questions, pale green boxes show research steps, purple boxes show the research and analysis methods and light yellow boxes show the chapter in which the research question is answered.

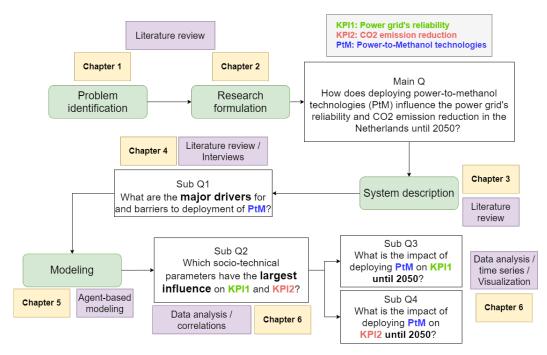


Figure 2.2: Research flow diagram showing the overview of research steps. Boxes colored in white, pale green, purple and light yellow show research questions, research steps, research methods and the reporting chapters, respectively.

The research begins by investigating the main question. In order to answer the main question, one shall first understand the conditions under which PtM technologies can possibly be deployed. In this regard, social and technical drivers exist that steer the developments. These drivers influence capacity of PtM technologies in the system and therefore, grid reliability and CO<sub>2</sub> emission reduction. Sub-question *SRQ*1 investigates these drivers.

After answering *SRQ*1, an extensive list of drivers are identified. However, these parameters are not equally effective. Some of the parameters have a higher influence on the system. If these parameters are identified, one can predict the future developments better and intervene successfully. An answer to *SRQ*2 sheds light on the important drivers and barriers within the system.

Once the most important parameters are identified, it is time to calculate the dynamics of the development. *SRQ*3 and *SRQ*4 are formulated to understand the range of viable states in each year until 2050. In this respect, the patterns of variations are indicative of the impact of PtM deployment on grid reliability and on CO<sub>2</sub> reduction. The answer to these two final questions concludes on how PtM deployment influences the grid reliability and CO<sub>2</sub> reduction until 2050.

#### 2.9. Summary

This chapter built the foundation of the research. In the following chapters, the research steps taken will be discussed to enable answering the research questions.

# 3

# System description

The system studied in this research consists of a technical system as well as an institutional system. The technologies and actors within the scope of this project define the technical system of interest. Knowledge of this system is crucial in order to conduct an analysis. Moreover, the regulations governing the technologies and actors in the technical system define the rules of the game and shape the institutional system of interest. This chapter provides brief overview of the technical and institutional systems of interest.

#### 3.1. Technical system

The focus of this research is on the factors that lead to deployment of power-to-methanol technologies and on the impact that power-to-methanol technologies will have on other elements of the energy system. The technical system that power-to-methanol technologies are part of, is hence of importance. This section outlines the elements of this system.

#### 3.1.1. Intermittent renewable power generation

The power system is changing in the Netherlands. The efforts to incorporate renewable power production in the power production portfolio has been going on for two decades. Even though the share of renewable energy in the power sector was less than 15% in 2019 (CBS, 2020b), a faster growth is expected in the next decade. In projected scenarios of the future of power generation, such as the scenarios investigated by Schoots and Hammingh (2019), up to two-third of the electricity is generated from renewable sources in 2030. This section describes the scenarios for expected growth of renewable power generation as well as the challenges that the power grid is facing due to this growth.

#### Renewable energy on the power grid: a review of scenarios

The Dutch *klimaataakkoord* urges to achieve a carbon-neutral power system by 2050. There are a lot of movements in the sector to achieve this goal. Apart from the onshore wind and rooftop solar panels that have been around for a while, offshore wind seems a promising alternative for the Netherlands to fulfill this carbon-neutrality goal.

One of the most recent scenario studies for the North Sea by PBL (Matthijsen et al., 2018) provides four scenarios for offshore wind installed capacity. Figure 3.1 shows an overview of the scenarios. Far right hand of this plot corresponds to high dynamics in the economy, technology, the climate and other areas. These scenarios are derived from the two scenarios in the Welfare, Prosperity and Quality of the Living Environment (WLO) outlook (CPB/PBL, 2015). The upper two panels in this diagram show the scenarios where extra policy is developed for the North Sea that contributes to the Paris Agreement Climate Agreement as well as the UN sustainable development goals. The lower two panels show policy-as-usual scenarios. In 2020, total installed

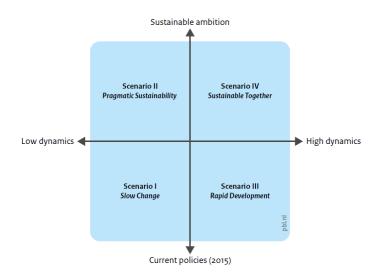


Figure 3.1: The background assumptions of the four scenarios for wind energy in the North Sea. Source: Matthijsen et al. (2018)

capacity of offshore wind power is 1 GW (Schoots & Hammingh, 2019). Table 3.1 shows the installed capacity of offshore wind in 2030 and 2050 in each of the scenarios. The road-map for offshore wind energy states that 11.5 GW of offshore wind is already planned and will be commissioned by 2030 (TenneT, 2020).

Scenario	Installed capacity (GW)		
Scenario	2030	2050	
Slow change	11.5	12	
Pragmatic sustainability	11.5	22	
Rapid development	11.5	32	
Sustainable together	11.5	60	

Table 3.1: PBL scenarios for wind power development in the North Sea. Source: Matthijsen et al. (2018).

The installed capacity of solar PV and onshore wind in 2020 are 9 GW and 4.7 GW, respectively (Schoots & Hammingh, 2019). It is expected that solar PV capacity increases up to 27 GW and onshore wind to 6.1 GW (Schoots & Hammingh, 2019). The maximum potential of the Netherlands to produce power from solar PV and onshore wind is estimated in PBL and ECN (2011) based on the total area available for installing PV panels (rooftops) and the total area available to place wind turbines on land. Based on this method, the maximum installed capacity for solar PV and onshore wind are 88 GW and 8 GW respectively.

Combining solar PV, onshore wind and offshore wind scenarios, table 3.2 shows the current state and the future of renewable power in the Netherlands in 2030 and 2050.

Year	Scenario	Installed capacity (GW)					
Iear	Scenario	Solar PV	Onshore	Offshore	All renew-		
		Solar PV	wind	wind	ables		
2020	All scenarios	9	4.7	1	14.7		
2030	All scenarios	27	6.1	11.5	44.6		
	Slow change Pragmatic sustainability		12	108			
2050		88	8	22	118		
2050	Rapid development	00	ð	32	128		
	Sustainable together			60	156		

Table 3.2: Scenarios of renewable power generation in the Netherlands from 2020 to 2050. Source: Matthijsen et al. (2018); Schoots and Hammingh (2019)

#### **Challenges of renewables**

Large share of renewable power plants in the energy mix has benefits for the energy transition. First of all, the operation of renewable power plants (except for geothermal power plants) has zero greenhouse gas emission. Therefore, the average emission from the power sector declines as more renewable power units are deployed. This explains why renewable energy has been high on agenda in the last decade (Schoots & Hammingh, 2019). Along with decarbonization, renewables contribute to the affordability of the power. The reason is simple: renewable power generation has zero fuel cost while conventional power plants have to pay for the fossil fuel they combust. Therefore, when a considerable amount of power is coming from renewable sources, the average price of electricity plunges. The day-ahead market prices might even take negative values if a lot of sun and wind energy is available but no large scale storage. In other words, if the total power production is more than there is demand for, the plant operators are even willing to pay something to the consumers to take the energy. The electricity prices in the Netherlands fell below zero in March 2020, due to a sudden decrease of power demand in the lock down state during COVID-19 pandemic.

Even though abundance of renewables pulls down the electricity prices, periods of renewable shortage are as probable as periods of renewable abundance. For example in winter, the power generation from solar PV might stay zero for several days in a row. As a result, in a power system with high penetration of renewables, frequent shortage and high peak prices are common. On the other hand, negative power price is not desirable by the producers. It creates negative return on investment and is harmful for current asset owners. This affects all power plants, including renewables. The prospect of having negative prices in the future can also discourage investments and slow down the pace of developments.

#### Curtailment or storage?

During high renewable production hours, an alternative is "curtailment", when renewable units are shut down. Curtailment of renewable power plants prevents negative prices in the day-ahead market. By suppressing generation, the transmission system operator (TSO) manages the balance between demand and supply and hence, maintains grid stability. The TSO compensates for the loss of asset owners.

In general, power generation from renewable sources is costly if supply exceeds demand. In the short term, either the generation units are not curtailed and negative prices develop or the TSO curtails surplus renewable generation. In the first case, the asset owners incur costs and in the other case, the TSO bears the costs. If large scale storage units were available, part of these costs could be avoided. Specifically, seasonal variations of renewables require storage capacity of weeks to months. Different alternatives for energy storage

are discussed in (Energy storage NL, 2019). According to Energy storage NL (2019), Power-to-X is the most suitable energy storage to control seasonal variations in the Netherlands.

#### 3.1.2. Green hydrogen

The Hydrogen Roadmap for Europe states that hydrogen is required in large scale to enable carbon-neutrality for EU (FCH JU, 2019). Hydrogen is the zero-carbon alternative fuel for heavy-duty transport -e.g. aviation and maritime- and high grade industrial heat (FCH JU, 2019). Production, transport and storage are the main stages in the hydrogen supply chain. This section describes selected aspects of these steps.

#### Production of green hydrogen

Hydrogen can be produced through water electrolysis using renewable power, in which case it is labeled as "green" hydrogen. The main electrolysis technologies are: Alkaline Electrolysis Cells (AEC), Proton Exchange Membrane Electrolysis Cells (PEMEC) and Solid Oxide Electrolysis Cells (SOEC) (Schmidt et al., 2017). AEC is the most mature technology among the three and is in use for a century (Schmidt et al., 2017). PEMEC has a higher power density and higher efficiency than AEC, though is more expensive (Schmidt et al., 2017). SOEC is the least developed technology and is not commercialized yet (IEA, 2019a). Table 3.3 lists the current and future values for several techno-economic characteristics of the three technologies.

	AEC			PEMEC			SOEC		
	2020	2030	long term	2020	2030	long term	2020	2030	long term
Electrical efficiency (%)	63-70	65-71	70-80	56-60	63-68	67-74	74-81	77-84	77-90
Load range (% nominal load)		10-110			0-160			20-100	
Stack lifetime (operating hours)	60000- 90000	90000- 10000	100000- 150000	30000- 90000	60000- 90000	100000- 150000	10000- 30000	40000- 60000	75000- 100000
Capital cost (US\$/ <i>kW<sub>e</sub></i> )	500- 1400	400-850	200-700	1100- 1800	650- 1500	200-900	2800- 5600	800- 2800	500- 1000

Table 3.3: Techno-economic characteristics of electrolysers technologies. Source: IEA (2019a)

#### Transport and storage of hydrogen

The infrastructure for transport and usage of hydrogen is expensive and is, thus, a bottleneck for hydrogen development. To transport hydrogen, first it can be liquefied, then stored in vessels and transported to the desired location with ship or truck. Another alternative is to transport it via pipelines. In the Netherlands, Gasunie is planning to have the *hydrogen backbone* ready by 2030 (Gasunie, 2019). It refers to a network

which connects the five main industrial clusters in the Netherlands with each other and with the transmission network in Germany. It will be realized using existing high pressure natural gas pipelines (Gasunie, 2019).

Hydrogen can be stored in salt caverns beneath the ground. This method has been implemented in the UK for many years (van Wijk & Chatzimarkakis, 2020). A recent study reveals that in the Netherlands, there is a technical potential to store 10.4 peta watt-hour hydrogen in salt caverns (Caglayan et al., 2020). Energy storage in salt caverns is cheaper than electricity storage in batteries by a factor of 100 (van Wijk & Chatzimarkakis, 2020).

#### 3.1.3. Green methanol

The term "green methanol" corresponds to the methanol which can be obtained by catalytic hydrogenation of  $CO_2$  molecules, using green hydrogen and renewable electric power. Whereas conventional processes for methanol production emit considerable amount of  $CO_2$  (between 0.8 to 3.1 ton  $CO_2$  for each ton methanol produced), green methanol production consumes  $CO_2$  and creates a negative emission. Hence it is labeled as green methanol. The reactions governing methanol synthesis through  $CO_2$  hydrogenation are (Rafiee, Rajab Khalilpour, Milani, & Panahi, 2018):

$$CO + 2H_2 \leftrightarrow CH_3OH \qquad \Delta H_{298} = -92 \ kJ/mol$$
 (3.1)

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \qquad \Delta H_{298} = -49.5 \ kJ/mol \tag{3.2}$$

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad \Delta H_{298} = -41 \ kJ/mol \tag{3.3}$$

A study by Otto, Grube, Schiebahn, and Stolten (2015) shows that power-to-methanol, among all possible  $CO_2$  utilization techniques, ranks high in terms of economic feasibility and contribution to  $CO_2$  reduction. Methanol is widely used in the industry and is a potential fuel for heavy transport (Quarton & Samsatli, 2020). A consortium of partners have launched the project  $MefCO_2$  that produces green methanol. This project aims at improving the business case for CCUS by using part of the captured  $CO_2$  and turning it into fuel for road and maritime, i.e. a revenue generation source (partnership, 2018). Located in Germany, this pilot project finished now and is one of the biggest flue gas  $CO_2$ -derived methanol synthesis plants in Europe, with 1 ton methanol production per day. Another demonstration of green methanol production is the George Olah plant in Iceland, the world's largest green methanol plant, which produces 22 GWh of methanol per year (Quarton & Samsatli, 2020).

At the system level, methanol production plant can have various configurations. Generally speaking, the main feedstocks are hydrogen and CO<sub>2</sub>. Each of the feedstocks may be supplied from an external source or be sourced internally (e.g. hydrogen produced via an internal electrolyser). The configuration of production plant influences the costs and energy demand of the plant. Table 3.4 lists the main techno-economic characteristics of a green methanol production plant for which the feedstocks are sourced externally. Future values are also estimated.

#### **3.1.4.** CO<sub>2</sub> supply

As explained in the previous section,  $CO_2$  is a feedstock needed for green methanol production. Besides sourcing of  $CO_2$ , the infrastructure to transport the captured  $CO_2$  is of high importance. The presence of a  $CO_2$  transport network is one of the requirements to realize  $CO_2$  capture (Lensink, 2020). In this section, first the main CCUS infrastructures in the Netherlands are introduced. Then information is presented about possible sources of  $CO_2$  in the Netherlands.

Figure	2020	2030	2050		
Technical lifetime (yr)			25		
Investment costs (M $\in$ /PJ <sub>MeOH</sub> )	11	8	7		
Fixed operational costs ( $M \in /PJ_{MeOH}/yr$ )	0.44	0.24	0.18		
Variable costs		Depends on the price of hydrogen and $CO_2$ .			
Electricity consumption $(PJ_e/PJ_{MeOH})$	0.05	0.04	0.03		
Hydrogen intake $(PJ_H/PJ_{MeOH})$	1.22	1.20	1.18		
$CO_2$ intake (Mton/ $PJ_{MeOH}$ )			0.07		

Table 3.4: Techno-economic characteristics of green methanol (indicated by *MeOH* subscript) production plant per unit installed capacity. Costs are based on the 2015 euro. Source: Detz (2019).

#### Athos, Porthos and OCAP

One of the major carbon utilization infrastructures is the OCAP infrastructure. OCAP supplies pure CO<sub>2</sub> that is coming from hydrogen production unit of Shell and bio-ethanol production plant Alco in Rotterdam (OCAP, 2018). 600 greenhouses in the western area of the Netherlands are using 0.5 million tons of CO<sub>2</sub> transported by OCAP every year. In the near future, OCAP is planning to double the infrastructure capacity (OCAP, 2018).

Whereas OCAP is meant to transport captured  $CO_2$  to greenhouses, two other projects are under development to facilitate CCUS: Porthos and Athos. Porthos is a project in the area of Port of Rotterdam. It is initiated by Port of Rotterdam Authority, EBN and Gasunie. Porthos is going to connect OCAP infrastructure and the interested industry in the port area to depleted gas fields in the North Sea, 20 kilometers offshore (Port of Rotterdam, EBN, & Gasunie, 2019). The infrastructure is able to handle 5 million tons of  $CO_2$  per year at 40 bar, and the total storage capacity is 37 million ton (Port of Rotterdam et al., 2019). Porthos project plans indicate that the system would be operational by 2023. Porthos is also able to carry  $CO_2$  to the industries that demand it for utilization. The costs of transporting and storing  $CO_2$  is paid by the capturing industries. No exact cost estimation is reported by Porthos yet, though calculations based on a 70% utilization factor for the infrastructure result in a 15  $\in$ /ton fee for storage and 45  $\in$ /ton for transport (Lensink, 2020).

Athos is a similar project initiated by the Port of Amsterdam Authority, EBN, Gasunie and Tata steel<sup>1</sup>. Tata steel has expressed her interest in storing  $CO_2$  in the empty reservoirs at the bottom of the North Sea, though other industrial parties can also participate. Carbon utilization is also possible if there is enough demand for  $CO_2$  in the future. The infrastructure is expected to be operational in 2027 and will be handling around 5 million tons of  $CO_2$  per year (van Bracht & Braun, 2018).

To summarize, from 2027 onward, it is possible to capture 10 million tons of CO<sub>2</sub> per year from the industrial areas in and around Rotterdam and Amsterdam, and to store it beneath the North Sea or utilize it in other industrial processes.

#### **Industrial capture**

The port of Rotterdam is responsible for 17% of the total CO<sub>2</sub> emissions of the Netherlands (Port of Rotterdam et al., 2019). Table 3.5 lists the main emitters in the industrial areas covered by Porthos and Athos project. These emitters are among the top emitters of the Netherlands. In total, 12 million ton of CO<sub>2</sub> per year is emitted from main emitters of the Amsterdam area and 25.75 million ton per year from the main emitters in the Rotterdam area.

<sup>&</sup>lt;sup>1</sup>Unlike Porthos, official information about the specifications of Athos project was not published at the time this thesis was written.

Name	Type of emitter	Area	Emission (Mton/yr)
Tata steel	Iron & steel	Amsterdam	6.21
Uniper centrale Maasvlakte	Coal-fired power plant	Rotterdam	5.95
Uniper centrale Maasvlakte 3	Coal-fired power plant	Rotterdam	4.67
Shell Pernis	Refinery	Rotterdam	4.25
Nuon power Velsen	Natural gas-fired power plant	Amsterdam	3.63
Essent Amercentrale	Coal-fired power plant	Rotterdam	3.52
Shell Moerdijk chemie	Petrochemical (Ethylene/Propylene)	Rotterdam	2.55
BP Raffinaderij	Refinery	Rotterdam	2.29
Nuon power IJmond	Natural gas-fired power plant	Amsterdam	2.15
Esso Raffinaderij	Refinery	Rotterdam	2.1
Gunvor Petroleum	Refinery	Rotterdam	0.42

Table 3.5: The top 11 emitters in the areas Rotterdam and Amsterdam. Source: EBN and Gasunie (2017).

The current prospect for  $CO_2$  handling infrastructure in these two areas is limited to Porthos and Athos projects. These two project provide a maximum handling capacity of 10 million ton per year. However, the total  $CO_2$  emissions from these areas is around 4 times this value. Therefore, some industries can not store their  $CO_2$  emissions. Those with the lowest capture costs will be the first to capture  $CO_2$ . Table 3.6 shows the estimated capture cost per ton  $CO_2$  avoided (excluding the infrastructure handling costs) for different emitters and different processes. These costs include energy costs, which is a combination of electrical and thermal energy. All industries have to pay for the connection to the infrastructure, which would cost them 4.5  $\notin$ /ton  $CO_2$  (Lensink, 2020).

Table 3.6: Capture cost per process in different industries. The numbers within brackets show the range of costs and the number before
brackets is the average cost. Sources: EBN and Gasunie (2017); Lensink (2020)

Type of emitter	Process	Capture cost ( $\in$ /ton CO <sub>2</sub> avoided)
	Hydrogen production	33 (23-42)
Definery	Process heaters	79 (42-126)
Refinery	Cracking	99 (79-128)
	Cogeneration production	104 (42-126)
Petrochemical plant	Ethylene/Propylene	71
	Post-combustion capture	57
Coal-fired power plant	Pre-combustion capture	43
	Oxyfuel capture	51
Natural gas-fired power plant	Post-combustion capture	79

Capture of  $CO_2$  and injection in the grid requires compression and costs energy. Depending on the capture method, energy consumption for carbon capture is different. Here, the estimated consumption in Lensink (2020) is used. The carbon capture process is assumed to consume 50 kilowatt-hours of electrical energy.

For compression, according to theory the power consumption of a compressor is given by (Nesbitt &

Actuators, 2007):

$$G = \frac{Z_{av}RT_I}{m}(r^m - 1)\frac{w}{\eta_p} + F,$$
(3.4)

where w is the kilogram mass flow per second,  $\eta_p$  is the polytropic efficiency of the gas, F is the mechanical power loss,  $Z_{av}$  is the average compressibility factor of the gas,  $T_I$  is the inlet temperature, r is the pressure ratio, and  $m = \frac{n-1}{n}$  where n is the polytropic index. Using rough estimates for the parameters in equation 3.4 (listed in section A.2), the power consumption of compressors for CCUS network can be found. According to Port of Rotterdam et al. (2019), the pressure of CO<sub>2</sub> in the Porthos infrastructure would be between 15 to 40 bar. Lensink (2020) reports that Porthos will use 22 bar for Carbon Capture and Utilization (CCU) network and 35 bar for Carbon Capture and Storage (CCS) network. Assuming the pressure of gas at the inlet of compressor be 1 bar, the pressure ratio (r) is 22 and 35 for CCU and CCS networks, respectively. Therefore, the power consumption for CCS is approximately 120 kilowatt-hour per ton and for CCU is roughly 100 kilowatt-hour per ton. These values are coherent with estimates in Lensink (2020).

#### **3.2.** Institutional system

The technical context of the problem is governed and constrained by the institutions: the rules and regulations regarding each part of the technical context. To understand the impact that power-to-methanol technologies will have on the other elements of the energy system, one should identify the institutional context as well. This section explains two main elements of the legislation that influence power-to-methanol, namely the EU Emission Trading System and the applicable subsidy schemes.

#### 3.2.1. Emission Trading System

European Emission Trading System (ETS) is a market-based mechanism for regulation of greenhouse gas (GHG) emissions from EU which is in place since 2005. Most of the GHG-intensive sectors of the economy are regulated in this system. The information presented in this section is mainly obtained from the ETS handbook (European Commission, 2015). ETS works as a "cap and trade" system. All participants need to obtain emission rights equivalent to their yearly emissions by purchasing allowances. They can do so in two ways. Either they have the right to get free allowances or they purchase allowances through auctions.

The supply of allowances is limited by the EU legislation at a cap which is reduced every year by 1.74%. This is intended to keep the price of allowances at a level which motivates emitters to reduce their emissions. If the price rises, however, there is a risk of "carbon leakage": GHG-intensive industries might move to countries with less restrictions on GHG emissions in order to avoid paying a high price for ETS allowances. By allocation of free rights, EU legislation has accounted for this factor. Carbon leakage risk is prominent for industries that have difficulty with reducing their emissions. These might be energy intensive industries like steel production that have no choice other than using fossil fuels, or petrochemical industries which are directly dependent on fossil fuels. Based on the degree of carbon-leakage risk, these industries are eligible to receive a number of free ETS allowances.

EU ETS is designed to regulate *direct* emissions. To date, circular industry is not fully accounted for in the EU legislation regarding GHG regulation. In the ETS handbook, allocation of free rights regarding the use of waste heat and waste gas is discussed. However, the concept of carbon utilization is by far unrecognized. An example of carbon utilization is the operation of OCAP in the west of the Netherlands. Several industries in this region are selling their  $CO_2$  to the horticulture area through OCAP pipeline (OCAP, 2018). However, they are not exempt from purchasing ETS allowances, neither are they eligible for free allocation. Current ETS provides exemption for carbon capture and storage, though  $CO_2$  is still accounted as emission even if it is captured and converted into other products (Group of Chief Scientific Advisors, 2018). In fact, carbon capture and utilization (CCU) can be a part of decarbonization efforts in sectors like chemical industry that currently have no economic way to avoid emissions (Group of Chief Scientific Advisors, 2018).

The discussion about carbon utilization processes, such as green methanol production, is ongoing to determine a proper way of allocating ETS allowances. Some experts suggest that with carbon utilization,  $CO_2$  emission is delayed and should not be included in the emissions from the installation which has captured the  $CO_2$  (Group of Chief Scientific Advisors, 2018). Others suggest that since the ETS motive is to ensure a transition to zero-carbon economy,  $CO_2$  emission should be still penalized even if utilized. The situation can be more complicated especially when  $CO_2$  is captured by a sector regulated by ETS, then used to produce a substance that is used in a sector not regulated by ETS scheme. To summarize, the current legislation provides derogation in case  $CO_2$  is captured and *stored* underground (CCS). Those sectors that capture their emissions to be *utilized*, however, are not exempted from ETS scheme.

#### 3.2.2. Subsidy schemes

The EU directives and Dutch regulations provide different support schemes for the technologies deemed useful for the energy transition. These technologies include renewable power generation and carbon capture. At the time this thesis is written, the main subsidy scheme in use in the Netherlands is SDE+ which only covers power production from renewable sources (Netherlands Enterprise Agency, 2018). From September 2020, it will be updated to SDE++ which covers more sectors and circumstances, e.g. CCS and green hydrogen (Rijksdienst voor Ondernemend, 2020b). SDE+ provides a feed-in tariff to compensate the difference between renewable power production costs and the market value of produced power. In other words, SDE+ subsidy aims to make renewable power competitive compared to fossil fuel-generated power. Depending on the technology, projects are eligible to receive subsidy for 8, 12 or 15 years. SDE+ subsidy scheme scheme has seemingly been successful in stimulating renewable power production although it exposes the investors to the risk of low power prices in the future, by eliminating the feed-in tariff when electricity price remains negative for a long period (at least six hours) (Netherlands Enterprise Agency, 2018).

As mentioned above, SDE++ is expected to provide subsidy for CCS. According to PBL study, CCS projects can be subsidized up to  $112 \notin$ /ton CO<sub>2</sub> for up to 15 years (Lensink, 2020). It should be noted that CCU is not considered in this plan. The criteria to receive CCS subsidy in SDE++ scheme is to transport the captured CO<sub>2</sub> directly to dedicated underground storage locations.

Green hydrogen production might also receive subsidy according to SDE++ publications. Considering AEC or PEMEC technologies for production, the subsidy level for green hydrogen production is determined by Lensink (2020). The subsidy will be paid for 15 years and depends on two factors. First of all, the price of natural gas is considered. The higher the price of natural gas, the higher is the subsidy. This way, green hydrogen can compete with gray hydrogen produced by steam methane reforming. The second factor is the operating hours of the electrolyser. If only renewable power is consumed for electrolysis, the electrolyser should be operated in a flexible manner, which translates into higher operating costs and lower incomes for the operator. Since more  $CO_2$  emission is avoided in this way, it is desired to incentivize flexible operation. Therefore the higher the operation hours of electrolyser, the less subsidy is allocated to the unit.

The DEI+ is another support scheme which deals with small scale prototypes of innovative technologies, including CCUS, Direct Air Capture (DAC) and flexibility options for the power grid (including green hydrogen) (Rijksdienst voor Ondernemend, 2020a). For the categories mentioned, DEI+ supports only pilot projects for a maximum of four years.

#### 3.3. Summary

In summary, the technical system of importance involve all stages of the supply chain to produce methanol. In particular, the equipment and actors involved with renewable power generation, production and transportation of green hydrogen and capture and transportation of  $CO_2$  shape the technical system under investigation. The main elements of institutional system investigated in this chapter were support mechanisms for each of relevant technologies and the  $CO_2$  emission control scheme of ETS.

## 4

### Power-to-methanol technology deployment: drivers and barriers

The main drivers for deployment of power-to-methanol technologies are identified through interviews with experts and literature review. These interviews also point to some barriers to the deployment of these technologies. In this chapter, first a general theory for identifying drivers of a renewable technology is presented based on the systematic literature review of Darmani, Arvidsson, Hidalgo, and Albors (2014). Next, findings from interviews are presented. The drivers identified in the interviews are placed into the framework created by Darmani et al. (2014). Based on the conclusions from interviews and the literature review, an answer is given to subquestion 1: *What are the major drivers of and barriers to deployment of power-to-methanol technologies*?

#### 4.1. A framework for drivers of renewable energy technology

Large scale deployment of renewable energy technologies is high on the agenda to control climate change. For this reason it is crucial to understand which factors drive the deployment of these technologies. Darmani et al. (2014) demonstrated a systematic literature review on this topic and classified the drivers into five main categories of incentives: Regional incentives, incentives for actors, network incentives, technology incentives and institutional incentives. These categories are explained in the following sections. The reader should note that the article focuses on renewable energy technologies such as wind or solar energy production. However, the technology of interest in this research is power-to-methanol which is intrinsically different from renewable energy technologies. The categories of drivers are interpreted accordingly so that they are applicable to the case of power-to-methanol technologies. The drivers are created when the incentives exist and a barrier exists when incentives are lacking.

#### 4.1.1. Regional incentives

Regional incentives enlisted by Darmani et al. (2014) refer to the specific geographical conditions that create a potential for a specific renewable energy technology. For example, the Netherlands is more suitable for harvesting wind energy as compared to solar energy due to the climate conditions of the region. Power-tomethanol technologies are hardly affected by regional natural conditions. Instead, other system parameters can create incentives specific to the region. To put it in perspective, power is a major element to have a complete power-to-methanol chain. The conditions of the power grid, e.g. the amount of renewable power available, can be categorized as a regional incentive.

#### 4.1.2. Technological incentives

As outlined by Darmani et al. (2014), technology is a main driver of change in a technology-based system. Technology incentives emerge from two aspects of technology: the specifications of the technology itself, and the availability of technology infrastructure. According to the definition by Darmani et al. (2014), technology infrastructure refers not only to the physical infrastructure (such as internet, power grid, etc.) but also to the knowledge infrastructure. This refers to the knowledge about system that provides perceptions of what technological development is desirable by the system. Technology specification and infrastructure can create incentives for power-to-methanol technologies as they do for renewable energy technologies.

#### 4.1.3. Incentives for actors

Actors are the decision makers in the system who force the development in a bottom-up manner. According to Darmani et al. (2014), the actors decide mostly based on economic incentives. If a certain decision has a positive economic impact on their assets, they are incentivized to take that decision. Second, actors seek a competent position among other actors. If a new investment gives them an advantage over other competitors, they are more likely to make the investment decision. Third, influenced by national climate goals, some companies have set targets to reduce their greenhouse gas emissions. These targets act as another incentive for investment in renewable energy technologies. Finally, the level of change acceptance in a system can influence actors' decision. If organization structure of actors is flexible enough, it encourages the transition to renewable energy technologies. All the elements that create incentive for renewable energy technologies can be influential for actors investing in power-to-methanol technologies.

#### 4.1.4. Network incentives

The network of companies, non-profit organizations, government and knowledge institutes creates another set of drivers. According to Darmani et al. (2014), this network might correspond to the supply chain network or the societal network. The effectiveness and efficiency of interactions in the supply chain network forms one of the most dominant group of incentives for renewable energy technologies (Darmani et al., 2014). On the other hand, the green movement in the societal network motivates actors to move towards renewable energy technologies. Regarding power-to-methanol technologies, the supply chain is complex and hence supply chain network drivers are important. Furthermore, the technology is supposed to provide low-carbon alternative fuel and thus, help with  $CO_2$  reduction. As a result, the incentives created by the societal network are relevant, too.

#### 4.1.5. Institutional incentives

The role of institutions in enhancing large scale deployment of renewable energy technologies is widely acknowledged (Darmani et al., 2014). The institutions can be divided into hard and soft institutions.

Hard institutions are formal institutions. In the context of energy system, these institutions correspond to energy policies. According to Darmani et al. (2014), policies have a three-fold effect. The formal statements of energy policies might provide support to certain producers or consumers. Next to policy formality, sta-

bility of policies create incentive for actors. Finally, coherence and conformity of regulatory frameworks in different regions and for different technologies can create incentives for the development of renewable energy technologies. Soft institutions refer to the norms in the market or in the society. According to Darmani et al. (2014), market norms include the degree of risk tolerance, entrepreneurial spirit and resource sharing. Market norms determine the extent of innovativeness and hence, drive renewable energy technologies. Societal norms correspond to social acceptance. For example, in some countries, people are willing to pay more for renewable power. Power-to-methanol technologies are influenced by hard and soft institutions.

#### 4.2. Interview setup

In total, a number of 22 unstructured interviews were conducted with energy experts The experts were selected from academia and industry and their expertise was related to energy transition. The role, expertise and affiliation of interviewees are listed in table C.1 of appendix C. The discussions with the energy experts were steered towards certain themes in order to make sure all aspects of related systems are covered. The themes are facts and current state of affairs, strategies of actors, current and short-term moves of actors, regulations and prospect of the future of energy transition, as explained in section 2.5.1.

The interviews were mostly one-on-one and conducted over phone. First, the interview was conducted and recorded. Some interviewees were contacted more than once at this step. Interviewees were not explicitly informed about the themes. Afterwards, the discussions were summarized into several statements per each theme. The experts revised and confirmed the summaries before reporting. The confirmed statements are listed in table C.2 to C.6 in appendix C. Statements are labeled and referred to in the rest of this chapter. Table 4.1 lists the labels for each theme and the corresponding table in appendix C.

Table 4.1: Labels of the statements, corresponding theme and reference to the full table of statements.

Theme	Labels	Table of statements
Facts and current state of affairs	SC-1 to SC-20	Table C.2
Strategies of actors	SSt-1 to SSt-23	Table C.3
Current and short-term moves of actors	SM-1 to SM-22	Table C.4
Regulations	SR-1 to SR-12	Table C.5
Prospect of the future of energy transition	SF-1 to SF-25	Table C.6

#### 4.3. Analysis of experts' opinion: framework of drivers and barriers

The experts highlight drivers of and barriers to power-to-methanol technologies in the interviews. These factors are analyzed using the framework explained in section 4.1. The drivers and barriers are categorized as regional, technological, actor, network and institutional drivers and barriers as explained in section 4.1. The following sections describe the findings in more detail.

#### 4.3.1. Regional drivers and barriers

The experts underlined *availability of feedstock* as a driver for deployment of power-to-methanol technologies. Green hydrogen is one of the main feedstocks. Availability of green hydrogen can be partly influenced by regional parameters. One of these regional factors is the number of hours that surplus power is available. Higher surplus hours allow for more green hydrogen production. However, as the surplus hours increase, it is possible to produce more hydrogen which creates higher electrical load on the power grid. This, in turn, reduces the amount of surplus energy (**SC-4**). Number of surplus hours can be considered a regional factor because it depends on the mix of renewable resources available in the region and the level of renewable deployment.

Direct conversion of offshore wind to green hydrogen when wind energy becomes more abundant in the future can become an economically feasible option (**SF-16**). Therefore, abundance of wind energy in the region can drive investments in green hydrogen production and hence, power-to-methanol. Nowadays how-ever, this configuration results in higher electricity cost for hydrogen production compared to an on-grid electrolyser (**SC-12**). The power sector is surprisingly neglecting this opportunity by directing the resources on wind development and delaying green hydrogen development (**SSt-1**). Furthermore, the capacity and distance of offshore wind farm from the land influence suitability of off-grid electrolysis. The larger the wind farm, the further it is placed and the more competitive green hydrogen becomes as compared to direct electrical connection to inland grid (**SSt-17**). In the Netherlands, there is currently an idea to develop between 60-100 GW wind power offshore, produce hydrogen from most of its production and transmit the rest to the power grid (**SM-3**).

The most challenging issue concerning increase of renewable power production is long term and seasonal storage (**SC-9**). Other than storage in a chemical medium, a number of large scale storage technologies are proposed as well but are mostly in the research phase (**SC-8**). Green methanol can be used as a medium to store excess energy of renewables and resolve grid congestion. In the Netherlands, energy storage in a chemical substance is on of the few feasible options for the long term (Boom, 2020). Other options such as pumped-storage hydroelectricity are not feasible due to geographical characteristics of the region.

Finally, for a country like the Netherlands, land availability is an important regional factor. Some configurations of power-to-methanol require a large area of land to be deployed. Whether the methanol production or hydrogen production is flexible, or the production sites are onshore/on-grid or offshore/off-grid create different configurations. For example, if the electrolyser is integrated in the methanol production unit and it is supposed to run flexible and only during surplus hours, huge hydrogen buffers are needed in order to ensure full-load methanol production. Increasing hydrogen buffer size means higher CAPEX as well as more space occupation (**SSt-21**). The land availability can thus be a barrier to some configurations and a drive for other configurations.

#### 4.3.2. Technological drivers and barriers

Power-to-methanol technologies have specific characteristics and rely on several infrastructures to be operable. The technology specifications and technology infrastructure can be driver for or barrier to power-tomethanol deployment.

#### **Technology specification**

Regarding technological specifications, the configuration of power-to-methanol system is playing a role. As discussed in section 4.3.1, some configurations are more costly or might not fit into the regional constraints. To put it in perspective, methanol production is a rather mature technology in the industry. The production often takes place in large scales and at a fixed rate. However, new technologies have been proposed that allow for flexible methanol production. In this way, the power demanded can be taken from the grid only during surplus hours. These technologies have not been demonstrated yet and appear risky to the investors (**SSt-22**). Moreover, the prospective buyers of green methanol have huge energy demands, hence they never rely on flexible contracts alone (**SSt-23**). On the other hand, if the green methanol plant operates at a fixed load

while using flexible hydrogen production (i.e. green hydrogen produced only during surplus hours), there will be a need for huge hydrogen buffers. Use of large buffers increase CAPEX and needs more land. As a result, some configurations appeal more than the others to the investors.

Purity of  $CO_2$  supplied to power-to-methanol units can impose technical requirements and act as barrier. Some catalysts for green methanol production are extremely sensitive to impurities like sulfur or heavy metals which are found in industrial flue gas (**SC-13**). As a result,  $CO_2$  should be purified either at the side of supply (i.e. the capturing industries) or at the side of demand (methanol production unit in this case). In both cases, CAPEX increases. Therefore, unless the quality of  $CO_2$  is maintained at the capturing stage, the increase of power-to-methanol CAPEX can act as a barrier to power-to-methanol technologies.

#### **Technology infrastructure**

Considering technology infrastructure, there are three technical infrastructures that play a role. Those are the electricity grid, carbon capture utilization and storage (CCUS) network and hydrogen transport network. First of all, there is an urgent need in the Netherlands to increase the capacity of the power grid. It is insufficient not only for all the new demand created from electrification efforts (SM-1), but also the new renewable power capacity which is planned to be realized in the near future (SF-3). The industry cannot fulfill its energy demand by electrification due to lack of sufficient transmission capacity (SF-4). Green hydrogen production is also seen as a load, which would create extra congestion in the already occupied grid, especially in the Rotterdam area (SC-1). The constraints of the power grid can significantly influence the amount of green hydrogen production and hinder green methanol production. It is worth mentioning that the reason and scale of congestion is important, too. The distribution system might be congested temporarily in case a large load is demanding power for a short while, such as for large construction projects. In these cases, storage systems can resolve congestion (SC-5). Next to the congestion problem which can be seen as a barrier to power-to-methanol technologies, the capacity of cross border interconnection is important. When the installed capacity of renewable power increases and the cross border interconnection has a low capacity, the renewable power becomes available for power-to-methanol process. If the interconnection is increased, the surplus power can be transmitted to other countries, leaving little energy available for green methanol production. In other words, if cross border interconnection is intensified, it allows power export which competes with power-to-methanol when it comes to grid balancing (SC-6).

Availability of feedstocks as an important factor discussed by the experts (look at section 4.3.1) can be influenced by development of transport infrastructures. In particular, green hydrogen developments depends heavily on development of a transport infrastructure, which is expensive (**SC-11**). In the Netherlands there is a possibility to modify the intensified natural gas network for hydrogen transport (**SF-11**). Gasunie has already started a pilot project to convert part of the gas network in the Netherlands to hydrogen transportation network (**SM-11**). Therefore, the perspective of having hydrogen transport network will drive actors to invest in green hydrogen. The situation for CO<sub>2</sub> as another feedstock is different from that of green hydrogen. The future for CO<sub>2</sub> capture is less ambiguous to the players (**SSt-19**). Companies know for a fact that decarbonization of the processes takes time, while they are currently forced to comply with emission reduction requirements. As a result, CCUS systems appear to be the only solution for the transition phase and are being financed (**SSt-20**). The Netherlands is paving the way for two front-runner projects in the Port of Rotterdam (Porthos) and Amsterdam and IJmuiden industrial region (Athos). These two CCUS networks are going to be connected through the OCAP pipeline to form an integrated CCUS infrastructure in the west of the Netherlands. The government has confirmed by means of the Tiki study that CCUS infrastructure is necessary in order to fulfill climate goals (**SM-14**). In conclusion, there is a strong driver for power-to-methanol when technology infrastructures are present. The experts did not mention any driver or barrier that could be categorized as "knowledge infrastructure" according to the definition by Darmani et al. (2014).

#### 4.3.3. Network drivers and barriers

The network of actors that is formed around a specific technology such as power-to-methanol can create drivers for or barriers to deployment of the technology. This network might be viewed from two different angles: the supply chain network or the social network.

#### Supply chain network

First and foremost, the coherence of actions on the production side and the demand side is an important driver of large scale deployment. Green hydrogen as an alternative fuel is a good energy carrier and energy storage medium (**SF-13**), though is only locally adopted. Such initiatives at the local scale cannot solve the climate change problem unless there is a global effort to shift to hydrogen (**SF-15**). If, for example, Port of Rotterdam takes an initiative and invests in bunker fuel stations for alternative fuel, e.g. hydrogen, ships can still get their fuel from other international ports. Therefore, Rotterdam might gradually attract less sea transport and lose its position as an important European hub (**SSt-15**). In particular for the maritime sector, if the shift to E-fuels is started from the demand side, it can drive activities at the production side. In fact, the mere *expectation* that a particular E-fuel will gain a share in the market is sufficient to drive deployment of that technology. Green methanol might have an advantage as bunker fuel over hydrogen and other E-fuels, since the propulsion technology needs only minor adaptations (**SF-23**).

Consumers of green methanol are important nodes in the supply chain network. Their requirements guide the activities at the production side. Currently, the actors in the transport sector, especially aviation and maritime, are potential buyers of alternative low carbon fuels (**SM-20**). These actors have huge energy demands, hence they never rely on flexible contracts alone (**SSt-23**). As a result, the technical configurations that achieve fixed production rates with a reasonable cost win out over the configurations that are offering flexible production at a lower cost. The type of consumer segment creates drivers for investment in certain types of asset and acts as a barrier for other types.

Green methanol is not the only low carbon alternative for bunker fuel. There are parallel supply chains that compete with that of green methanol. In fact, continuing to use fuel for propulsion instead of electric propulsion is logical only if electrification is troublesome (**SSt-10**). The transport sector is going more and more electric. Buses and even heavy duty road transport is going electric (**SF-25**). In the shipping sector, some initiatives are taken for electrification of small-scale ships. Bio-fuel also has a potential to be used in this sector (**SM-21**). For long distance shipping, however, electric options are not feasible. Ammonia is seen as a good alternative for this purpose (**SC-17**). Even a conceptual idea has been developed recently to produce green hydrogen in Sahara, and convert it to ammonia to be used in Europe (**SM-16**). The more competitive alternatives, the smaller the market share for green methanol will be. Presence of competition is a barrier to deployment of power-to-methanol technologies.

Upstream in the supply chain of power-to-methanol, suppliers of feedstock to power-to-methanol process are critical actors. Although the timely development of a CCUS infrastructure is driving power-to-methanol technologies, CO<sub>2</sub> supply comes with uncertainties. Due to economic growth, CO<sub>2</sub> emissions will rise in the course of next decade, though would be limited in the far future as the decarbonization efforts begin to show results (**SF-17**). Therefore, if utilization processes like power-to-methanol are realized now, CO<sub>2</sub> supply will not be adequate in the future and alternatives like Direct Air Capture should be considered (**SF-17**). In other words, CCUS may act as a catalyst to a future of CO<sub>2</sub> supply by DAC (**SF-18**). However, the supply of CO<sub>2</sub> is still uncertain and is a barrier to power-to-methanol deployment. The CCUS network can have a totally opposite effect as well. The development of CCUS network enables higher production rates of blue hydrogen<sup>1</sup>. Cost-wise, blue hydrogen might be competitive to green hydrogen (**SC-15**). However, blue hydrogen is not a suitable feedstock for power-to-methanol because it creates a loop of CO<sub>2</sub> : carbon is captured when blue hydrogen is produced and again combined with blue hydrogen to produce methanol. This process does not contribute to carbon reduction and only increases energy consumption. In conclusion, high production rate of blue hydrogen is a disincentive for green hydrogen production and hence, a barrier for power-to-methanol. Besides competition with blue hydrogen, green hydrogen production faces other issues in the Netherlands. The business case for green hydrogen production is currently very difficult (**SF-7**). There is only a limited amount of renewable power available for green hydrogen production. However, import of green hydrogen can compensate for the lack of production in the country. In fact green hydrogen can be cheaply produced in locations where plenty of solar energy is available throughout the year (**SF-9,SF-14**). If production and/or import of green hydrogen takes off, it drives deployment of power-to-methanol technologies.

#### Societal network

The only driver mentioned by the experts regarding the societal network relates to the interaction between the government and the actors in supply chain network. When actors consider new investment in development, manufacture or operation of low carbon technologies, they try to foresee the future gains of the technology. Subsidies do play a significant role here (**SSt-1**). For example, the future of renewable power plants is more predictable thanks to the consistent and sufficient subsidy allocation to all types of renewable power production (**SSt-9**). Regarding hydrogen production, however, no subsidy has been allocated so far. This makes actors to play "wait-and-see" (**SSt-2**). To put it in a nutshell, coherence and transparency of support mechanisms for all steps of power-to-methanol process are strong drivers within the societal network for the technology. In contrast, lack of coherence and transparency is a barrier.

#### 4.3.4. Actor drivers and barriers

Actors have different motives for their actions. They have targets for the future, want to achieve a competitive position in the market, consider economic factors and have certain structural character regarding flexibility to change.

#### Targets

There are national targets to mitigate climate change by reducing greenhouse gas emissions. Regulations are often enforced in order to push actors to take measures. However, some actors are setting individual goals in order to build up reputation. If aviation and maritime sectors are regulated tightly, E-fuels are promising alternatives for them to switch to carbon-neutral propulsion (**SF-19**). A straightforward way to meet decarbonization requirements for ocean shipping could be to continue using hydrocarbon fuels, though combined with an onboard CCUS system to reproduce its fuel (**SM-22**). In the transport sector, the inland shipping is controlled easier compared to aviation and maritime (**SR-11**), hence is more inclined to shift to alternative fuels. In short, individual actors have CO<sub>2</sub> reduction targets that drive their decision making.

#### Competence

As stated in previous sections, green hydrogen is an important feedstock. Investment in green hydrogen is prominently strategic, meaning that companies tend to think decades ahead (**SSt-12**). Short term finance is

<sup>&</sup>lt;sup>1</sup>Blue hydrogen is produced in the same way as the gray hydrogen is produced, i.e. through steam gas reforming. The difference is that the CO<sub>2</sub> produced in the process is captured and stored instead of being released in the air.

not as determinant of the investment decision as is the tendency to reach a dominant position in the market. The same strategic stance can hold for investors in power-to-methanol technologies. The experts did not make a specific comment on this, though.

#### **Economic factors**

When a new technology is introduced into the market, it takes a while before it is widely deployed. There is a minimum level of technology adoption named "critical mass" after which the growth becomes exponential. Hydrogen production has not reached its critical mass yet (**SSt-14**). Launch of initiatives like "NortH<sub>2</sub>" and "2×40 GW" creates hopes for the future supply of green hydrogen through the backbone (**SM-5**, **SM-9**). There are also studies conducted which investigate production of green hydrogen with solar energy in other countries and transportation of it to the Netherlands (**SM-4**). When green hydrogen production has reached its critical mass, a good perspective is seen for the supply of green hydrogen to power-to-methanol process and hence, green methanol production can speed up faster.

A strong driver of power-to-methanol deployment is the revenue stream and the return on investment. Costs of green hydrogen production is thus important. In the future, when offshore wind energy becomes abundant, offshore green hydrogen production with dedicated wind farms might become economically feasible (**SF-16**). Therefore, high growth rate of offshore wind power plants drives deployment of green hydrogen and hence, power-to-methanol. It is also expected that the CAPEX of electrolysers will decline in the near future as automation and mass-production of electrolyser cells become feasible (**SF-10**). Mass-production of electrolyser cells can reduce green hydrogen production costs and hence, green hydrogen price. CO<sub>2</sub> is the other feedstock needed for power-to-methanol process. However, experts did not explicitly mention economic factors regarding CO<sub>2</sub> utilization system. Obviously, the price of green hydrogen and the trade price of CO<sub>2</sub> being utilized in power-to-methanol process appear in the calculation of power-to-methanol return of investment. High feedstock price is a barrier to power-to-methanol and a driver for the feedstock production side, and vice versa.

Finally, the trade price of green methanol is a basic economic parameter that influences the investment decision on power-to-methanol technologies. This element was also not explicitly mentioned by the experts, although is simple to note its importance. If other factors are isolated, high methanol price can positively influence the business case while low price is a disincentive for the actors. However, for such ground breaking technologies to be realized, there should be sufficient demand for it. Study of the market drivers for the shift to alternative fuels by vehicle owners (Linzenich, Arning, Bongartz, Mitsos, & Ziefle, 2019) indicate that high price for green methanol might be a barrier in some circumstances. In this study, five attributes of the alternative fuel and the impact they have on the decision of consumers have been investigated. Among all, the price of alternative fuel is reported to have the highest decision impact. Therefore, the higher the price of fuel, the lesser the adoption at the demand side. Low demand for the alternative fuel is a disincentive for its production. Therefore, it is not straightforward to determine whether high price for green methanol is a driver for or a barrier to power-to-methanol deployment.

#### Structure

The companies make decisions based on their vision of the future of energy transition (**SSt-1**). Even though there are uncertainties regarding the future energy system, there are clear indications that all sectors are trying to convert to alternative, low carbon technologies. If the transition goes well, the demand for  $CO_2$ emitting fuels will decline. Therefore, investment in production of these fuels will turn into a worse business case in the future (**SF-20**). As an investor, it seems wise to align with the shift to low carbon technologies (**SSt-7**). The moment assets are bought, companies have to assess the risk they are facing from a potential zero-carbon future (**SSt-5**). Methanol production might seem an uninteresting option in this regard. In fact if enough demand is created, hydrogen would be a better choice for energy transition compared to hydrogen-based chemicals (**SF-8**). Therefore, when the transition moves on, the degree to which an actor is flexible to adapt to new routine creates incentive or disincentive for the actor to invest in power-to-methanol. If an actor is willing to accept radical changes, they are more willing to invest in green hydrogen than in green methanol.

#### 4.3.5. Institutional drivers and barriers

Institutional drivers are grouped as soft or hard institutions. In the discussions with experts, soft institutions were not mentioned. Therefore, this section discusses only the aspects related to hard institutions. According to the theory (section 4.1), drivers and barriers created by hard institutions can arise from three qualities of policy: policy formality, policy stability and policy conformity. Policy formality corresponds to the actual regulations set by the government to enable meeting climate goals. Policy stability refers to how predictable the regulations are, and policy conformity means how policies are aligned in different regions and for different technologies.

#### **Policy formality**

Regulation of different sectors of the economy has initiated moves to adopt low carbon technologies. As stated in section 3.2.1, ETS scheme is one of the main policy instruments designed to enforce decarbonization. Some emitters, however, have no feasible option for decarbonization in short term. For example, steel production is energy intensive and has no feasible alternative option to meet its energy demand. In order to meet decarbonization goals, they are thus interested in utilization of their CO<sub>2</sub> emission to produce jet fuel (**St-18, SM-19**). Another similar initiative which was among the first carbon utilization projects realized is Twence's CO<sub>2</sub> utilization to produce sodium bi-carbonate (**SM-12**). In short, strict carbon reduction targets imposed on the sectors that have difficulty in decarbonization turns into a driver for power-to-methanol (and other carbon utilization) technologies.

Relevant policies are not only aiming to prevent  $CO_2$  emissions, but also to support low carbon technologies. Current support mechanisms in the Netherlands as discussed in section 3.2.2 do not have a specific support scheme for alternative fuel production technologies such as power-to-methanol. However, the feed-stocks, i.e. green hydrogen production and  $CO_2$  capture, are supported. Devising a precise support mechanism for power-to-methanol technologies can be a strong driver of the technology.

#### Policy stability

Whether it is about support or limitation, regulations are changing constantly and so do the rules of game for actors (**SR-1**). With regard to green methanol production, the main uncertainty is with respect to ETS emission right allocation. Currently there is a discussion regarding ETS emission rights in case the captured  $CO_2$  is utilized instead of storage. It is not made clear in the ETS scheme who is held accountable for the  $CO_2$  that is released into the air from the product of  $CO_2$  utilization after its end of life (**SR-8**). Currently, greenhouses are taking  $CO_2$  from the OCAP pipeline, though are not paying for ETS emission rights (**SR-9**). Furthermore, companies which inject their captured  $CO_2$  in OCAP do not receive free emission rights. This scheme is indeed line with the philosophy of ETS emission rights to penalize  $CO_2$  emission, though is under discussion (**SR-10**). The uncertainty of regulations is a disincentive for actors to invest in power-to-methanol technologies.

#### **Policy conformity**

The critical infrastructures such as power grid, hydrogen backbone and CCUS are changing slowly. In the next decade, we are not expecting radical changes regarding the infrastructure. This is mainly due to the complexity that the set of all regulations create in the institutional framework of developments (**SR-3**). Policies for different sectors create a difficult environment for development of low carbon technologies such as power-to-methanol.

#### 4.4. Summary

In the previous section, expert opinion was analyzed and placed into the framework of incentives for deployment of renewable energy technologies developed by Darmani et al. (2014). This analysis answers subquestion 1: *What are the major drivers of and barriers to deployment of power-to-methanol technologies*?

#### 4.4.1. Framework: drivers and barriers of power-to-methanol technologies

Figure 4.1 shows the framework with the drivers and barriers. White boxes indicate drivers and pale red boxes contain barriers to the deployment of power-to-methanol technologies. Gray boxes show the factors that could be both a driver or a barrier through the course of technology deployment and depending on the conditions. Furthermore, the reader can recognize gaps in the framework, highlighted as "knowledge gap". These are the factors that were discussed neither in the interviews nor in the reviewed literature.

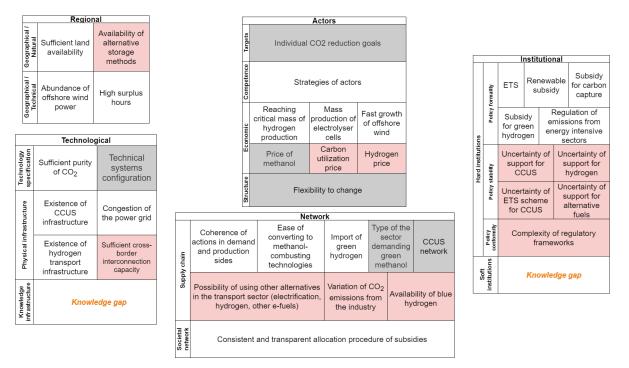


Figure 4.1: Drivers for and barriers to deployment of power-to-methanol technologies. White boxes: drivers, pale red boxes: barriers, gray boxes: driver and/or barrier.

#### 4.4.2. Knowledge gaps in the framework

The two main areas that are overlooked by the experts are "knowledge infrastructure" and "soft institutions". Knowledge infrastructure is constructed of the plethora of research institutes, universities, acknowledged

researchers, experts and technology know-hows. The knowledge infrastructure is available to other actors in the field. As the knowledge infrastructure related to a technology is strengthened, the deployment of that technology becomes easier. Soft institution is another aspect largely missing in the expert opinion. Soft institutions are formed from norms, cultures and values of the community related to the technology.

Other than the two factors missing in the interview results, some of the drivers and barriers are apparently are not elaborated. First, incentives can arise from the societal network around the technology, though the only driver mentioned in this category was the relation between actors and the government and the procedure of subsidy allocation. In fact, study suggests that public support or opposition can influence low carbon projects to a great extent de Vries (2016). However, the connection between actors and the community did not appear in the interview result. The public opinion regarding power-to-methanol technologies worth of studying not only for the sake of science but also for the business of consultancy.

The second driver that was vaguely addressed is the impact of organizational structure of actors. The current results only show that the flexibility of actors is important. However, although there are studies that emphasize the cooperation of actors (e.g. Mallett (2013)), a typology of actors, their organizational structure and their flexibility to change is not found in the literature analyzed so far.

Finally, the only issue related to policy conformity incentives was the fact that regulations have created a complex institutional framework for low carbon technologies and this is hindering developments. However, conformity of the policies related to power-to-methanol technologies in different countries in the EU seems to be a matter of importance as well. This topic was not discussed in the interviews. However, the interviewees brought up the discussion about necessity of collaboration with other countries in the EU in order to make a change with respect to Power-to-X options (e.g. **SF-9,SF-15**).

At the decision making stage, lack of attention to the factors that influence power-to-methanol technologies can have effects. The decision makers might picture the situation incompletely and differently. Most of the interviewees have consultancy or management roles (table C.1). If they are unaware of some drivers and barriers, they will not be able to provide the right advise to the private sector. This can cause actions at the private sector that are not aligned with other actors. For example, when a firm has been formerly active in a business, she has accumulated in-house expertise. If that expertise can be used for green methanol production processes, it gives them a competitive position to enter that market. However, if she or her consultants are unaware of the effect of knowledge infrastructure, they will miss the opportunity. In general, it is best for the consultants to have the complete picture. It is not only important for the private sector but also for the public sector. A policy to support or not support power-to-methanol technologies can easily go wrong if the policy makers have incomplete view of the drivers and barriers of the technology. This shows the importance of empty or incomplete fields in the framework. It should be noted, however, that no policy makers based on the results presented here. There are unexplored matters regarding drivers for and barriers to power-to-methanol technologies that is worth of further investigation.

# 5

### Modeling

In this chapter the scope of the model, assumptions, model logic, inputs, outputs and external data are discussed. Wherever a reference is made to the model assumptions, the label (in the format **A-x** where "x" is a number) is mentioned in brackets. All assumptions are listed in appendix A and formulas for the model logic can be found in appendix B.

#### 5.1. Scope of the model

The vast number of drivers for power-to-methanol technologies renders the problem highly complex. Not all drivers are quantified in the model. In fact, the drivers are put in three groups. The first group of drivers are excluded from the model. In this group fall the drivers which have a complicated impact on the system. Quantification of their influence is, hence, not feasible and requires a separate study. An example is the impact of the flexibility of actors. The import of green hydrogen is also not possible to model, because the dynamics of green hydrogen import correspond to a global development which is extremely complex. Land availability is another driver in this category.

In order to manage the research within the time scope, several assumptions are made regarding the second group of drivers. In this way, the impact of these drivers on the system remain limited and under control. A good example is the existence of CCS infrastructure, which is assumed to be in place regardless of the drivers that influence its development. The assumptions with regard to technical configuration of the system also fall into this category. Highlights of assumptions are discussed in section 5.2 and elaborated upon in appendix A.

The third group of the drivers are included in the model, either as input or as model parameters. The impact of these drivers can be quantified using the model investigated thoroughly. At least one driver from each main category of drivers, i.e. regional, technological, actors, network and institutional drivers, is quantified in the model. These drivers are:

- Surplus hours (Regional),
- · Abundance of offshore wind power (Regional),
- Congestion on the power grid/Demand increase from electrification (Technological/Physical infrastructure),

- Strategies of actors/Investment in green hydrogen (Actors/Competence)
- Price of methanol (Actors/Economic),
- Carbon utilization price (Actors/Economic),
- Hydrogen price (Actors/Economic),
- Variation of CO<sub>2</sub> emission from the industry (Network/Supply chain),
- Coherence of actions in demand and production sides/Existing demand for methanol as fuel (Net-work/Supply chain),
- EU ETS (Institutional/Policy formality),
- Subsidy for carbon capture (Institutional/Policy formality),
- Uncertainty of ETS scheme for CCUS (Institutional/Policy stability).

Variation of  $CO_2$  emissions is considered as a decreasing factor in the amount of emissions and abundance of offshore wind is included by renewable scenarios. Input parameters are discussed further in section 5.5.4.

#### 5.2. Assumptions

To build up the model, several assumptions are made. Initially, the *boundary* of the technical system that is going to be modeled is set using primary assumptions. Other assumptions mostly correspond to the *logic* of the model, i.e. how the real world is quantified in the model. A few assumptions are made in order to deal with *uncertain* factors and parameters. For example, the future support for and regulation of green hydrogen production is not clear. In order to model uncertain factors like regulatory uncertainty, assumptions are made. A complete list of assumptions is found in appendix A. The highlights of assumptions in these three categories are listed below:

- Green hydrogen production takes place during surplus hours only. However, CO<sub>2</sub> capture and green methanol production are not flexible (boundaries of system).
- Green hydrogen and CO<sub>2</sub> needed for green methanol production are obtained from external sources (boundaries of system).
- Porthos, Athos and OCAP form one single CCUS infrastructure (boundaries of system).
- All actors make investment decisions based on their estimation of Net Present Value (NPV)(logic of model).
- If CO<sub>2</sub> is utilized at a certain rate, an equal amount of capacity is released in the CCUS network (logic of model).
- No subsidy is granted for green hydrogen and green methanol production (uncertain parameters).
- Industries capturing CO<sub>2</sub> would need to buy the emission rights (uncertain parameters).

#### 5.3. Rules of action

As explained in section 2.6, the actors modeled in this research are the investors in green hydrogen production (electrolysers), carbon capture and green methanol production. This section describes the decision making rules for each actor. A brief explanation of how each action might influence model KPI's (grid balance and  $CO_2$  reduction) is also provided.

#### 5.3.1. Investment in green hydrogen

Green hydrogen production is possible whenever surplus electricity is available (**A-1**). It is indeed be possible to run the electrolysers constantly, though it would not be called "green" anymore, since the power is not coming from carbon-free sources (**A-2**). As a result of this assumption, no decision on green hydrogen production is made unless the investors expect surplus power becomes available. They estimate whether surplus power will be available or not by extrapolating the trend. There are two types of investment behavior. If renewable energy grid balance  $GB_{RE}$  (given by equation 2.3) is positive in the year of decision and the investment is perceived as profitable, most of the actors become interested in the investment. In that case, market incentive is provided to capture all excess energy and several actors make investment in electrolysers. This results in a total production capacity equal to the excess renewable energy available. If  $GB_{RE}$  is negative and is expected to turn positive within a decision window of  $t_D$  years, the investors consider placing investment in a conservative production capacity ( $P_{min,H_2}$ ) if it might be profitable. The expected grid balance,  $GB_{RE,exp}$ , is calculated by a linear extrapolation of  $GB_{RE}$  in each year:

$$GB_{RE,exp} = GB_{RE,t_0} + \frac{\Delta GB_{RE}}{\Delta t} t_D , \qquad (5.1)$$

where  $GB_{RE,t_0}$  is the RE grid balance in the decision year. When an investment is placed, depending on the year, the investor makes a choice about electrolyser technology (**A-3**). Whether or not the investment in electrolyser is expected to be profitable depends on the value of Net Present Value (NPV) calculated with the formula (**A-4,A-5,A-6**):

$$NPV_{H2} = -CAPEX_{H_2} + \sum_{t=1}^{L_{H_2}} \frac{\pi_{H_2}}{(1+i)^t} , \qquad (5.2)$$

where  $CAPEX_{H_2}$  is the capital cost per unit hydrogen production of electrolyser (**A-7**),  $L_{H_2}$  is the lifetime of electrolysers,  $\pi_{H_2}$  is the price of hydrogen per unit energy content of hydrogen (**A-8**) and *i* is the discount rate. If  $NPV_{H_2} > 0$  the investment is profitable and the investor decides to invest.

Since hydrogen production is expected to help with seasonal storage, the production capacity of electrolysers is set to the amount of surplus power that is available at the time of investment (**A-9**). The electrolyser efficiency is determined based on the choice of technology (**A-10**) in the range of 63 to 74 percent (look at section A.2). It should be noted that new investment in electrolysers is conditioned on the presence of the hydrogen backbone (**A-11**). From the moment that a connection to the hydrogen backbone is made till the end of simulation, the user purchases green hydrogen through the hydrogen backbone and cannot switch to other hydrogen sources (**A-14**). When green hydrogen is available, it is first utilized for green methanol production. In case there is more hydrogen available than demanded for green methanol production, it can be sold to other industries that take hydrogen as feedstock. In this way, less gray hydrogen is used and the  $CO_2$  emission from gray hydrogen production is saved.

#### 5.3.2. Investment in carbon capture

The industries modeled here are all covered by ETS scheme (A-15). Therefore, they are paying for ETS emission rights. In the year that CCUS infrastructure is available (A-16,A-17), they can consider capturing CO<sub>2</sub> (A-19). No priority is given to industries, i.e. they can all request a connection of the size they want (A-20) if there is a business case for them (A-21).

There are two different types of business case. First, if no demand for  $CO_2$  is demonstrated yet, the industries calculate the NPV of new carbon capture facilities with the equation:

$$NPV_{Cap.} = -C_{Conn.} + \sum_{t=1}^{15} \frac{\bar{\pi}_{ETS} + S_{Cap.} - C_T - C_S}{(1+i)^t} + \sum_{t=16}^{L_{Cap.}} \frac{\bar{\pi}_{ETS} - C_{Cap.} - C_T - C_S}{(1+i)^t} .$$
(5.3)

In this equation,  $C_{Conn.}$  is the cost of making a connection to the CCUS network (**A-23**),  $\bar{\pi}_{ETS}$  is the average estimation of the price of ETS rights that each industry has at the time of decision making for the next 5 years (**A-22**),  $S_{Cap.}$  is the amount of subsidy that is granted for CCS in the first 15 years of its operation,  $C_T$  is the transport cost,  $C_S$  is the storage cost paid to the CCUS network operator,  $L_{Cap.}$  is the lifetime of capture technology,  $C_{Cap.}$  is the approximate yearly costs of carbon capture technology (including CAPEX and OPEX) and *i* is the discount rate.

In case there is a demonstrated demand for  $CO_2$  (i.e. operational methanol production plants were constructed before), the industries include the revenue from selling  $CO_2$  in their calculations. They have to exclude the savings they had from not buying ETS emission rights (**A-24**). The following formula shows the NPV is this case:

$$NPV_{Cap.} = -C_{Conn.} + \sum_{t=1}^{15} \frac{\pi_U + S_{Cap.} - C_{Cap.} - C_T}{(1+i)^t} + \sum_{t=16}^{L_{Cap.}} \frac{\pi_U - C_{Cap.} - C_T}{(1+i)^t} .$$
(5.4)

Here,  $\pi_U$  is the price of utilized CO<sub>2</sub> (A-25) and the storage costs are excluded from calculations.

In reality, industrial capture can be partly utilized and partly stored. However, this configuration creates infinite number of possibilities for decision making (i.e. the share of stored to utilized  $CO_2$ ) and requires collaboration of actors. In this model, industries calculate their business cases either by the assumption of 100% storage or 100% utilization. The actual decision is made by the CCUS network operator (**A-27**).

In the year which investment in carbon capture becomes profitable, the industry starts to capture. However, if the CCUS network is utilized to its maximum capacity, they have to withhold their investments (**A-28**). If capacity becomes available later (**A-29**) they can proceed with their investments provided that the new market conditions create a positive business case for them.

Industrial carbon capture uses power and hence reduces the grid balance. Both capture and compression processes require electricity. Obviously, carbon capture has a direct impact on  $CO_2$  reduction. Furthermore, total  $CO_2$  emission by industries decrease on a yearly basis due to improving the process efficiencies and electrification of the processes (**A-31**).

#### 5.3.3. Investment in green methanol

If there is sufficient hydrogen and  $CO_2$  available, it is possible to produce methanol to be used as fuel for shipping (**A-36**). Investors in green methanol production calculate the NPV of a new methanol production plant using the formula:

$$NPV_{MeOH} = -CAPEX_{MeOH} + \sum_{t=1}^{L_{MeOH}} \frac{\pi_{MeOH} - OPEX_{MeOH}}{(1+i)^t} ,$$
(5.5)

where  $CAPEX_{MeOH}$  and  $OPEX_{MeOH}$  are the upfront investment costs and operational costs of methanol production plant per unit energy content of methanol,  $\pi_{MeOH}$  is the price of methanol (A-37,A-38),  $L_{MeOH}$  is the lifetime of the plant, and i is the discount rate. Operational costs include the costs of input energy (electricity) and feedstock (hydrogen and CO<sub>2</sub>), and is calculated by:

$$OPEX_{MeOH} = OPEX_{fix,MeOH} + f_{H_2}\pi_{H_2} + f_{CO_2}\pi_{CO_2} + f_e\pi_e , \qquad (5.6)$$

in which  $OPEX_{fix,MeOH}$  is the fixed operational costs of the plant (i.e. labor, maintenance, etc.),  $f_x$  represent the amount of input *x* required for unit production of methanol and  $\pi_x$  is the unit price of input *x*. The investor decides on the capacity of the plant based on the availability of hydrogen and CO<sub>2</sub> (A-40).

Green methanol production requires electricity, thus increases load on the power grid and reduces the grid balance. Moreover, it contributes to  $CO_2$  reduction in different ways: first, green methanol substitutes dirty fuels for shipping and reduces emission from that sector, and second, the process takes  $CO_2$  from the CCUS network and allows for more capture from the industries. A third element to  $CO_2$  reduction is created when more green methanol is produced than the amount demanded by the shipping sector. In this case, green methanol takes a share in the market for methanol and an amount of  $CO_2$  production is avoided due to down-scale of normal methanol production.

#### 5.4. Calculation of KPI's

The main KPI's of this model are RE grid balance and  $CO_2$  reduction. The equations used to calculate the KPI's and related variables are presented in this section.

#### 5.4.1. Calculation of grid balance

As explained in section 2.7.1, the renewable energy (RE) grid balance in each year is calculated by equation 2.3:

$$GB_{RE} = GB - E_{Conv.} .$$

In this equation, *GB* stands for grid balance which is the overall yearly balance of demand and supply. It can be attributed to the surplus of renewable power available to the grid which is equal to the total surplus renewable production deducted by the *dedicated* demand for renewables. Dedicated demand can be, for example, demand for green hydrogen and green methanol production. Therefore, RE grid balance is calculated as:

$$GB_{RE} = P_{RES}T_{RES} - D^* - E_{Conv.}, \qquad (5.7)$$

where  $P_{RES}$  is the installed capacity of renewables,  $T_{RES}$  is the approximate number of surplus hours,  $D^*$  is the yearly dedicated demand for renewables and  $E_{Conv.}$  is the yearly production of conventional power plants. The power demand that renewable sources are dedicated to satisfy,  $D^*$ , is calculated as:

$$D^* = P_{H_2} T_{H_2} + P_{MeOH} T_{MeOH} + \Delta \epsilon_{Cap.} \tilde{P}_{Cap.} T_{Cap.} , \qquad (5.8)$$

where  $P_x$  is the production capacity of substance x (x can be  $H_2$  or MeOH),  $T_x$  is the total hours of operation related to substance x in a year,  $\Delta \epsilon_{Cap}$  is the total amount of CO<sub>2</sub> which is captured and  $\tilde{P}_{Cap}$  is the power demand per unit CO<sub>2</sub> captured. In other words, it is assumed that the power demand for green hydrogen production, green methanol production and CO<sub>2</sub> capture is satisfied by renewable power.

RE grid balance ( $GB_{RE}$ ) gives an indication of how much is the power grid occupied by renewables. A negative balance means the renewables are not sufficient to supply power to the grid. Negative RE balance on the grid is equivalent to systemic "shortage" periods of renewables, hence a need for flexible, conventional power plants. A positive RE grid balance, on the other hand, means that renewables are playing a major role

in the power system. Although positive balance is also not suitable for the grid, it is an indication of a "green" power system. In general, stable RE grid balance that remains close to zero is desirable.

#### 5.4.2. Calculation of CO<sub>2</sub> reduction

Incorporating green hydrogen and green methanol in the energy system is an endeavor to facilitate energy transition. The potential of green methanol to contribute to energy transition can be measured by the amount of CO<sub>2</sub> emission reduction that is achieved in the course of deploying power-to-methanol technologies. Total CO<sub>2</sub> reduction is found in each year using the formula:

$$\Delta \epsilon_{Tot.} = \Delta \epsilon_{Power} + \Delta \epsilon_{Cap.} + \Delta \epsilon_{H_2} + \Delta \epsilon_{MeOH} , \qquad (5.9)$$

where  $\Delta \epsilon_x$  is the amount of CO<sub>2</sub> emission avoided by the changes related to sector *x*. Sectors (*x*) are renewable power production (*Power*), industrial capture (*Cap.*), hydrogen production (*H*<sub>2</sub>) and methanol production (*MeOH*).

The climate agreement indicates the vision for  $CO_2$  reduction by percentage of reduction compared to 1990 emission levels. The percentage of  $CO_2$  emission reduction is calculated using the formula:

$$p_{sect.} = \frac{\sum_{x \in sect.} \Delta \epsilon_x}{\epsilon_{ref,x}} , \qquad (5.10)$$

in which  $p_{sect.}$  is percentage of CO<sub>2</sub> reduction in a specific sector,  $\Delta \epsilon_x$  is the amount of CO<sub>2</sub> reduction due to change *x* in the corresponding sector and  $\epsilon_{ref,x}$  is the reference value of emissions for that sector. Sectors are power, industry and the whole economy. This section presents the steps for calculation of CO<sub>2</sub> reduction due to a change in system.

#### Reduction from renewable power production

 $CO_2$  reduction takes place in the power sector ( $\Delta \epsilon_{Power}$ ) due to increase in renewable power production. When the share of renewables increases, because the marginal cost of renewable power production is close to zero, fossil-fueled power plants are pushed to lower merit order (i.e. they can sell less power to the market). Therefore, for unit power supply from renewables, an amount of  $CO_2$  emission is avoided that is equal to the average  $CO_2$  emission from conventional power plants. The following formula gives the  $CO_2$  reduction in the power sector:

$$\Delta \epsilon_{Power} = \delta \tilde{\epsilon}_{Power} S_{RES} , \qquad (5.11)$$

where  $\delta \tilde{\epsilon}_{Power}$  is the CO<sub>2</sub> emission per unit power supply from conventional power plants and  $S_{RES}$  is the supply of renewable power.

#### Reduction due to industrial capture

The amount of emission reduction due to industrial capture is a direct CO<sub>2</sub> reduction calculated as:

$$\Delta \epsilon_{Cap.} = \sum_{i=1}^{11} \Delta \epsilon_i , \qquad (5.12)$$

in which  $\epsilon_i$  is the amount of CO<sub>2</sub> captured by industry *i*. The sum over all 11 modeled industries (listed in table 3.5) gives the direct emission reduction due to industrial capture. The maximum amount that each industry can capture in year *n* is:

$$\Delta \epsilon_{i,max_n} = \epsilon_{i,0} r^{(n-2020)} - \Delta \epsilon_{i,n-1}, \tag{5.13}$$

in which  $\epsilon_{i,0}$  is the industry's emission in 2020, r is the CO<sub>2</sub> emission reduction rate due to improvement of processes and electrification and  $\Delta \epsilon_{i,n-1}$  is the total amount of captured emission before year n. In this equation, n varies between 2020 to 2050.

#### **Reduction from hydrogen production**

Green hydrogen production has an indirect effect on  $CO_2$  reduction. If the hydrogen demand for green methanol production is fulfilled, green hydrogen can substitute gray hydrogen that is used in the industry. As a result, the demand for gray hydrogen decreases and hence, less gray hydrogen is produced. Therefore, for unit green hydrogen that does not end up in methanol production, an amount of  $CO_2$  emission is avoided that equals the amount of  $CO_2$  emission from gray hydrogen production. The  $CO_2$  reduction by green hydrogen production is given by:

$$\Delta \epsilon_{H_2} = \delta \tilde{\epsilon}_{H_2} (P_{H_2} T_{H_2} - f_{H_2} P_{MeOH} T_{MeOH}), \qquad (5.14)$$

where  $\delta \tilde{\epsilon}_{H_2}$  is the CO<sub>2</sub> emission per unit gray hydrogen production,  $P_x$  is the total capacity of production of substance *x*,  $T_x$  is the total hours of operation related to substance *x* in a year and  $f_{H_2}$  is the amount of hydrogen required for unit production of green methanol.

#### **Reduction from methanol production**

Same as green hydrogen, green methanol production influences  $CO_2$  emissions indirectly. If the methanol demand in the shipping sector is fulfilled (**A-36**), green methanol can substitute normal methanol (produced from natural gas) that is used in the industry. As a result, the demand for normal methanol decreases and hence, less normal methanol is produced. Therefore, for unit green methanol that does not end up in fuel tanks for shipping, an amount of  $CO_2$  emission is avoided that equals the amount of  $CO_2$  emission from normal methanol production. The  $CO_2$  reduction by green methanol production is given by:

$$\Delta \epsilon_{MeOH} = \delta \tilde{\epsilon}_{MeOH} (P_{MeOH} T_{MeOH} - \alpha_{MeOH} D_{Shipping}), \qquad (5.15)$$

where  $\delta \tilde{\epsilon}_{MeOH}$  is the CO<sub>2</sub> emission per unit normal methanol production,  $P_{MeOH}$  is the total capacity of green methanol production,  $T_{MeOH}$  is the total hours of green methanol production in a year,  $D_{Shipping}$  is the total energy demand by the shipping sector and  $\alpha_{MeOH}$  is the percentage of energy demand by the shipping sector that is fulfilled by green methanol.

#### Other compartments of CO<sub>2</sub> reduction

The four compartments of  $CO_2$  reduction discussed above are not the only contributors. In reality,  $CO_2$  reduction also happens when green methanol is used as an alternative, low carbon fuel in the shipping sector. Furthermore, when green hydrogen and green methanol reach substantial production levels, market share of gray hydrogen and normal methanol decreases. As a result, demand for natural gas as a feedstock for gray hydrogen and methanol production declines. In the long term, this results in a reduction in natural gas extraction which in turn leads to a reduction in  $CO_2$  emissions from exploration and exploitation of gas fields. Due to high complexity, the two elements of  $CO_2$  reduction mentioned above are not included in the calculations of  $CO_2$  emission in this research. Hence, the calculated results indicate the lower bound of  $CO_2$  reduction.

#### 5.4.3. Calculation of intermediate variables

In sections 5.4.1 and 5.4.2, the formulas used for calculation of grid balance and CO<sub>2</sub> reduction were presented. On the right hand side of these formulas appear some intermediate variables. These variables are the total capacity of hydrogen production ( $P_{H_2}$ ), the total capacity of methanol production ( $P_{MeOH}$ ) and the total amount of industrial CO<sub>2</sub> capture ( $\Delta \epsilon_{Cap}$ .). These variables depend on the decisions that investors make and are calculated in each year of the simulation.

#### 5.5. Numerical values in the model

In this section, the numerical values of inputs, parameters for actors, factors involved in decision making and for calculation of outputs are listed.

#### 5.5.1. Parameters for actors

The most heterogeneous group of actors are industrial emitters. In this model, the top 11 emitters in the regions of Rotterdam and Amsterdam are modeled. Table 5.1 list their emissions and capture costs.

Table 5.1: The emissions and capture costs for the emitting industries in the model. Source: EBN and Gasunie (2017).

Nome	<b>Emission</b> $[\epsilon_{i,0}]$	Capture cost	
Name	(Mton/yr)	[ <i>C<sub>Cap.</sub></i> ] (€/ton)	
Tata steel	6.21	69	
Uniper centrale Maasvlakte	5.95	57	
Uniper centrale Maasvlakte 3	4.67	57	
Shell Pernis	4.25	78.9	
Nuon power Velsen	3.63	79	
Essent Amercentrale	3.52	57	
Shell Moerdijk chemie	2.55	43	
BP Raffinaderij	2.29	78.9	
Nuon power IJmond	2.15	79	
Esso Raffinaderij	2.1	78.9	
Gunvor Petroleum	0.42	78.9	

#### 5.5.2. Variables for decision making

As explained in section 5.3, actors rely on different variables to make decision. The parameters used for decision making are listed in table 5.2.

Table 5.2: Variables and parameters used by actors in decision making.

Variable	Definition	Value			Course of
	Definition	2020	2030	2050	– Source
i	Discount rate		4.5%		van den Boomen,
					Schoenmaker, Ver-
					laan, and Wolfert
					(2017)
$CAPEX_{H_2}$	Investment cost of elec-	500	400	200	IEA (2019a)
	trolysers $(\in /kW_e)$				
$L_{H_2}$	Lifetime of electrolysers		20		– Danish Energy
	(yr)				Agency and En-
					erginet (2020)
				Cor	ntinued on the next page.

Variable	Definition		Value	Courses	
variable	Definition	2020	2030	2050	– Source
$\bar{\pi}_{ETS}$	Average ETS emission right price (€/ton CO <sub>2</sub> )	-	increases n 20.55 in <sub>050</sub> in 2050	per 2020	EEX (2020), table 5.4
C <sub>Conn.</sub>	Costs of making a con- nection to CCUS network (€/ton CO <sub>2</sub> )		4.5		Lensink (2020)
$C_T$	CCUS transport costs (€/ton CO <sub>2</sub> )		45		Lensink (2020)
$C_S$	CCUS storage costs (€/ton CO <sub>2</sub> )		15		Lensink (2020)
L <sub>Cap</sub> .	Lifetime of carbon capture technologies (yr)		25		Lensink (2020)
CAPEX <sub>MeOH</sub>	Capital expenditure for green methanol plant (mln. $\in /PJ_{MeOH}$ )	11	8	7	Detz (2019)
OPEX <sub>fix,MeOF</sub>	<sup>I</sup> Fix operational expendi- ture for green methanol plant (mln. €/PJ <sub>MeOH</sub> )	0.44	0.24	0.18	Detz (2019)
L <sub>MeOH</sub>	Lifetime of green methanol production plant (yr)		25		Detz (2019)
$f_{H_2}$	Hydrogen requirement per unit methanol production $(PJ_{H_2}/PJ_{MeOH})$	1.22	1.2	1.18	Detz (2019)
fco <sub>2</sub>	$CO_2$ requirement per unit methanol production (M ton $CO_2/PJ_{MeOH}$ )		0.07		Detz (2019)
fe	Electrical energy require- ment per unit methanol production $(PJ_e/PJ_{MeOH})$	0.05	0.04	0.03	Detz (2019)
$\pi_e$	Electricity price (€/MWh)	43	57	57	Schoots and Han

Table 5.2: Variables and parameters used by actors in decision making (continued).

mingh (2019)

#### 5.5.3. Variables for KPI calculations

Calculations of KPI's are explained with formulas in section 5.4. The numerical values of the parameters used in those formulas are listed in table 5.3.

Variable	Definition	Value (2020 to 2050)	Source
E <sub>Conv</sub> .	Power dispatched from conventional power	97.5	CBS (2020a)
	plants per year (TWh)		
$T_{MeOH}$	Production hours of green methanol plant	8760	A-42
	(hr/yr)		
$T_{Cap.}$	Operation hours of $CO_2$ capture unit (hr/yr)	8760	A-33
$\delta\epsilon_{Power}$	CO <sub>2</sub> emission per unit power supply from	650	CBS (2018)
	conventional power plants (ton $CO_2/MWh$ )		
$\delta \epsilon_{H_2}$	CO <sub>2</sub> emission per unit gray hydrogen pro-	70	IEA (2019b)
	duction (kg $CO_2/GJ_{H_2}$ )		
$\delta\epsilon_{MeOH}$	CO <sub>2</sub> emission per unit normal methanol	2.3	IEA (2019a)
	production (ton CO <sub>2</sub> /ton MeOH)		
D <sub>Shipping</sub>	Energy demand by the shipping sector (PJ)	100	CPB and PBL (2015)
r	CO <sub>2</sub> reduction by electrification and pro-	0.8%	Schoots and Ham-
	cess improvements		mingh (2019)

Table 5.3: Variables and parameters used for calculation of KPI's.

#### 5.5.4. Model inputs

Whereas the aforementioned parameters take specific values, inputs vary in a range. This has two reasons: first, the values of inputs are often uncertain and cannot be determined with accuracy. The second reason is due to the exploratory nature of the study. The general approach in agent-based modeling is to capture different possible behaviors in the system by varying the input values in a meaningful range. In an experiment, each of these parameters take a specific value in the corresponding range. Experiments are explained in section 5.7. Table 5.4 shows numerical input parameters that can be manipulated by the user and the range of variation.

Another input parameter provided by the user is the "scenario" of renewable power production up to 2050. This input determines the numerical value for variable  $P_{RES}$ , the total installed capacity of renewables in each year. Four choices are possible for the renewable scenario: "Slow change" corresponds to the lowest development rate expected, which results in a total of 108 gigawatt installed capacity of wind and solar energy in 2050. "Pragmatic sustainability" suggests slightly higher development rate, with 118 gigawatt installed capacity in 2050. "Rapid development" and "Sustainable together" are the other two scenarios, which predict 128 and 156 gigawatt installed capacity in 2050, respectively. The value of installed capacity in each of the scenarios were introduced in table 3.2 and are summarized in table 5.5.

#### 5.6. Model verification and validation

This model includes decision making processes as well as technical processes. The logic and numerical calculations of the model should be *verified* in order to circumvent subtle mistakes. Furthermore, in order to make sure the processes are aligned and coherent with real life, the model should be *validated*. Validation is Table 5.4: Input variables and the range of values.

Variable	Definition	Range of values
Renewable scenario	The scenario for renewable power produc-	Explained in table 5.5
	tion until 2050.	
$\alpha_{MeOH}$	Share of energy demand for shipping, ful-	0-100%
	filled by green methanol	
$t_D$	Decision window of investment in electrol-	Any value
	ysers (yr)	
$P_{min,H_2}$	Electrolyser capacity of early movers (MW)	Any value
$\pi_{H_2}$	Hydrogen price	1-2.5 €/kg
$\pi_U$	Average price of utilized CO <sub>2</sub>	10-90 €/ton
$\pi_{MeOH}$	Green methanol price	250-450 €/ton
$\pi_{ETS,2050}$	ETS emission right price in 2050	40-160 €/ton
S <sub>Cap</sub> .	Carbon capture subsidy	0-100 €/ton capture
$T_{RES}$	Surplus hours	500-3000 hr/yr
$T_{H_2}$	Hours of hydrogen production	500-2500 hr/yr

Table 5.5: Scenarios of renewable power production up to 2050. Source: Matthijsen et al. (2018) & Schoots and Hammingh (2019).

Installed capacity (GW)		
2020	2030	2050
14.7	44.6	108
14.7	44.6	118
14.7	44.6	128
14.7	44.6	156
	<b>2020</b> 14.7 14.7 14.7	2020         2030           14.7         44.6           14.7         44.6           14.7         44.6           14.7         44.6

the procedure to determine how well is the implemented model coherent with the real world (Rand & Rust, 2011). This section presents a brief explanation of verification and validation steps.

#### 5.6.1. Verification

The first version of model outputs were analyzed to find potential errors in calculations. This has been done with the help of one energy expert. Some mismatches were identified and corrected. Among all tests that have been performed, the following are highlighted:

- The amount of energy stored in hydrogen and methanol in a year should be less than the amount of renewable energy made available in that year.
- The total energy content (high heating value) of green methanol produced in a year should be less than the amount of energy content (high heating value) of green hydrogen produced in a year.
- The amount of green methanol produced in a year should be less than or equal to the amount allowed by the availability of  $CO_2$ .
- The amount of CO<sub>2</sub> reduction from industrial capture should be less than or equal to the total amount of emissions from modeled industries.

- The amount of CO<sub>2</sub> reduction from hydrogen production and renewable power production should be always zero or positive.
- No hydrogen production before 2030.
- No CO<sub>2</sub> capture before 2027.

#### 5.6.2. Validation

One way of model validation is by comparing results with historical data. However, the model presented in this research creates projections for the future of the energy system. As a result, historical data is not available to validate the model outputs with. Instead of output validation, this model is "face validated" using expert opinion. As explained by Rand and Rust (2011), properties, mechanisms and aggregate patterns of agent-based models can be validated on face without making use of quantitative data. For face validation, researcher should step out of the context and use common sense to make sure the model behavior is valid (Salkind, 2010).

In total, seven energy experts critically reviewed the assumptions and attributes of the model and assessed its overall performance. The logic of decision making, the technical and institutional scope of the project and general patterns in model output were discussed during the meetings with experts. The model logic was improved based on expert opinion. The following points were suggested to improve the model logic:

- Statement: Investors in hydrogen tend to look ahead and predict what comes next.
- **Improvement**: The actors have two modes of investment. The first mode of decision making corresponds to the case which renewable power is not abundant. The actors extrapolate the trends and if they see a positive balance in the next five years, they invest in a conservative capacity. The second type of decision making happens when enough renewable power is available to invest in a large capacity. In that case, all actors can take part and utilize a part of excess energy in order to produce green hydrogen.
- **Statement**: If an industry makes a connection to the hydrogen backbone, they rely on a long term contract to have their hydrogen demand supplied from the pipelines.
- **Improvement**: According to this statement, the model logic is adjusted so that the amount of hydrogen directed to industries cannot be reverted for use for methanol production.

Besides the improvements made in model logic, experts stated their expectations from the model outputs. These expectations are used as the basis for validating general patterns in the output data. The following statements can be expected from the model based on the scope:

- It is expected to see the investments in hydrogen gain importance when the share of renewable power production increases.
- It is expected to see delays in the decision making processes.
- It is expected to see investment cycles because the collaboration among actors is neglected.
- It is expected to see higher CO<sub>2</sub> reduction for higher renewable scenarios.

Finally, the experts criticized several assumptions. These critiques will be addressed in the discussion:

- Import of hydrogen is excluded from the model. However, experts believed that import of hydrogen is going to play a major role in the future. Excluding this import from the model can have consequences on the outcomes.
- Import and export of electricity is also ignored in the model. However, experts note that import and export of electricity is another method to maintain the grid balance. Excluding this factor results in unrealistic numbers for grid balance.
- The geographical scope of this project is the Netherlands. However, experts believe that production of hydrogen-based E-fuels is more feasible in countries with ample amount of renewable power compared to the Netherlands.
- There are alternatives to methanol production. All those alternatives are competing with methanol. Different cases simulated with this model can capture this competition to some extent.

#### 5.7. Experiments

The method of simulation and data analysis with agent-based models is similar to experimenting with a real system. In an experiment, every input has a value in the viable range. Therefore, unique combinations of model inputs provide a setup for experiments. The results of all experiments are then analyzed and aggregated to identify patterns that are common or distinctive in a group of experiments. With this model, three groups of experiments were conducted. These groups are listed in table 5.6 and explained further in this section.

Experiment group	Explanation	Corresponding RQ
Exploration of correlation	$T_{RES}$ has a constant value for all years and for all scenarios, other inputs vary in a wide range in order to explore interdependencies among variables.	SRQ-2
Low flexibility for the grid	$T_{RES}$ increases linearly with time, and takes significantly higher values for higher renewable scenarios. Other parameters vary in a range that allow methanol production at some point before 2050.	SRQ-3, SRQ-4
Flexible grid	$T_{RES}$ increases linearly with time, and takes relatively higher values for higher renewable scenarios. Other parameters vary in a range that allow methanol pro- duction at some point before 2050.	

Table 5.6: Groups of experiments, explanations and corresponding research questions.

#### 5.7.1. Exploration of correlation

This group of experiments are designed in order to provide an answer to the second subquestion:

• *SRQ2* Which socio-technical parameters have the largest influence on the power grid's reliability and CO<sub>2</sub> emission reduction?

All input parameters of the model are varied in a wide range. In these experiments, methanol production might or might not happen. In these experiments, surplus hours are kept constant throughout the simulation. Table 5.7 lists the values that inputs take. Each unique combination of input parameters build one experiment. In total, 72000 experiments are conducted in this group. To make sure stochastic elements are not causing instability, each experiment will be repeated 3 times and the results will be aggregated.

Variable	Definition	Range of values			
$\alpha_{MeOH}$	Share of energy demand for shipping, fulfilled by green methanol	10, 50, 90 %			
$t_D$	Decision window of investment in electrolysers (yr)	5			
$P_{min,H_2}$	Electrolyser capacity of early movers (MW)	500			
$\pi_{H_2}$	Hydrogen price (€/kg)	1, 1.5, 2, 2.5, 3			
$\pi_U$	Average price of utilized CO <sub>2</sub> (€/ton)	30, 50, 70, 90			
$\pi_{MeOH}$	Green methanol price (€/ton)	250, 300, 350, 400, 450			
$\pi_{ETS,2050}$	ETS emission right price in 2050 (€/ton)	40, 100, 160			
S <sub>Cap</sub> .	Carbon capture subsidy (€/ton)	0, 40, 80, 120			
$T_{RES}$	Surplus hours (hr/yr)	500, 1000, 1500, 2000, 2500			
$T_{H_2}$	Hours of hydrogen production	Same value as $T_{RES}$			
Renewable scenarios					
Slow change, Pragmatic sustainability, Rapid development, Sustainable together					

Table 5.7: Input variables and the range of values in experiment group: exploration of correlation.

#### 5.7.2. Low flexibility for the grid

This group of experiments are designed in order to enable answering the third and fourth subquestions:

- *SRQ3* What is the impact of deploying power-to-methanol technologies on power grid's reliability until 2050?
- *SRQ4* What is the impact of deploying power-to-methanol technologies on CO<sub>2</sub> emission reduction until 2050?

In these experiments, it is assumed that flexibility options are limited for the power grid. As a result, the more installed capacity of renewable power production is realized, the more number of surplus hours are created by renewables. Number of surplus hours increase linearly with time. Furthermore, the conditions that do not provide a business case for green methanol production are excluded in this group of experiments. The demand for green methanol in the shipping sector is assumed to be constant and equal to half of the total energy demand in the sector. Table 5.8 lists the values of variables in this group of experiments. In total, 7200 experiments are conducted in this group. To make sure stochastic elements are not causing instability, each experiment is repeated 3 times and the results are aggregated.

#### 5.7.3. Flexible grid

This group of experiments are designed in order to enable answering the third and fourth subquestions:

- *SRQ3* What is the impact of deploying power-to-methanol technologies on power grid's reliability until 2050?
- *SRQ4* What is the impact of deploying power-to-methanol technologies on CO<sub>2</sub> emission reduction until 2050?

In these experiments, it is assumed that the system operator promotes several flexibility options as the share of renewables increases. As a result, the more installed capacity of renewable power production is realized, only a moderate increase in the number of surplus hours is observed. It is assumed that the number of surplus hours increase linearly with time. In this group of experiments, the conditions that do not provide a business case for green methanol production are excluded. The demand of methanol in the shipping sector is assumed to be constant and equal to half of total energy demand in the sector. Table 5.8 lists the values of variables in this group of experiments. In total, 7200 experiments are conducted in this group. To make sure stochastic elements are not causing instability, each experiment will be repeated 3 times and the results will be aggregated.

		Experiments: Flexible grid/Low fle	xibility grid		
Variable	Definition			Range of values	
$\alpha_{MeOH}$	Share of energy demand for shipping, fulfilled by green methanol		50%		
$t_D$	Decision window of investment in electrolysers (yr)			5	
$P_{min,H_2}$	Electrolyser capacity of early movers (MW)			500	
$\pi_{H_2}$	Hydrogen price (€/kg)			1, 1.2, 1.4, 1.6, 1.8	
$\pi_U$	Average price of utilized CO <sub>2</sub> (€/ton)			30, 50, 70, 90	
$\pi_{MeOH}$	Green methanol price (€/ton)		300, 350, 390, 430, 450		
$\pi_{ETS,2050}$	ETS emission right price in 2050 (€/ton)		40, 100, 160		
S <sub>Cap</sub> .	Carbon cap	ture subsidy (€/ton)		0, 20, 40, 60, 80, 100	
$T_{H_2}$	Hours of hy	drogen production		Same value as $T_{RES}$	
		Renewable scenarios			
	Slow change,	Pragmatic sustainability, Rapid develo	pment, Sustain	able together	
		Surplus hours (T <sub>RES</sub> )			
Experiments		Low flexibility grid	Flexible grie	d	
low change	9	0 in 2020, 500 in 2030 and 1000 in 2050			
Pragmatic sustainability		0 in 2020, 500 in 2030 and 1500 in 2050	0 in 2020, 50	00 in 2030 and 1200 in 20	
Rapid development		0 in 2020, 500 in 2030 and 2000 in 2050	0 in 2020, 50	00 in 2030 and 1300 in 20	
Sustainable together		0 in 2020, 500 in 2030 and 3000 in 2050	0 in 2020, 50	00 in 2030 and 1500 in 20	

Table 5.8: Input variables and the range of values in all experiments.

#### 5.8. Summary

In this chapter, the rules of action were discussed. Furthermore, important parameters were introduced. The setup of the model is clarified by listing the numerical values for the parameters and range of inputs. Finally, the groups of experiments are explained. In the next chapter, the findings from all experiments are analyzed and discussed.

# 6

### **Results of experiments**

In this chapter, the results of all experiments conducted with the model are presented. First, in section 6.1, important points before investigating the results are discussed. Next in section 6.2, the results of exploration experiment is presented to provide an answer to subquestion 2: *Which socio-technical parameters have the largest influence on the power grid's reliability and CO<sub>2</sub> emission reduction?* Afterwards, "flexible grid" and "low flexibility grid" experiment results are presented to analyze RE grid balance and CO<sub>2</sub> reduction in these experiments. Section 6.4 answers subquestion 3: *What is the impact of deploying power-to-methanol technologies on power grid's reliability until 2050?* and section 6.5 answers subquestion 4: *What is the impact of deploying power-to-methanol technologies on CO<sub>2</sub> emission reduction until 2050?*.

#### 6.1. Analysis of data

The main KPI's of the model and the equations were introduced in section 2.7. In this chapter, the numerical results derived using the model are presented. The reader should note the following points before delving into the results:

- The model is simulated up to and including 2050.
- For the "exploration" experiments, the presented conclusions are drawn only based on the final year values (in 2050).
- For the "flexible grid" and "low flexibility grid" experiments, the presented results correspond to the experiments in which methanol production takes place at some point before 2050.

Moreover, in the discussion in section 6.4, RE grid balance is considered acceptable if it remains close to zero in the range  $\pm 10\% D_0$ , where  $D_0$  is the yearly power demand (excluding demand from green hydrogen production, green methanol production and carbon capture). In this model,  $D_0$  is approximately 100 TWh (CPB/PBL, 2015), hence the acceptable range is  $\pm 10$  TWh.

Finally, CO<sub>2</sub> reduction is reported in percentage reduction with respect to the reference level in order to ease comparison with the goals. The Dutch "klimaatakkoord" envisages a goal to reduce total CO<sub>2</sub> emissions by 49% in 2030 compared to 1990 levels, and to achieve a carbon-free economy in 2050 (Klimaatberaad, 2019).

In 1990, total  $CO_2$  emission from mobile and stationary sources summed up to 163 million ton, manufacturing and non-energy industry had 52 million ton and power sector had 39.8 million ton  $CO_2$  emission (CBS, 2020c). Table 6.1 lists the contributors to reduction in each sector and the reference values.

Sector	Contributors	Reference value (Mton)	
Power sector	Renewable power production	39.8	
	Industrial capture		
Industry	Hydrogen production	52	
	Methanol production		
Whole economy	Power		
	Industrial capture	163	
	Hydrogen production		
	Methanol production		

#### 6.2. Exploration results: influential parameters

In the exploration experiments, input parameters are varied in a wide range and the influence on RE grid balance and  $CO_2$  reduction are studied. The correlation matrix between parameters is calculated to understand the influence. The higher the correlation of two parameters, the more influential is one on the other. All correlation factors larger than 0.1 are labeled as significant. For ease of analysis, the input parameters are categorized into hydrogen parameters, CCUS parameters and methanol parameters. Table 6.2 lists the input parameters in each category.

Table 6.2: Input parameters and the categories for "exploration" experiments.

Hydrogen parameters		
Renewable hours (h)	Number of hours that renewable power is available for hydrogen pro-	
	duction.	
Hydrogen price (€/kg)	Market price of hydrogen.	
Hydrogen capacity (PJ)	Total amount of hydrogen that is produced in a year.	
	CCUS parameters	
ETS 2050 price (€/ton)	ETS price in 2050.	
Carbon utilization price (€/ton)	The price paid to the capturing industry for every unit $\operatorname{CO}_2$ which is	
	utilized for methanol production.	
Carbon capture subsidy (€/ton)	Subsidy paid to the capturing industry for every unit $\mathrm{CO}_2$ which is cap-	
	tured.	
Methanol parameters		
Methanol price (€/ton)	Market price of methanol.	
Methanol demand (%)	The share of fuel energy demand by the shipping sector which would	
	be satisfied by methanol.	
Methanol production (PJ)	Total amount of methanol that is produced in a year.	

#### 6.2.1. Influential parameters for renewable energy grid balance

Correlation of renewable energy (RE) grid balance with hydrogen parameters are calculated and depicted in a heat-map in figure 6.1. The results show that the number of renewable hours is a critical factor for RE grid balance. It has a high positive correlation with RE grid balance, which indicates higher renewable hours result in higher RE grid balance, as expected. After renewable hours, hydrogen production is the second important factor in row, with a positive correlation. Hydrogen price has a minor influence. Hydrogen production as an intermediate variable is also greatly dependent on renewable hours. Note that the diagonal values are omitted since the correlation of any variable with itself is equal to one.

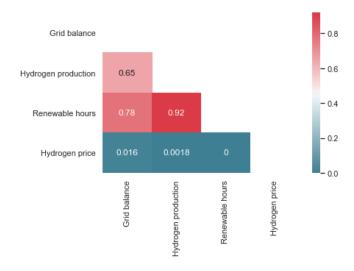


Figure 6.1: Heat-map showing correlation of hydrogen parameters with RE grid balance.

CCUS parameters, however, are loosely correlated with RE grid balance. The values of correlation factors between CCUS parameters and RE grid balance are lower. Figure 6.2 shows the heat-map of correlation matrix between RE grid balance and CCUS parameters. Carbon capture subsidy and ETS price have small negative correlation with RE grid balance while  $CO_2$  utilization price has a positive correlation. This is expected: the higher the subsidy, the more  $CO_2$  is captured in the industry, the more electrical load on the grid and hence, the less RE grid balance becomes. ETS price has the same influence: the higher the ETS price, the more interest in carbon capture and the less RE grid balance becomes. Positive correlation of carbon utilization price with RE grid balance is, however, difficult to explain.

Compared to CCUS parameters, methanol parameters show closer correlation. Figure 6.3 shows the heatmap of correlation matrix between RE grid balance and methanol parameters. Most of the values are close to zero. The only parameter that has (loose) correlation with RE grid balance is methanol production. The higher the methanol production, the higher the RE grid balance is. Based on the heat-maps, renewable hour, hydrogen production and methanol production are important factors that determine RE grid balance.

#### 6.2.2. Influential parameters for CO<sub>2</sub> reduction

Correlation of  $CO_2$  reduction with hydrogen parameters are calculated and depicted in a heat-map in figure 6.4. The results show that the amount of hydrogen production is a critical factor for  $CO_2$  reduction. It has a high positive correlation with  $CO_2$  reduction which indicates more  $CO_2$  reduction as more hydrogen is produced, as expected. After hydrogen production, renewable hours is the second important factor in row, with a positive correlation. Finally, renewable hours also determine the amount of hydrogen production



Figure 6.2: Heat-map showing correlation of CCUS parameters with RE grid balance.

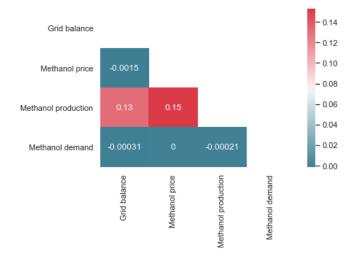


Figure 6.3: Heat-map showing correlation of methanol parameters with RE grid balance.

to a great extent. Influence of renewable hours on  $CO_2$  reduction is both direct and indirect: it influences reduction directly because the more renewable hours we have on the grid, the more renewable energy is available to replace dirty power. Renewable hours influence  $CO_2$  reduction indirectly, as more renewable hours result in more hydrogen production and hence, more  $CO_2$  reduction from hydrogen.

As the direct influence of renewable hours on  $CO_2$  reduction is trivial, the correlations with  $CO_2$  reduction in the industry are also calculated. Figure 6.5 depicts the heat-map of correlation matrix between  $CO_2$  reduction in the industry and hydrogen parameters. The results are similar to the results for total  $CO_2$  reduction, with hydrogen production and renewable hours being the most influential parameters with positive correlation.

To analyze influence of CCUS parameters, only the amount of  $CO_2$  reduction in the industry is considered to exclude the trivial amount resulting from renewable power production. Figure 6.6 shows the heat-map of correlation matrix between  $CO_2$  reduction in the industry and CCUS parameters. Carbon capture subsidy and ETS price have small positive correlation with  $CO_2$  reduction while carbon utilization price has little to no correlation. This is expected: the higher the subsidy, the more  $CO_2$  is captured in the industry. ETS price has the same influence: the higher the ETS price, the more interest in carbon capture. The carbon utilization

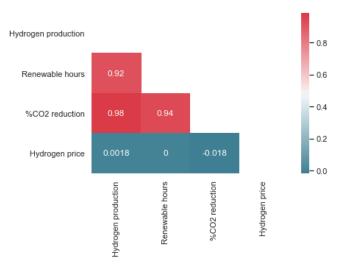


Figure 6.4: Heat-map showing correlation of hydrogen parameters with total CO<sub>2</sub> reduction.

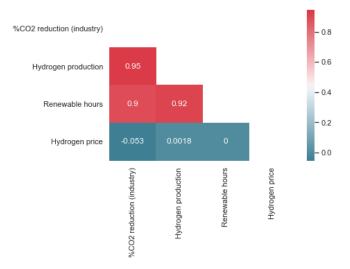


Figure 6.5: Heat-map showing correlation of hydrogen parameters with CO2 reduction in the industry.

price has little influence on CO<sub>2</sub> reduction.

Compared to CCUS parameters, methanol parameters show closer correlation with  $CO_2$  reduction. Here, again the reduction due to renewable power production is excluded and only  $CO_2$  reduction in the industry is considered. Figure 6.7 shows the heat-map of correlation matrix between  $CO_2$  reduction in the industry and methanol parameters. Methanol production has a relatively close correlation with  $CO_2$  reduction. The higher the methanol production, the higher the  $CO_2$  reduction. However, the higher the methanol demand in the shipping sector, the lower the  $CO_2$  reduction will be. This is due to the fact that part of  $CO_2$  reduction in the industry is coming from substitution of green methanol with normal methanol. When the demand in the shipping sector increases, less green methanol can be directed to the industry to replace normal methanol, for which the production process has a high  $CO_2$  emission rate. Methanol price has a low, indirect influence on  $CO_2$  reduction with a positive correlation.

Based on the above figures, renewable hour, hydrogen production, methanol production, methanol demand and carbon capture subsidy are important factors that determine CO<sub>2</sub> reduction in total and in the industry.



Figure 6.6: Heat-map showing correlation of CCUS parameters with CO<sub>2</sub> reduction in the industry.

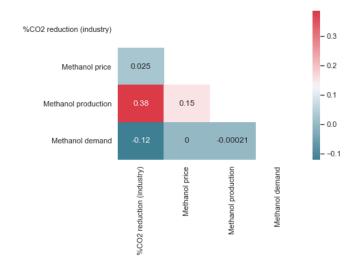


Figure 6.7: Heat-map showing correlation of methanol parameters with CO<sub>2</sub> reduction in the industry.

#### 6.3. Summary of influential parameters

The results presented in this section provide an answer to the subquestion 2: *Which socio-technical parameters have the largest influence on the power grid's reliability and CO<sub>2</sub> emission reduction?* In a nutshell, renewable hours, hydrogen production and methanol production are the most influential parameters on both RE grid balance and CO<sub>2</sub> reduction. The subsidy provided for carbon capture technologies and the demand for methanol are also parameters that influence  $CO_2$  reduction. RE grid balance is not significantly influenced by these parameters. All other parameters seem to be loosely correlated with RE grid balance and  $CO_2$  reduction. However, those parameters might influence intermediate parameters like methanol capacity which has a high correlation with RE grid balance and  $CO_2$  reduction. Table 6.3 summarizes the parameters being analyzed and the type of correlation discovered between them and RE grid balance and  $CO_2$  reduction. All correlation factors larger than 0.1 are labeled as significant.

Category	Parameter	Type of correlation	
		RE grid balance	CO <sub>2</sub> reduction
Hydrogen parameters	Renewable hours (h)	Significant, Positive	Significant, Positive
	Hydrogen price (€/kg)	Insignificant	Insignificant
	Hydrogen capacity (PJ)	Significant, Positive	Significant, Positive
CCUS parameters	ETS 2050 price (€/ton)	Insignificant	Insignificant
	Carbon utilization price (€/ton)	Insignificant	Insignificant
	Carbon capture subsidy (€/ton)	Insignificant	Significant, Positive
Methanol parameters	Methanol price (€/ton)	Insignificant	Insignificant
	Methanol demand (%)	Insignificant	Significant, Negative
	Methanol production (PJ)	Significant, Positive	Significant, Positive

Table 6.3: Correlation of parameters with RE grid balance and CO<sub>2</sub> reduction.

#### 6.4. Renewable energy (RE) grid balance

In this section, the results of RE grid balance in "low flexibility" and "flexible grid" experiments conducted with the model are presented and compared. It is worth mentioning that the excess renewable power is stored in hydrogen and methanol. Therefore, negative or positive RE grid balance should be analyzed in tandem with the amount of energy storage in hydrogen and methanol.

#### 6.4.1. RE grid balance in experiments "flexible grid"

The results of simulation in the "flexible grid" shows that depending on the scenario of renewable power generation, RE grid balance can take various values. The scatter plot of values of RE grid balance in 2050 is shown in figure 6.8 per scenario. Each point corresponds to one experiment in the group. The results show that for two scenarios, namely "Slow change" and "Pragmatic sustainability", the amount of balance remains within the acceptable range of  $\pm 10\% D_0$ . All scenarios end up with a positive RE grid balance in 2050. For "Sustainable together" scenario, the 2050 value of RE grid balance can take very high positive values. In "Sustainable together" scenario, the 2050 values of RE grid balance show a wide spread though the data appear to be clustered in four groups. The same structure of data can be observed for "Rapid development" scenario, with a smaller spread.

Figure 6.9 shows the probability distribution of RE grid balance values for these two scenarios. The size of boxes are proportional to the probability that RE grid balance takes a value in the respective range, and the black line shows the mean value. This figure shows that in scenario "Sustainable together", RE grid balance most probably takes a large value in 2050. The correlation between RE grid balance and other variables of the model in this scenario shows no specific pattern, i.e. it is not obvious what is the reason that values of RE grid balance are clustered.

For all scenarios but "Pragmatic sustainability", there is a meaningful relation between hydrogen production capacity and RE grid balance in 2050. Figure 6.10 shows the scatter plot of RE grid balance 2050 values versus the amount of hydrogen production in all scenarios. What can be clearly seen is that RE grid balance decreases as the hydrogen production increases in all scenarios but "Pragmatic sustainability". A loose correlation is also observed between RE grid balance and the amount of methanol production. One can recognize the darker data points (corresponding to higher methanol production) are mostly below light data points (corresponding to lower methanol production).

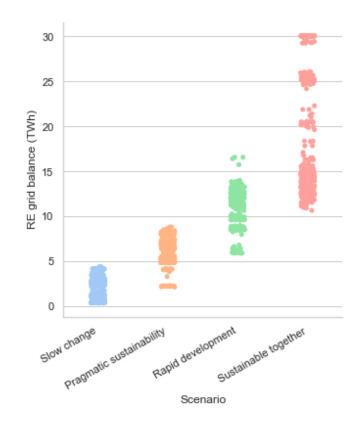


Figure 6.8: RE grid balance in 2050, flexible grid experiments, per renewable scenario.

Analysis of RE grid balance development throughout the simulation from 2020 to 2050 reveals interesting patterns, too. Figure 6.11 shows the variation of RE grid balance over time per scenario. In this figure, solid

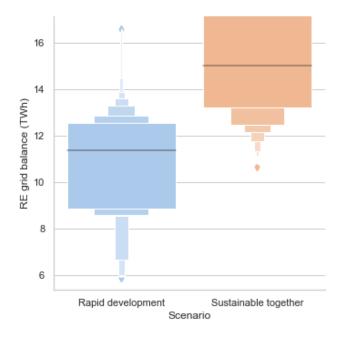


Figure 6.9: Probability distribution of RE grid balance in 2050, flexible grid experiments, in scenarios "Sustainable together" and "Rapid development". Black line shows the mean value in each scenario.

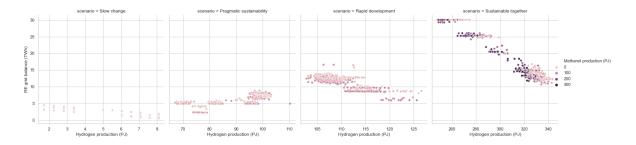


Figure 6.10: RE grid balance in 2050 versus hydrogen production, flexible grid experiments, in all scenarios. Color of data points show the amount of methanol production in the corresponding experiment.

line shows the average value of RE grid balance at a time and the shade represent the standard deviation of data.

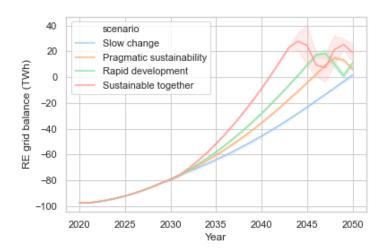


Figure 6.11: RE grid balance from 2020 to 2050, flexible grid experiments, in all scenarios. Solid line shows the mean value and the shade shows standard deviation of data.

What stands out in figure 6.11 is the oscillatory behavior of RE grid balance. After 2030, the RE grid balance overshoots and oscillates, with higher overshoot for higher scenarios. The reason for oscillations can be explained by the fact that after 2030, the hydrogen backbone becomes available and actors begin to invest in electrolysers. Electrolysers increase the power demand and hence, decrease the RE grid balance. Having hydrogen available, investment in green methanol takes off. As a result, the demand increases further and RE grid balance falls steeper. When the renewable production increases further, the RE grid balance increases again. Positive RE grid balance is an incentive for more hydrogen production and methanol production thereafter, which results in decline of RE grid balance again. This consequent rise and fall of RE grid balance creates an oscillatory pattern corresponding to hydrogen investment cycle.

Furthermore, figure 6.11 shows that "Sustainable together" scenario creates a large deviation of RE grid balance. A close investigation of RE grid balance in all scenarios reveal that RE grid balance exhibit two essentially different patterns. Figure 6.12 shows these two distinctive patterns. The left panel in this figure shows a pattern for which RE grid balance reaches a very high value of more than 40 tera watt hour in 2045, and then peaks again in less than five years. In this short period, RE grid balance can take negative values, too. Whether or not RE grid balance falls below zero depends on the price of methanol and hence, methanol

production rate. In contrast, the right panel shows a peak in 2044 of about 20 tera watt hour which is followed by a second, higher peak reaching up to 40 tera watt hour happening in less than five years. Between the two peaks, RE grid balance remains above zero. A close investigation of the data shows that the pattern shown in the right panel is more probable among all experiments. The pattern shown in the left panel occur only in cases which hydrogen price is significantly low. Furthermore, carbon capture subsidy or carbon utilization price contribute to the spread of trajectories. For a more detailed overview of patterns, look at figures D.1 and D.2 in appendix D.

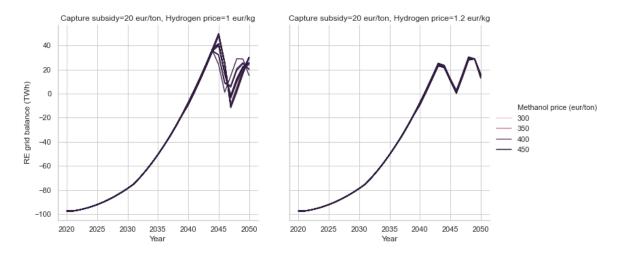


Figure 6.12: Two distinctive patterns in RE grid balance from 2020 to 2050, flexible grid experiments, for "Sustainable together" scenario.

#### 6.4.2. Renewable energy (RE) grid balance in experiments "low flexibility grid"

The results of simulation in the "low flexibility grid" shows that depending on the scenario of renewable power generation, RE grid balance can take various values. The results presented here only correspond to the cases which methanol production takes place.

The scatter plot of values of RE grid balance in 2050 is shown in figure 6.13 per scenario. Each point corresponds to one experiment in the group. The results show, surprisingly, that only in the "Rapid development" scenario that negative RE grid balance in 2050 is possible. The amount of negative balance, however, falls within the acceptable range of  $\pm 10\% D_0$ . Other scenarios end up with a positive RE grid balance in 2050. For "Sustainable together" scenario, the 2050 value of RE grid balance can take very high positive values. In "Slow change" and "Pragmatic sustainability" scenario, values of RE grid balance show an almost continuous spread. However, in "Rapid development" scenario, results are clustered in four groups. In "Sustainable together" scenario, almost all experiments return similar value for RE grid balance in 2050.

RE grid balance shows different correlations with total yearly hydrogen production in different scenarios. This is depicted in figure 6.14. This figure shows that in "Slow change" and "Rapid development" scenarios, the more hydrogen production is realized the lower the RE grid balance becomes. However, "Pragmatic sustainability" scenario shows a *positive* correlation between green hydrogen production and RE grid balance. In "Sustainable together" scenario, there is almost no correlation between green hydrogen production and RE grid balance.

Turning now to RE grid balance development throughout the simulation from 2020 to 2050, figure 6.15 reveals interesting patterns. This figure hows the variation of RE grid balance over time per scenario. In this figure, solid line shows the average value of RE grid balance at a time and the shade represent the standard

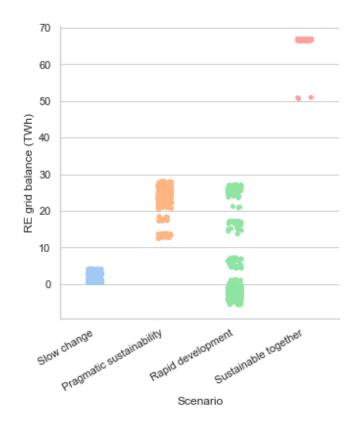


Figure 6.13: RE grid balance in 2050, low flexibility grid experiment, per renewable scenario.

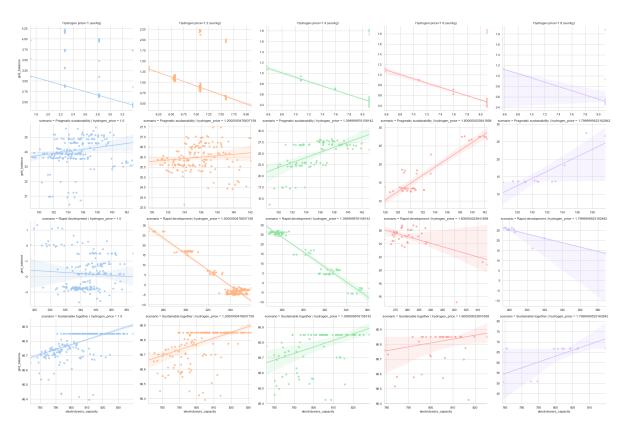


Figure 6.14: RE grid balance in 2050 versus hydrogen production, low flexibility grid experiment, in all scenarios. Columns show different values of hydrogen price and rows show different scenarios.

deviation of data. What stands out in this figure is the oscillatory behavior of RE grid balance. After 2030, the RE grid balance overshoots and oscillates, with higher overshoot for higher scenarios. The amplitude of oscillations appears to diverge in "Sustainable together" scenario.

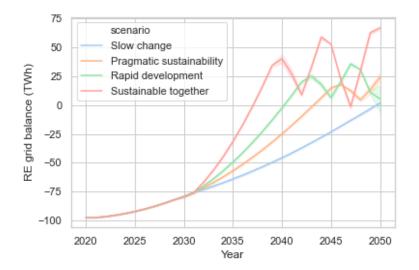


Figure 6.15: RE grid balance from 2020 to 2050, low flexibility grid experiments, in all scenarios. Solid line shows the mean value and the shade shows standard deviation of data.

The reason for oscillations can be explained by the fact that after 2030, the hydrogen backbone becomes available and actors begin to invest in electrolysers. Electrolysers increase the power demand and hence, decrease the RE grid balance. Having hydrogen available, investment in green methanol takes off. As a result, the demand increases further and RE grid balance falls steeper. When the renewable production increases further, the RE grid balance increases again. Positive RE grid balance is an incentive for more hydrogen production and methanol production thereafter, which results in decline of RE grid balance again. This consequent rise and fall of RE grid balance creates an oscillatory pattern corresponding to hydrogen investment cycle. Recalling the fact that the power grid has less flexibility options in these experiments, the investment cycles for hydrogen have a high impact on RE grid balance. Furthermore, figure 6.15 shows that in "Rapid development" scenario, RE grid balance deviates in a wide range.

The relationship between RE grid balance and model parameters in "Rapid development" scenario is investigated in order to identify the cause of these variations. Figures D.4 to D.6 in appendix D show that essentially different RE grid balance patterns emerge in different experiments. A combination of ETS price in 2050, price of carbon utilization, carbon capture subsidy and hydrogen price contributes to create two different patterns in RE grid balance. These two patterns are illustrated in figure 6.16. In one set of experiments (an example shown in the right panel), after 2030 RE grid balance oscillates between zero and a positive value with a diverging amplitude and relatively constant mean. Most of the experiments create this pattern and hence, the averaged value over all experiments exhibit the same pattern. A few of experiments result in a different behavior (an example shown in the left panel). In these experiments, after 2030 the RE grid balance oscillate but with a lower amplitude than the former pattern. The mean value of RE grid balance increases gradually in contrast to the former case which shows a constant mean value. By looking at the total methanol production which is realized by 2050 in each experiment, one can recognize that low methanol production facilitates

gradual increase of RE grid balance over time and dampens the amplitude of oscillation. Figure D.7 illustrates the pattern of methanol production in this scenario.

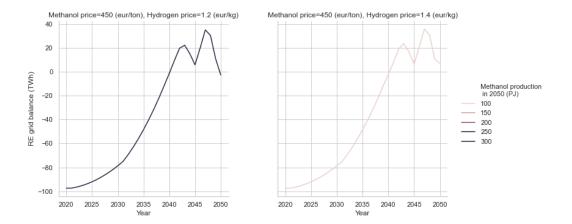


Figure 6.16: Two patterns of RE grid balance from 2020 to 2050 in the low flexibility grid experiments, "Rapid development" scenario. Color of lines show the value of methanol production in 2050.

#### 6.4.3. Summary: RE grid balance in the two experiment sets

RE grid balance exhibits oscillatory behavior in both group of experiments. The oscillation can be attributed to hydrogen investment cycle. When the flexibility options are limited in the grid, the amplitude of oscillations diverge quickly and the frequency of oscillations are higher. For the high renewable scenarios essentially different emergent patterns are observed on RE grid balance for both experiment sets. The characteristics of individual experiments resulting in each of those patterns were discussed in the previous subsections. In both experiment sets, RE grid balance in 2050 takes diverse values.

It is important to note that oscillation of RE grid balance is not a desirable state for the power grid. Oscillations -especially with high amplitude- creates uncertainty for the system operator and makes it difficult to plan for flexibility options. The actors such as investors in electrolysers will also suffer from the uncertainty. Furthermore, the fact that very different system behaviors for a certain range of system parameters might occur is undesirable in real life. In these cases, very different projections of the future exist that require different actions. For example, when the hydrogen price is low and with a flexible power grid, RE grid balance might oscillate with a divergent or convergent amplitude. When predictions show a diverging amplitude, system operator should plan for more balancing options while this action might lead to a negative balance when the amplitude is converging itself.

Based on the discussion, an answer is given to the subquestion 3: *What is the impact of deploying power-to-methanol technologies on power grid's reliability until 2050?* The results indicate that power-to-methanol cannot be considered as the only flexibility option for the power grid, especially if the growth rate of renewable power production is substantial. It can prevent uncontrolled rise of RE grid balance and reduce the need for curtailment, though it is not the ultimate solution.

#### 6.5. CO<sub>2</sub> reduction

In this section, the results of CO<sub>2</sub> reduction in "low flexibility" and "flexible grid" experiments conducted with the model are presented and compared.

#### 6.5.1. CO<sub>2</sub> reduction in experiments "flexible grid"

Figure 6.17 shows the percentage of  $CO_2$  reduction that is achieved in the economy in 2030 and 2050 in all scenarios. This figure shows that in 2050, the amount of  $CO_2$  reduction in the investigated sectors can reach beyond 70% in the highest scenario, though remains at about 20% in the worst case. The highest reduction can be achieved in the highest renewable scenario and the worst case corresponds to the lowest renewable production scenario. In the power sector, the amount of  $CO_2$  reduction due to power production of renewables only accounts for 9% in 2030 which is significantly lower than the 49% goal (look at figure D.8 in appendix D). One shall note, however, that in reality a flexible power grid can achieve higher reduction levels in case flexibility options are also carbon-neutral.

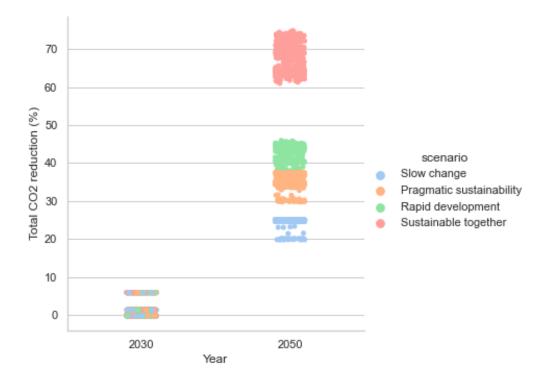


Figure 6.17: Total CO<sub>2</sub> reduction percentage in 2030 and 2050 in different renewable scenarios, flexible grid.

The total  $CO_2$  reduction in the industry is illustrated in figure 6.18. Unlike total emission reduction, there is no straightforward relationship between the renewable power scenario and emission reduction in the industry. In 2030, the most optimistic situation leads to a reduction of about 10% in the industry. The reader should note that this is the amount achieved only from the carbon reduction efforts in the Port of Rotterdam and IJmuiden industrial regions. In 2050, it is possible to achieve high reduction of more than 95% in the industry, provided that the renewable power production grows according to the predictions of "Sustainable together" scenario. Negative  $CO_2$  reduction occurs in cases where methanol is demanded in the shipping sector while green methanol is not yet produced.

What is striking in figure 6.18 is that the values of  $CO_2$  reduction are clustered. In 2030, only 3 levels of  $CO_2$  reduction is possible. In 2050, the values are clustered as well, with a wide spread for one of the clusters. In order to understand the cause of clustering and spread of values,  $CO_2$  reduction percentage in all experiments are plotted against all variables of the model (please look at figures D.9 and D.10). From the analysis it is understood that  $CO_2$  capture has a strong impact on the percentage of  $CO_2$  reduction in the industry. Before

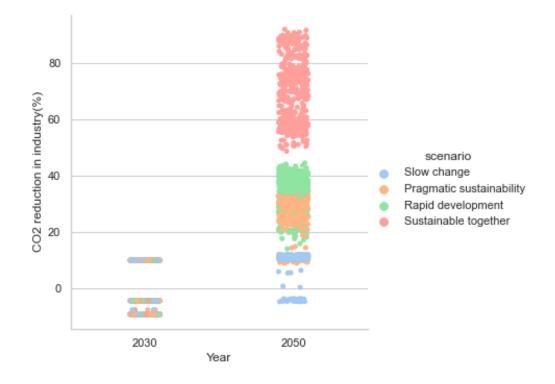


Figure 6.18: CO<sub>2</sub> reduction percentage in the sector industry in 2030 and 2050 in different renewable scenarios, flexible grid.

the capacity of CCUS network is fully utilized (i.e. total carbon captured is less than 10 million tons), the industries in the region (listed in table 3.5) will either capture the whole emission they have or not capture any  $CO_2$ . This behavior results in discrete amounts of  $CO_2$  reduction from industrial capture. When the capacity of CCUS network is fully utilized, industries may partly capture their emissions, provided that an amount of  $CO_2$  is extracted from the CCUS network for methanol production. Therefore, a continuum of  $CO_2$  reduction is created in different experiments. Note that without methanol production, it is still possible to achieve  $CO_2$  reduction levels of up to 80% (please look at figure D.11 in appendix D) which is a mere result of increasing green hydrogen production.

Having discussed the patterns observed in the  $CO_2$  reduction data, it is now interesting to have a closer look at the role each change (i.e. hydrogen production, methanol production and industrial capture) has in the  $CO_2$  reduction from industry. Figure 6.19 shows the amount of reduction in million tons, achieved by each development in 2050. The rows show different scenarios and the columns show different capture subsidy levels. This figure shows that for the "Slow change" and "Pragmatic sustainability" renewable scenarios, hydrogen and methanol are barely playing a role in  $CO_2$  reduction. Most of the reduction is due to investments in  $CO_2$  capture in the industry. For "Rapid development" and "Sustainable together" scenarios, carbon capture subsidy is playing a role. The higher subsidy is allocated to carbon capture, the higher  $CO_2$ reduction is achieved from methanol production and the lower  $CO_2$  reduction from hydrogen production. In other words, subsidizing  $CO_2$  capture technologies in cases which  $CO_2$  utilization is possible, is equivalent to prioritizing  $CO_2$  utilization products like methanol or other E-fuels over hydrogen.

Before moving on to the next section, it is valuable to analyze the timely manner of  $CO_2$  reduction. Figure 6.20 shows the total  $CO_2$  reduction (right panel) and  $CO_2$  reduction in the industry (left panel) from 2020 to 2050. What stands out in this figure is the slow rate of  $CO_2$  reduction in the industry before 2040. Up until

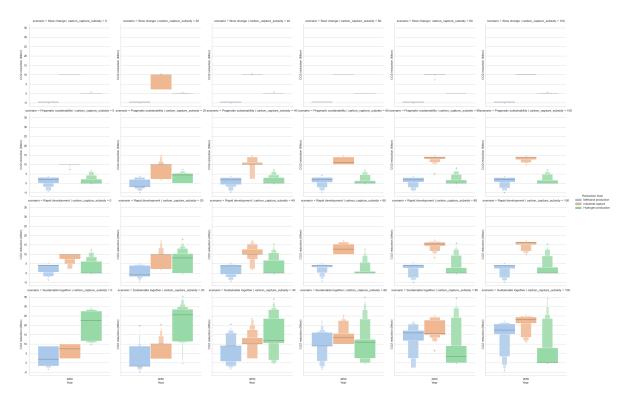


Figure 6.19: CO<sub>2</sub> reduction for each change in 2050 per scenario and carbon capture subsidy

2043, the rate of  $CO_2$  reduction is very low and the main reduction is achieved from renewables and industrial capture. After 2043, hydrogen production and methanol production start (look at figure D.12) and allow for more reduction, with higher scenarios showing a higher potential for  $CO_2$  reduction.

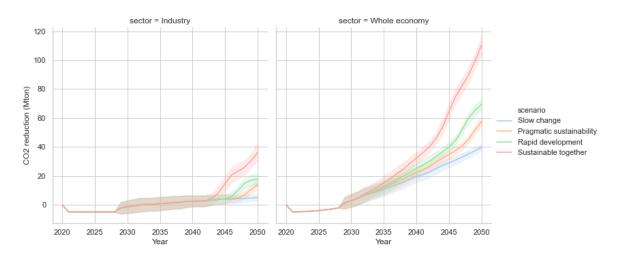


Figure 6.20: CO<sub>2</sub> reduction from 2020 to 2050 in the industry and in the whole economy, flexible grid.

#### 6.5.2. CO2 reduction in experiments "low flexibility grid"

Figure 6.21 shows the percentage of  $CO_2$  reduction that is achieved in the economy in 2030 and 2050 in all scenarios. This figure shows that in 2050, the amount of  $CO_2$  reduction in the investigated sectors can reach up to 140% in the highest scenario, though remains at about 20% in the worst case. The highest reduction can

be achieved in the highest renewable scenario and the worst case corresponds to the lowest renewable production scenario. In the power sector, the amount of  $CO_2$  reduction due to power production of renewables only accounts for 9% in 2030 which is significantly lower than the 49% goal (look at figure D.13 in appendix D).

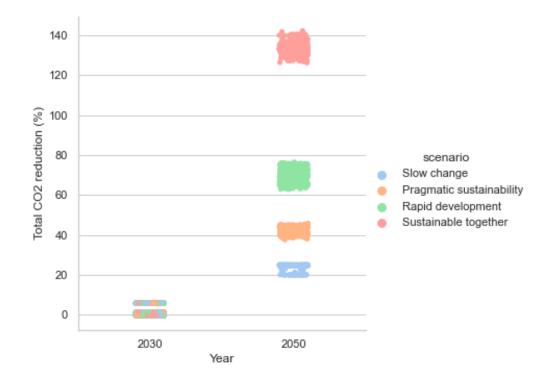


Figure 6.21: Total CO<sub>2</sub> reduction percentage in 2030 and 2050 in different renewable scenarios, low flexibility grid.

The total  $CO_2$  reduction in the industry is illustrated in figure 6.22. In 2030, the most optimistic situation leads to a reduction of 15% in the industry. The reader should note that this is the amount achieved only from the carbon reduction efforts in the Port of Rotterdam and Amsterdam industrial regions. In 2050, it is possible to achieve extremely high reduction of about 200% in the industry, provided that the renewable power production grow according to the predictions of "Sustainable together" scenario. In general, higher scenarios result in higher  $CO_2$  reduction in the industry. Negative  $CO_2$  reduction occurs in cases where methanol is demanded in the shipping sector while green methanol is not yet produced.

What is striking in figure 6.22 is that the values of  $CO_2$  reduction are clustered. In 2030, only 3 levels of  $CO_2$  reduction is possible. In 2050, the values are clustered as well, with a wide spread for one of the clusters. In order to understand the cause of clustering and spread of values,  $CO_2$  reduction percentage in all experiments are plotted against all variables of the model (please look at figures D.14 and D.15 in appendix D). From the analysis it is understood that  $CO_2$  capture has a strong impact on the percentage of  $CO_2$  reduction in the industry. Before the capacity of CCUS network is fully utilized (i.e. total carbon captured is less than 10 million tons), the industries in the region (listed in table 3.5) will either capture the whole emission they have or not capture any  $CO_2$ . This behavior results in discrete amounts of  $CO_2$  reduction from industrial capture. When the capacity of CCUS network is fully utilized, industries may partly capture their emissions, provided that an amount of  $CO_2$  is extracted from the CCUS network for methanol production. Therefore, a continuum of  $CO_2$  reduction is created in different experiments. Note that without methanol production, it

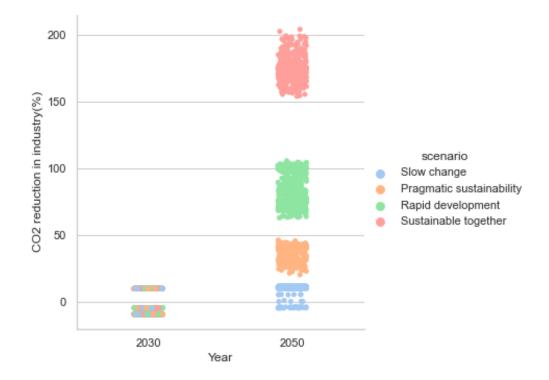


Figure 6.22: CO2 reduction percentage in the sector industry in 2030 and 2050 in different renewable scenarios, low flexibility grid.

is still possible to achieve very high CO<sub>2</sub> reduction levels of up to more than 175% (please look at figure D.16 in appendix D) which is a mere result of increasing green hydrogen production.

Having discussed the patterns observed in the  $CO_2$  reduction data, it is now enlightening to have a closer look at the role each change (i.e. hydrogen production, methanol production and industrial capture) has in the  $CO_2$  reduction from industry. Figure 6.23 shows the amount of reduction in million tons, achieved by each development in 2050. The rows show different scenarios and the columns show different capture subsidy levels. This figure shows that for the "Slow change" and "Pragmatic sustainability" renewable scenarios, hydrogen and methanol are barely playing a role in  $CO_2$  reduction. Most of the reduction is due to investments in  $CO_2$  capture in the industry. For "Rapid development" and "Sustainable together" scenarios, carbon capture subsidy is playing a role. In all scenarios, the higher the subsidy paid for capture technologies, the more significant is the role of methanol production in  $CO_2$  reduction as compared to hydrogen production and industrial capture. In other words, subsidizing  $CO_2$  capture technologies in cases which  $CO_2$  utilization is possible, is equivalent to prioritizing utilization products like methanol or other E-fuels over hydrogen.

It is now valuable to analyze the timely manner of  $CO_2$  reduction. Figure 6.24 shows the total  $CO_2$  reduction (right panel) and  $CO_2$  reduction in the industry (left panel) from 2020 to 2050. What stands out in this figure is the slow rate of  $CO_2$  reduction in the industry before 2040. Up until 2038, the rate of  $CO_2$  reduction is very low and the main reduction is achieved from renewables and industrial capture. After 2038, hydrogen production and methanol production start (look at figure D.17) and allow for more reduction, with higher scenarios showing a higher potential for  $CO_2$  reduction.

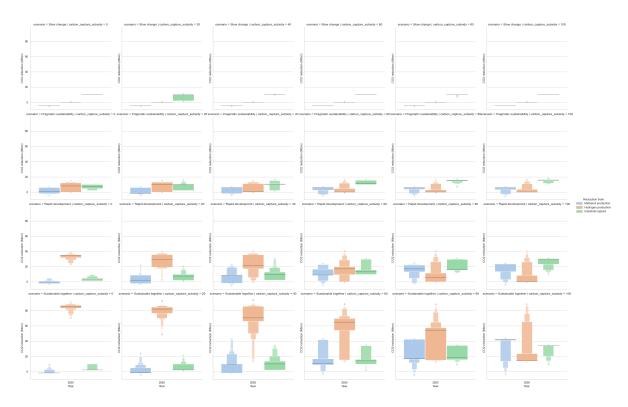


Figure 6.23: CO<sub>2</sub> reduction for each change in 2050 per scenario and carbon capture subsidy

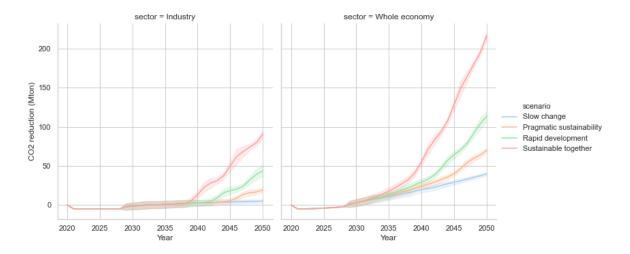


Figure 6.24:  $CO_2$  reduction from 2020 to 2050 in the industry and in the whole economy, low flexibility grid.

#### 6.5.3. Summary: CO<sub>2</sub> reduction in the two experiment sets

 $CO_2$  reduction in both sets of experiments remains constant until hydrogen production and industrial  $CO_2$  capture projects are realized. After hydrogen production and methanol production take off,  $CO_2$  reduction increases monotonically. For a flexible grid, since there are other flexibility options to absorb renewable power, hydrogen production gains less importance, hence starts later. In most of the experiments with a flexible grid setting,  $CO_2$  reduction begins to increase only after 2042. For a less flexible grid, however, this can happen earlier. The experiments conducted here show  $CO_2$  reduction rate can take off as early as 2038. In all experiments, total  $CO_2$  reduction is higher for higher scenarios. In "low flexibility" experiments, the industrial  $CO_2$  reduction has a clear relationship with renewable scenario. No such correlation can be identified from "flexible grid" experiments.

Regarding  $CO_2$  reduction goals, a flexible grid is less promising as it provides less incentives for hydrogen production. When the grid flexibility relies mainly on green hydrogen production, a large amount of hydrogen can be produced that can lead to full decarbonization of the economy in 2050 in some renewable scenarios. Decarbonization goals appear to be easily met in the industry in "low flexibility" experiments. Although in most of the cases the main contributor to  $CO_2$  reduction is hydrogen production, methanol production also has a two-fold effect: first, high production rate of green methanol influences normal methanol production and leads to  $CO_2$  reduction, and second, methanol production utilizes  $CO_2$  and creates space in a fully utilized CCUS network. In this way, more industrial actors are able to capture their  $CO_2$  emissions.

Based on the discussion in this section, an answer is given to subquestion 4: *What is the impact of deploying power-to-methanol technologies on CO<sub>2</sub> reduction until 2050?* The results show that it is possible to achieve carbon reduction goals by deploying power-to-methanol technologies, provided that the growth of renewable power supply is fast enough to allow for sufficient hydrogen and methanol production rates. In any case, power-to-methanol technologies have no influence before 2030 and hence, are not helping with the 2030 reduction goals.

#### 6.6. Summary

In summary, the following answers can be given to the second, third and fourth research questions:

## SRQ-2: Which socio-technical parameters have the largest influence on the power grid's reliability and CO<sub>2</sub> emission reduction?

Exploration experiments and data analysis revealed that renewable hours, hydrogen production and methanol production are the most influential parameters on both RE grid balance and  $CO_2$  reduction. The subsidy provided for carbon capture technologies and the demand for methanol are also parameters that influence  $CO_2$  reduction. RE grid balance is not significantly influenced by these parameters. All other parameters seem to be loosely correlated with RE grid balance and  $CO_2$  reduction.

### SRQ-3: What is the impact of deploying power-to-methanol technologies on power grid's reliability until 2050?

Experiments with "flexible grid" and "low flexibility grid" were conducted and various visualizations of data were created to answer this question. In all experiments, it is observed that the impact of deploying power-to-methanol technologies on RE grid balance is the creation of an oscillatory pattern. Since power-to-hydrogen is the first step of power-to-methanol process, the oscillation on the RE grid balance can be attributed to the investment cycle for hydrogen. The higher the growth rate of renewables, the larger the amplitude of

oscillation gets. Furthermore, if there are not enough flexibility options available for the grid, the RE grid balance rises on average.

# SRQ-4: What is the impact of deploying power-to-methanol technologies on CO<sub>2</sub> emission reduction until 2050?

Experiments with "flexible grid" and "low flexibility grid" were conducted and various visualizations of data were created to answer this question. In all experiments, deploying power-to-methanol technologies begin to pay off only around 2040 even in the most ambitious renewable scenario. The factor that prevents high CO<sub>2</sub> reduction before 2040 is hydrogen. Power-to-hydrogen becomes a feasible option only when sufficient amount of renewable power is available on the grid. When hydrogen production reaches the critical mass, methanol production also becomes feasible. What is crucial to understand is that when few flexibility options are available for the power grid, hydrogen production takes off earlier and hence, CO<sub>2</sub> reduction reaches higher levels.

# 7

# Conclusions, recommendations and discussion

In this chapter, first the answers to the subquestions provided in previous chapters are combined to conclude an answer to the main research question: *How does deploying power-to-methanol technologies influence the power grid's reliability and CO<sub>2</sub> emission reduction in the Netherlands until 2050?* Based on the conclusion, a number of recommendations that can be given to the industry and science are listed. Furthermore, the implications of the model assumptions and the limitations of the study are discussed. Finally, a guideline for future research in this direction is presented.

#### 7.1. Conclusions

In this research, the influence of power-to-methanol technologies on power grid's reliability and CO<sub>2</sub> reduction has been studied. An agent-based model was developed in order to explore possible future scenarios created by deployment of power-to-methanol technologies, in case the green methanol is primarily supplied to the shipping sector as an alternative low-carbon fuel. The model outcomes were explored using two sets of experiments. These two experiments simulate two hypothetical cases: "flexible grid" experiments in which the power grid is assumed to have several flexibility options, and "low flexibility grid", that the grid cannot easily adapt to high renewable power production. For a flexible grid, as more renewable power supply is realized, the surplus hours increase slightly. For a grid with low flexibility, however, surplus hours increase greatly when more renewable power capacity is realized.

The results of the experiments show that deploying power-to-methanol technologies has a considerable influence on power grid's reliability. At the highest level of aggregation, the balance between renewable power supply and the conventional power supply is an indication of the reliability of the power grid. This factor is called "RE grid balance" in this report. A positive RE grid balance means more renewable power is available than demanded by the grid. If RE grid balance remains positive for an extended period, it implies frequent curtailment of renewable power production and a disincentive for further investments in renewables. On the other hand, when the RE grid balance is predominantly negative, it implies a need for extensive flexibility options (e.g. batteries or hydroelectric plants) or a necessity for conventional power plants. Therefore,

desired is that RE grid balance remains close to zero. The analysis of RE grid balance shows that deploying power-to-methanol technologies creates an oscillatory pattern on the RE grid balance. In other words, the RE grid balance swings between zero and a positive value when the circumstances allow for substantial deployment of power-to-methanol technologies. The amplitude of the oscillations is positively correlated with the growth rate of renewable power supply. The faster the increase in renewable power supply, the bigger is the amplitude of oscillations. Furthermore, oscillations have higher frequency in high renewable scenarios. In the most ambitious renewable scenario, i.e. "Sustainable together" scenario, RE grid balance goes from peak-to-peak in five years, which is very quick compared to the time scales of grid development. The analyses shows that oscillation on the RE grid balance are due to an investment cycle for hydrogen. Positive RE grid balance is a positive investment signal for power-to-hydrogen and then green methanol production. With a coherent increase of green hydrogen and green methanol production, power demand increases and RE grid balance decreases. Declining RE grid balance turns into a disincentive for investment in hydrogen, which allows for a growth of RE grid balance after a short while. The cycle starts over when RE grid balance reaches a sufficiently large positive value. In addition to oscillations, a grid with inadequate flexibility means shows a rising average balance. The desirable state for the power grid is to have a rather constant balance close to zero. Without any power-to-hydrogen and power-to-methanol technology being realized, RE grid balance would have risen indefinitely. These technologies help to contain the growth of RE grid balance and maintain better conditions for the grid. However, they cannot be considered as the only flexibility providers for the power grid.

The experiments show that deploying power-to-methanol technologies can influence CO<sub>2</sub> reduction to a great extent. In the course of the next seven years, no  $CO_2$  reduction is observed in the simulation. From 2027 when carbon carbon capture utilization and storage (CCUS) network is realized, industries begin to capture their emissions. Soon after 2030, the capacity of the CCUS network is fully utilized while some industries have not yet captured their emission. As a result, CO<sub>2</sub> reduction is limited until power-to-methanol attracts the attention of investors. Even then, power-to-methanol technologies begin to pay off only around 2040. Given that sufficient CO<sub>2</sub> is available to start power-to-methanol supply chain, it becomes clear that powerto-hydrogen is the limiting step from 2027 to 2040. Green hydrogen production becomes a feasible option only when sufficient amount of renewable power is available on the grid. This does not happen before 2035 in most of the experiments. When power-to-methanol technologies are widely deployed, there is a threefold impact on CO<sub>2</sub> reduction. First and foremost, power-to-methanol process extracts CO<sub>2</sub> from the CCUS network. This way, capacity is released in the network and more industries can capture their emissions. Second, power-to-methanol funds green hydrogen production. In some cases, methanol production can stimulate green hydrogen production to the extent that more green hydrogen is produced than demanded for methanol production. This surplus green hydrogen can be directed to the industry to substitute gray hydrogen that comes with substantial  $CO_2$  emissions. Last but not least, in some cases more green methanol can be produced than demanded for as fuel. Therefore, green methanol can be used as feedstock in the chemical industry and replace normal methanol which is produced from a carbon-emitting process. Considering fulfillment of carbon reduction goals, it is striking that a grid with fewer flexibility options creates a better situation for CO<sub>2</sub> reduction. This is mainly due to the fact that all excess renewable power is directed to powerto-methanol as the only flexibility option for the grid. Therefore, hydrogen and methanol production begin to rise earlier in time and hence, CO<sub>2</sub> reduction can reach higher levels by 2050. Under these circumstances, it is possible to achieve carbon reduction goals by deploying power-to-methanol technologies, provided that the growth of renewable power supply is fast enough. In any case, power-to-methanol technologies have no

influence before 2030 and hence, are not helping with the 2030 reduction goals.

To put it in a nutshell, deployment of power-to-methanol technologies can help to contain RE grid balance and hence improve power grid's reliability to some extent, but it cannot be considered as the only alternative to make the power grid reliable. On the other hand, power-to-methanol technologies can greatly help in meeting carbon reduction goals in the industry.

#### 7.2. Recommendations

#### 7.2.1. Promoting power-to-methanol technologies

Based on the results of the simulations, the policy maker is recommended to support power-to-methanol technologies as a viable and promising flexibility option which enables achieving high levels of  $CO_2$  reduction. There are two bottlenecks that should be removed in order to exploit the potential of power-to-methanol technologies. The first bottleneck is the availability of surplus renewable power. Green hydrogen production does not suggest a good business case unless renewable power is abundant and thus cheap. As a result, the support for renewable power projects should remain in the agenda of energy transition. The second bottleneck is the market price of methanol. The experiments with the model showed that methanol production becomes interesting for the investors only if the price of methanol is above  $350 \notin/ton$ , which is significantly higher than the highest price of 2020, which was  $260 \notin/ton$ . This large difference suggests that for green methanol production to be interesting, it should be supported by subsidies or a system like guarantee of origin (GoO) which is used for renewables.

Another recommendation for the policy maker considering energy transition is to watch out for mismatching signals for different sectors. This research particularly reveals a risk about incoherent actions in the supply and demand side of the market for green methanol. In some cases, methanol is demanded as a bunker fuel while far too little green methanol is produced to satisfy the demand. The shipping sector in turn, buys normal methanol and this *increases* CO<sub>2</sub> reduction from methanol production processes. Even if green methanol is produced later, the emission cannot be easily reverted. If the policy agenda aims at promoting alternative fuels for the shipping sector, the viability of producing that fuel should be taken into account.

Finally, the policy makers should be wary of the lock-in effect. Using alternative fuels like methanol requires a change (even minor) in the propulsion technology. The actors might need support to take this step and modify their assets. However, the technology is still carbon emitting. If the policy maker envisages a full decarbonization of a sector, the next step to switch from methanol to a zero-emitting fuel such as hydrogen still needs financial support. The policy maker is thus advised to allocate the financial support for current and future transition steps in a smart way, to decrease the risk of lock-in on carbon emitting technologies.

#### 7.2.2. Collaboration of actors

The system operator is responsible to maintain grid reliability. Large variations of renewable power supply are troublesome for the grid. These sharp changes provide alternating signals to investors in flexibility provider systems such as large scale storage. When the market is not predictable for these investors, they "wait and see", i.e. delay investments. The system operator is thus facing more from fluctuations of grid balance. Lack of enough investments in flexibility options means in reality, the outcomes would come close to the results of "low flexibility grid" experiments. In those experiments a persistent rise of RE grid balance was observed for high scenarios. If the system operator fails to expand the cross-border interconnection capacity in time, the oscillation and rise of RE grid balance makes the grid unreliable.

The system operator cannot influence the rate of deployment of power-to-methanol technologies. However, she can recognize the underlying reason for the oscillations and gradual increase of RE grid balance. The main factor that fuels these oscillations is the investment cycle for green hydrogen production. The investors in green hydrogen consider their individual interests when considering an investment. The same holds for investors in green methanol production. They do not involve the system operator in their decision making. However, this decision making process undermines the fact that the power should be supplied from the power grid. What happens to the power grid is not communicated in time with potential investors in green hydrogen and green methanol. Opening room for discussion, long term joint strategies and enabling flow of information can alleviate the problems that the system operator faces regarding RE grid balance.

#### 7.2.3. Investing in power-to-methanol technologies

The industry is recommended to consider all aspects of power-to-methanol technologies. Even if demand is established for green methanol, it is not recommended to start investments unless the grid can transmit sufficient renewable power for this purpose. Otherwise, high and volatile hydrogen prices influence the business case in the future. Furthermore, the production of green methanol varies in a wide range throughout the simulations. This variation suggests high volatility of the market for green methanol production. The system seem to show a chaotic behavior regarding methanol production. This might be due to lack of support for power-to-methanol technologies which creates an unstable ground for developments.

#### 7.3. Discussion

In this research, assumptions were made that have clear consequences. Some of them should be relaxed in order to have a more realistic model.

#### 7.3.1. Technology assumptions

The results presented here are only valid for one configuration of methanol production which is full load operation. Furthermore, green hydrogen production is external to green methanol production, which makes it necessary to have hydrogen backbone ready. However, a configuration with on-site green hydrogen production is also possible. Sourcing of  $CO_2$  only happens through CCUS network as well. However, on-site Direct Air Capture (DAC) is a feasible option in real world. Exploration of the system behavior when DAC is playing a role can be a good addition to this study.

#### 7.3.2. Market assumptions

The market price for hydrogen, methanol and utilized carbon is set at a constant value throughout the simulation. This assumption was made in order to keep the scope of the problem manageable within the time limit. However, one can expect the demand for green hydrogen and green methanol vary in time and so does the market price. Furthermore, in reality there would be other types of contracts between actors that enable investors to hedge part of their risks. By concluding bilateral contracts, the price might be different from the market price. It is worthwhile to investigate the system behavior when negotiation of bilateral contracts creates dynamic prices.

In the hydrogen market, green hydrogen is competing with blue hydrogen. Provided that the CCUS network is available in time, blue hydrogen might have a better business case. Furthermore, import of hydrogen is supposed to play an important role in the future of hydrogen supply in the Netherlands. The imported hydrogen competes with the hydrogen produced in the Netherlands. Hydrogen might also be converted to methanol in other countries and then be transported to the Netherlands. The competition of imported green methanol with the green methanol produced in the Netherlands creates a totally different ecosystem and hence, might greatly influence the findings of this research. In this regard, a new degree of freedom should be considered by the investors in green hydrogen.

#### 7.3.3. System assumptions

In reality, high renewable power production which is not balanced properly, demotivates further investment in renewable power production. Therefore, the energy system might follow an ambitious, fast-growing renewable scenario but it is highly probable that we shift to slower growth rates in case the grid is not able to balance out the fluctuations and residual balance. This research assumed that investments in renewable power goes on irrespective of changes in the system.

Furthermore, increasing the capacity of cross-border interconnections can alleviate the congestion problem and decrease the need for storage units. Therefore, if the developments regarding international connections were included in the model, it would have influenced the RE grid balance and less renewable power would have been available in the Netherlands for hydrogen production.

It is assumed that onshore and offshore hydrogen production have the same cost, whereas offshore wind combined with hydrogen can create a good business case for wind farm, hydrogen and the system operator. In essence, formation of consortia is a common practice to address mutual interests of actors; an aspect which was not modeled in this research. That might be one of the causes of the oscillations observed in the results of RE grid balance.

#### 7.4. Future work

#### 7.4.1. Complete the framework of drivers

The interviews with experts were analyzed and placed into the framework of drivers developed by Darmani et al. (2014) in chapter 4. In the discussion in section 4.4, it was concluded that the incentives created from knowledge infrastructure and soft institutions are overlooked by the interviewees. Further literature review also did not turn in relevant results. Therefore, researchers are encouraged to delve into the subject and investigate drivers caused by these two factors. This could be done by means of conducting interviews with a larger and more diverse group of interviewees. In particular, policy makers shall be involved in the interviews in order to make sure they have a complete overview of the drivers and barriers. Moreover, the framework can be used to formulate a Q-analysis in order to identify groups of perspectives among various actor.

Other than the two aforementioned factors that were missing in the interviews, three factors were not elaborated enough. Incentives arisen from the societal network around the technology, incentives created from the structure of the actors and incentives created from policy conformity were discussed only briefly. The connection between actors and the community and social acceptance can play role in further deployment of power-to-methanol as a new technology. The type and structure of actors are other elements that can be studied further. Finally, policy researchers are urged to investigate the effect of policy conformity within the regulatory framework on deployment of power-to-methanol technologies.

#### 7.4.2. Improving the model of power grid

The grid is assumed to expand in the same pace as the demand and supply increase. This might not be the case in reality. In future work, grid constraints should be considered. This can be done most conveniently by including the system operator as the agent responsible for the grid. Furthermore, the perspective on grid reliability can be improved by adding two dimensions to the model of grid:

- Calculation of total RE grid balance, taking into account the amount of power produced by conventional power plants and the rate of coal phase out,
- Using hourly production curve of renewable power for calculation of more detailed reliability measures such as Loss of Load Expectation (LoLE).

Finally, direct use of hydrogen in fuel cells in a power-to-hydrogen-to-power setting is not studied here. In the future, the model can be expanded to include power-to-hydrogen-to power. This will bring valuable insights for the system operator.

#### 7.4.3. Competition of E-fuels

Green methanol is not the holy grail of energy transition. Ammonia and methane are strong competitors for methanol. With minor modifications, the model developed here can be used to simulate methane and ammonia production and the role they can have in the energy mix. As a further development of the model, users of or investors in E-fuels can have the possibility to decide between two or more options.

#### 7.4.4. Including market models

In the current model, price of green hydrogen and green methanol are constant throughout the simulation. The influence that the demand side can have on the price is not quantified. A next step that can lead to more insight into the topic is to include a market model for hydrogen and methanol. A model for the carbon utilization market can also be useful in understanding the future of carbon utilization technologies. By including a market model, the role of hydrogen import can be studied easier.

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# A

# Assumptions

In this chapter, model assumptions, data assumptions and the range of uncertainties are summarized.

#### A.1. Model assumptions

#### Green hydrogen

A-1	Electrolysers only operate during surplus hours.
A-2	The distinction between green hydrogen and other types of hydrogen is made by a system like "GvO"
	(Garantie van Oorsprong - Guarantee of origin). Therefore, inefficient loop of "natural gas $\rightarrow$ blue
	hydrogen $\rightarrow$ methanol" can be avoided.
A-3	Until 2030, the prominent technology of electrolysis is Alkaline Electrolysis Cell (AEC). Afterwards,
	Protone Exchange Membrane Electrolysis Cell (PEMEC) becomes favorable.
A-4	No subsidy is granted to the green hydrogen investors.
A-5	In the financial calculations of hydrogen supplier and consumer, the cost of connection to hydrogen
	transport network is not included. It is assumed that this cost is negligible compared to other upfront
	costs.
A-6	Hydrogen transport costs are neglected because no information is available about it.
A-7	Electrolyser CAPEX is equal to the minimum of the projected range in the scenarios (see table 3.3).
A-8	Green hydrogen is traded at a fixed price throughout the simulation.
A-9	There is no limit on the capacity of electrolysers.
A-10	Every time a new investment in electrolyser is made, its efficiency is set to a random value in the
	range of technically possible efficiencies.
A-11	Hydrogen backbone and hydrogen storage is available from 2030. Without hydrogen backbone,
	trade of hydrogen is not possible.
A-12	Currently, all hydrogen that is produced by the industry is gray hydrogen using steam gas reforming
	from natural gas.
A-13	Hydrogen production can happen offshore, though there is no distinction between onshore and off-
	shore hydrogen production in terms of costs.

A-14	Connection to the hydrogen backbone is governed by a long-term contract.
CO <sub>2</sub> supp	ly
A-15	In the model, the top 11 emitters in the Rotterdam and Amsterdam can capture their emissions.
	Other smaller industries are not included.
A-16	Porthos and Athos infrastructures are in place from 2027.
A-17	Porthos and Athos are connected through OCAP and form the carbon capture, utilization and storage
	(CCUS) infrastructure for the areas Amsterdam and Rotterdam.
A-18	OCAP pipeline has sufficient capacity to fully connect Porthos and Athos.
A-19	$CO_2$ is only traded through the CCUS network. There is no point-to-point transport of $CO_2$ .
A-20	Industries might choose to capture $CO_2$ only partially. This can happen if the CCUS network has
	insufficient capacity available. They can capture the rest of their emissions later.
A-21	All modeled industries have equal rights to connect to the CCUS network.
A-22	Industries estimate ETS price to be constant and equal to the average of the scenario for ETS price
	over the next five years.
A-23	Costs of making a connection to the CCUS network is equal for all industries.
A-24	When $CO_2$ is utilized, ETS emission right should be purchased by the industrial emitter.
A-25	$CO_2$ is traded for utilization at a fixed price throughout the simulation.
A-26	Carbon utilization price consists of an average value plus a random variation between 0 and 10% of
	the average.
A-27	The CCUS network operator decides on the amount of $CO_2$ which is stored or utilized.
A-28	The CCUS network operator will refuse to give access to industries only if the capacity of infrastruc-
	ture is fully utilized.
A-29	When $CO_2$ is utilized, capacity is released on the CCUS network by an amount equal to $CO_2$ uptake.
A-30	Before injection in the CCUS network, $CO_2$ is purified to the extent needed for green methanol pro-
	duction process.
A-31	Due to improvement of processes, the amount of $CO_2$ emission from industries decrease by a con-
	stant rate every year.
A-32	ETS price varies around the average by a random amount between 0 to 10% of the average price.
A-33	Carbon capture from industries operate 24/7.
A-34	Both carbon capture and carbon utilization receive the same amount of subsidy, for 15 years.
A-35	Electricity demand of the industry grows with a rate of 1% per year. The increase due to economic
	growth and decrease due to efficiency improvement are accounted for.
Green me	
A-36	There would be little change in the industrial demand for methanol. The increase in methanol de-
	mand comes from the shipping sector shifting to methanol as alternative fuel.
A-37	Green methanol is sold at the same price as normal methanol.
A-38	Green methanol is sold at a fixed price throughout the simulation.
A-39	While making financial calculations, investors in green methanol assume a random uncertainty in
	the price of methanol, between zero and 10% of methanol price.
A-40	Assumed is that green methanol production unit can be as big as desired by the investor, provided
• • •	that sufficient input (i.e. hydrogen and $CO_2$ ) is available.
A-41	Green methanol production unit sources hydrogen and $CO_2$ externally.
A-42	Green methanol production unit operates full load 24/7.

A-43 No subsidy is granted to the green methanol investors.

#### Power system

- A-44 For green hydrogen, green methanol and carbon capture, power is sold at the wholesale price.
- A-45 The power grid expands at a rate sufficient to handle all the new supply and demand.
- A-46 The new demand on the power grid includes: demand from electrolysers, demand for carbon capture technologies, demand for methanol production.
- A-47 All power plants other than renewables (i.e. solar and wind) are fully controllable. This means first the uncontrollable renewables are dispatched and then the deficit power is provided by conventional power plants.
- A-48 No more new conventional power plant is constructed after 2020.
- A-49 Renewable power supply is coherent with one of the four scenarios discussed in Matthijsen et al. (2018) and summarized in section 3.1.1.

Other

- **A-50** The delay between making decision about the investment and placing the investment (i.e. having the system operational) is less than a year.
- A-51 Most of the future scenarios give values for parameters in 2030 and 2050 and not in the years between. To estimate the values for other years, a linear interpolation is used.
- A-52 All energy sectors are fully liberalized, i.e. all decision makers are private entities.
- A-53 Limitations with regard to land use are neglected.

# A.2. Data assumptions

Data	Assumption	Source
US\$ to €	0.92	XE (2020)
Wholesale electricity price	From 2020 to 2030: linear increase from 43 to 57 €/MWh; from 2030 to 2050: constant at 57 €/Mwh.	Schoots and Ham mingh (2019)
Electricity demand	From 2020 to 2030: linear decrease from 1082 TWh to 99 TWh; from 2030 to 2050 lin- ear decrease from 99 to 98 TWh.	CPB and PBL (2015) Two degree centra scenario
Electrolyser efficiency (%)	63 to 74	IEA (2019a)
<i>CO</i> <sub>2</sub> emission from conven- tional power plants (ton/GWh)	650. Note: value taken from earlier years where almost no renewable power was generated.	CBS (2018)
Average ETS price (€/ton)	From 2020 to 2050, rises linearly from 20.5 to a value in the range between 40 to 160.	CPB and PBL (2015) EEX (2020)
CO <sub>2</sub> reduction due to electri- fication and improvements of process (%/yr)	0.8	Schoots and Ham mingh (2019)
Hydrogen energy content (MJ/kg)	141.8. Note: High Heating Value (HHV) is taken.	van Gerwen, Ei jgelaar, and Bosma (2019)
<i>CO</i> <sub>2</sub> emission from gray hydro- gen production (ton/GJ)	0.07. Note: Hydrogen production by steam gas reforming process with natural gas.	IEA (2019b)
Methanol energy content (MJ/kg)	23.84. Note: High Heating Value (HHV) is taken.	van Gerwen et al (2019)
$CO_2$ emission from conven- tional methanol production (ton $CO_2$ /ton methanol)	2.3. Note: Estimates vary between 0.8 to 3.1 and the global average is 2.3.	IEA (2019a)
Discount rate	4.5%	van den Boomen e al. (2017)
Total capacity of CCUS in- frastructure in Rotterdam- Amsterdam region (Mton)	10	van Bracht and Braun (2018)
<i>CO</i> <sub>2</sub> emission reduction in the energy sector (%/yr)	0.8	Schoots and Ham mingh (2019)

Table A.3: Thermodynamic variables used to estimate the power consumption of carbon capture technologies.

Variable	Value	Note
F	5% of polytropic work.	-
n	1.30	-
$\eta_p$	0.7	-
$Z_{av}$	0.97	From Adisoemarta, Frailey, and Lawal (2004), at $220F$
		and 500 psi.
$T_I$	400 K	-

# B

# Variables and Formulas

### B.1. Formulas for calculation of grid balance

 $GB = E_{RES} + E_{Conv.} - D \; .$ 

 $GB_{RE} = GB - E_{Conv.}$ ,

 $GB_{RE} = P_{RES}T_{RES} - D^* - E_{Conv.},$ 

$$\begin{split} D^* &= P_{H_2} T_{H_2} + P_{MeOH} T_{MeOH} + \Delta \epsilon_{Cap.} \tilde{P}_{Cap.} T_{Cap.} \; , \\ GB_{RE,exp} &= GB_{RE,t_0} + \frac{\Delta GB_{RE}}{\Delta t} . t_D \; . \end{split}$$

## B.2. Formulas for calculation of CO<sub>2</sub> reduction

 $p_{sect.} = rac{\sum_{x \in sect.} \Delta \epsilon_x}{\epsilon_{ref,x}}$  ,

 $\Delta \epsilon_{Tot.} = \Delta \epsilon_{Cap.} + \Delta \epsilon_{Power} + \Delta \epsilon_{H_2} + \Delta \epsilon_{MeOH} \text{ ,}$ 

$$\Delta \epsilon_{Cap.} = \sum_{i=1}^{11} \Delta \epsilon_i$$
 ,

 $\Delta \epsilon_{Power} = \delta \tilde{\epsilon}_{Power} S_{RES}$  ,

 $\Delta \epsilon_{H_2} = \delta \tilde{\epsilon}_{H_2} (P_{H_2} T_{H_2} - f_{H_2} P_{MeOH} T_{MeOH}) \ , \label{eq:electropy}$ 

 $\Delta \epsilon_{MeOH} = \delta \tilde{\epsilon}_{MeOH} (P_{MeOH} T_{MeOH} - \alpha_{MeOH} D_{Shipping}) ,$ 

## **B.3.** Formulas for calculation of business case

$$\begin{split} NPV_{H2} &= -CAPEX_{H2} + \sum_{t=1}^{L_{H2}} \frac{\pi_{H2}}{(1+i)^{t}} , \\ NPV_{Cap.} &= \sum_{t=1}^{15} \frac{\bar{\pi}_{ETS} + S_{Cap.} - C_{Cap.} - C_{Conn.} - C_T - C_S}{(1+i)^{t}} + \sum_{t=16}^{L_{Cap.}} \frac{\bar{\pi}_{ETS} - C_{Cap.} - C_{Conn.} - C_T - C_S}{(1+i)^{t}} , \\ NPV_{Cap.} &= \sum_{t=1}^{15} \frac{\pi_U + S_{Cap.} - C_{Cap.} - C_{Conn.} - C_T}{(1+i)^{t}} + \sum_{t=16}^{L_{Cap.}} \frac{\pi_U - C_{Cap.} - C_{Conn.} - C_T}{(1+i)^{t}} . \\ NPV_{MeOH} &= -CAPEX_{MeOH} + \sum_{t=1}^{L_{MeOH}} \frac{\pi_{MeOH} - OPEX_{MeOH}}{(1+i)^{t}} , \end{split}$$

 $OPEX_{MeOH} = OPEX_{fix,MeOH} + f_{H_2}\pi_{H_2} + f_{CO_2}\pi_{CO_2} + f_e\pi_e$  ,

# C

# Supplementary material: interviews

In this appendix, a list of role, expertise and affiliation of the interviewees are presented. Furthermore, the confirmed statements of interviewees are presented.

#### **C.1. Interviewees**

Most of the energy experts were advisors and consultants in strategy, sustainable industry, energy transition, investment, hydrogen and sector coupling. Two academics were consulted as well, with expertise in low carbon technologies and policy analysis. Table C.1 lists the organizations and the roles of experts.

Role	Expertise	Affiliation
Professor	Low carbon systems and technologies	TU Delft
Associate professor	Policy analysis, energy economics	TU Delft
Consultant	Electrical power systems and industry	Royal HaskoningDHV
Consultant	Energy transition	Royal HaskoningDHV
Consultant	Energy systems	Royal HaskoningDHV
Consultant	Strategy and technical	Royal HaskoningDHV
Strategic consultant	Smart energy	Royal HaskoningDHV
Senior consultant	Investment	Royal HaskoningDHV
Advisor	Sustainable industry	Royal HaskoningDHV
Advisor	Strategy	Eneco
Advisor	Strategy	Eneco
Senior advisor	Process, water management and energy	Royal HaskoningDHV
Senior advisor	Energy transition	Royal HaskoningDHV
Expert	Environment and Energy	Royal HaskoningDHV
Manager	Business strategy (energy, hydrogen, sector coupling)	Accenture
Senior project manager	Energy transition	Royal HaskoningDHV

Table C.1: Role, expertise and affiliation of interviewees.

### **C.2. Confirmed statements**

In this section the results per theme are presented. In each theme, different categories are identified. Statements are labeled for the ease of reference in the rest of this document.

#### C.2.1. Facts and current state of affairs

Table C.2 lists all the statements regarding the technical facts of the system and current state of affairs. Statements are labeled from SC-1 to SC-20, where *S* stands for *Statement* and *C* stands for *Current state*.

Table C.2: Expert statements about "Facts and current state of affairs".

Category	Label	Statement
	SC-1	If we are going to have distributed electrolysers, the power grid in the
Davison and J		Port of Rotterdam is not sufficient up to 2030.
Power grid	SC-2	The urgent questions for the power grid are: how to resolve disbalance?
		How to compensate for the lack of generation capacity?
	SC-3	After 2030, surplus hours might increase to up to 2000 hours in a year.
	SC-4	Increase of surplus hours is limited because it feeds back to the deci-
		sion making about renewable power investments.
Power grid / Energy	SC-5	If there is a temporary congestion issue, e.g. a very large load for a short
		while during constructions, storages are interesting as they can resolve
storage		congestion.
	SC-6	When it comes to stabilization and congestion management, cross-
		border interconnection competes with storage options.
	SC-7	Storage might solve the congestion problem but is not the final solu-
		tion.
Enorgy storage	SC-8	Large scale storage units are mostly in the research phase.
Energy storage	SC-9	Regarding renewable energy, the most challenging storage issue is not
		short term but long term, seasonal storage.
	SC-10	For offshore wind, the combination of a light cable connection for base
Hydrogen		load combined with a hydrogen solution for peak production is possi-
		ble.
	SC-11	Hydrogen infrastructure is so expensive. That's a bottleneck for hydro-
		gen.
	SC-12	If you convert offshore wind directly to hydrogen, then the electricity
		price to operate the electrolyser is currently higher than when it is con-
		nected to the grid.
	SC-13	Some catalysts for methanol production are very sensitive to impurities
CCUS		(e.g. sulfur or heavy metals). You should either put a purification unit at
		the source of $\mathrm{CO}_2$ or at the methanol production unit. Then the CAPEX
		increases on either side.
		Continued on the next page.

Category	Label	Statement
	SC-14	Direct Air Capture has no sulfur, thus a great source of $\mathrm{CO}_2$ for
		methanol production. However, it is expensive at the moment and the
		carbon footprint depends on the source of power production used for
		DAC.
	SC-15	Investment in CCS is linked with the production of blue hydrogen. This
		influences green hydrogen production.
Transport soctor	SC-16	Aviation sector has a high inertia to change.
Transport sector	SC-17	Ammonia is seen as a good alternative fuel for long distance shipping.
	SC-18	It is important to note energy systems emerge in parallel and in real life,
Other		they have influence on each other.
	SC-19	Partnerships involve actors from the whole supply chain.
	SC-20	There are two reasons to be interested in e-fuels: first, transport of hy-
		drogen is an issue, and second, export and import of e-fuels are easier.

Table C.2: Expert statements about "Facts and current state of affairs" (continued).

### C.2.2. Strategies of actors

Table C.3 lists all the statements regarding the strategies of actors regarding investment in and operation of their assets. Statements are labeled from SSt-1 to SSt-23, where *S* stands for *Statement* and *St* stands for *Strategies of actors*.

Table C.3: Expert statements about "Strategies of actors".

Category	Label	Statement
	SSt-1	A company makes decisions based on her vision about the future.
Comment		Subsidies do play a role here.
General	SSt-2	There are many studies but no coherent action. Most of the compa-
		nies are waiting to see if the government is going to provide sufficient
		support.
	SSt-3	The period of rethinking a decision depends on the technical and eco-
		nomic lifetime of the technical system.
	SSt-4	The period of rethinking a decision depends on the type of the com-
		pany. Larger corporations tend to have longer decision periods.
	SSt-5	Nowadays, many industries are based in the Netherlands, but that has
Considering energy		a historical reason: cheap gas from Groningen. Now that the gas field
transition		is closed, industries might leak out of the Netherlands. The moments
		new assets are bought, companies have to decide on this.
	SSt-6	We should incorporate climate change in every decision that we take
		NOW. We can't afford to forget the climate anymore!
	SSt-7	Strategically, it is wiser to start the shift to no-carbon fuels instead of
		producing carbon-based e-fuels.
	•	Continued on the next page.

Table C.3: Expert statements about "Strategies of actors (continued)".

Category	Label	Statement
	SSt-8	If methanol is good for industrial processes, it's ok, but we should
		mind that we don't spend energy to produce a fuel which is going to
		emit $CO_2$ again if combusted.
Desirente et en	SSt-9	The future of renewable energy generation is much more predictable.
Power sector		SDE takes care of subsidies for all types of renewable power genera-
		tion.
	SSt-10	As long as there is a way to use the energy in electrons, end users adapt
		and shift to electrical technologies. Then there is no reason to use the
		less efficient way and produce hydrogen from electrical energy.
	SSt-11	The most logical configuration is to run electrolysers (almost) off-grid,
		with a large renewable unit dedicated to it.
	SSt-12	Big companies think decades ahead when it comes to investments in
Hydrogen		hydrogen. Investment in hydrogen is more strategically motivated.
		Short term finance doesn't play much role.
	SSt-13	There is an option to combine hydrogen production with offshore
		wind. However, the industry is currently focusing on wind and de-
		laying hydrogen!
	SSt-14	Green hydrogen production has not reached the critical mass. If there
		is a minimum adoption of green hydrogen production, the develop-
		ment goes exponentially afterwards.
	SSt-15	For sea-going heavy-transport, in the Netherlands e.g. shipping, both
		hydrogen and hydrocarbons might be an option. If the Port of Rotter-
		dam decides to supply hydrogen instead of fossil fuels, the ships might
		easily get their fuel from other bunkering ports (like Hamburg, Singa-
		pore or Shanghai). Therefore, the development to hydrogen-fueled
		shipping can't be forced from the supply side.
	SSt-16	Industrial users of an electrolyser would probably like to run their
	000 10	electrolyser full time, in order to keep the processes running continu-
		ously.
	SSt-17	The larger the wind plant, the further offshore it is placed. The further
	551-17	the wind plant, the more expensive it is to transmit electricity. The
		more expensive electricity transmission, the more interesting hydro-
		gen production is.
	SSt-18	
CCUS	551-10	For Tata steel, since they have no option for decarbonization in short
CCUS	664 10	term, they are motivated to utilize their carbon emissions.
	SSt-19	The landscape is more predictable for CO <sub>2</sub> storage as compared to hy-
		drogen.
	SSt-20	Even with $CO_2$ utilization, most of the $CO_2$ is surplus and should be
		stored. Therefore, companies more or less know what is going to hap-
		pen and are investing in storage infrastructure.
		Continued on the next page.

Category	Label	Statement
	SSt-21	Using intermittent renewable sources for constant methanol produc-
E-fuel (methanol)		tion implies a need for huge buffer capacity. On the other hand, the
		use of space should be optimized.
	SSt-22	New technologies for flexible methanol production are possible, al-
		though they appear to be risky to investors.
	SSt-23	End consumers of E-fuels have huge energy demands. They never rely
		on flexible contracts alone.

Table C.3: Expert statements about "Strategies of actors (continued)".

#### C.2.3. Current and short-term moves of actors

Table C.4 lists all the statements regarding the current and short-term moves of actors. Statements are labeled from SM-1 to SM-22, where *S* stands for *Statement* and *M* stands for *Moves of actors*.

Category	Label	Statement
Power sector	SM-1	Currently, more and more EV's are adopted by people which means
Power sector		there would be a huge problem with local distribution networks.
	SM-2	North west european countries are planning to have a large interna-
		tional network in the north sea. Together with the gas transmission
		network, the energy system is built up.
	SM-3	There is an idea to have between 60-100 GW wind power offshore, and
		make hydrogen from 90% of its production and transmit the rest to the
		power grid.
	SM-4	Port of Rotterdam has commissioned a study to investigate how hy-
Hydrogen		drogen could be produced in Oman using solar power, and then con-
		verted into Ammonia, Methanol and liquified hydrogen and transport
		it to Rotterdam.
	SM-5	There is a large company in the north: NortH2 which is going to pro-
		duce hydrogen in large scale and inject it into gas grid.
	SM-6	Car factories are also promoting hydrogen cars.
	SM-7	A consortium of Shell Nederland, Gasunie, Groningen Sea Port
		launched NortH2 project.It's only feasibility analysis, although it's a
		major hydrogen project announced.
	SM-8	A consortium of Vattenfall, Gasunie and Equinor started a study for
		blue hydrogen, in order to convert natural gas of Equinor to blue hy-
		drogen. The $\text{CO}_2$ goes into empty offshore gas fields of Norway. The
		hydrogen is mainly used in Groningen Magnum power plant and the
		surplus is sold in the Dutch hydrogen market.
	<b>(</b>	Continued on the next page.

Table C.4: Expert statements about "Current and near-term moves of actors".

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Category	Label	Statement
	SM-9	The 2x40 GW green hydrogen initiative, as part of the EU Green Deal,
		aims to connect hydrogen production in Africa and Ukraine to indus-
		trial hydrogen demand in Europe.
	SM-10	Rozenburg is the first urban area in the Netherlands that has provided
		hydrogen heating to dwellings.
	SM-11	Gasunie has a pilot project on conversion of part of high pressure gas
		pipelines to hydrogen backbone.
	SM-12	One of the first carbon capture and utilization initiatives was taken
CCUS		by Twence to utilize their $\ensuremath{\text{CO}}_2$ emissions and produce sodium bi-
		carbonate.
	SM-13	OCAP is going to expand in the near future to connect to other poten-
		tial sources.
	SM-14	Athos and Porthos projects are frontrunners of their type. By means
		of the Tiki study, the Dutch government confirmed that we need this
		infrastructure to reach our goals.
	SM-15	There is a demonstration unit in Iceland that produces methanol by
		CO <sub>2</sub> hydrogenation.
E-fuels	SM-16	There is a concept idea to produce renewables in large scale in Sahara
		and convert it to Ammonia to ship it to Europe.
	SM-17	Rotterdam-The Hague airport started a study on production of Kero-
		sine by DAC and green hydrogen.
	SM-18	Stedin is planning to invest in small-scale methane production units
		in cities, for peak shaving purposes on the demand side.
	SM-19	Tata steel is going to have an e-fuel production plant to produce jet
		fuel.
	SM-20	Aviation and maritime are potential buyers of E-fuels.
Transport sector	SM-21	In the shipping sector, some initiatives are taken for electrification.
		Biofuels also have a potential.
	SM-22	The easiest way for the shipping sector to meet decarbonization re-
		quirements is to use hydrocarbons and produce them onboard.

Table C.4: Expert statements about "Current and near-term moves of actors" (continued).

#### C.2.4. Regulations

Table C.5 lists all the statements regarding the current and near-term moves of actors. Statements are labeled from SR-1 to SR-12, where *S* stands for *Statement* and *R* stands for *Regulations*.

Category	Label	Statement
	SR-1	Rules of the game are changing a lot.
General	SR-2	The earlier a company applies for subsidies, the more money available
		and the more probable the company gets accepted.
	SR-3	In the next decade or so, nothing would probably change regarding the
		infrastructure. This is mainly due to the complexity of regulations that
		make a difficult situation.
	SR-4	For offshore wind plants, TSO is involved in the process from the begin-
Renewables		ning.
Reflewables	SR-5	For onshore wind TSO and DSO are not informed before all the research
		and permitting steps are fulfilled. They are obliged to provide the con-
		nection, though.
	SR-6	TSO is OBLIGED by law to accept the amount of RES which is offered,
		though they can charge you for providing excess capacity on the grid!
		This might in turn make you reconsider your decision.
	SR-8	There is a controversy regarding carbon capture and utilization in the
CCUS		ETS scheme. It is not clear who owns the emission right when the uti-
		lized carbon is released into the air after its end of life.
	SR-9	Green houses using $CO_2$ from OCAP are not paying for ETS.
	SR-10	Companies that capture CO <sub>2</sub> and inject it in OCAP pipline don't receive
		free emission rights under current scheme. This is under discussion.
Transport soater	SR-11	Compared to aviation and maritime, there is more control over inland
Transport sector		shipping from regulations.
	SR-12	Aviation emissions are global and not regulated tightly.

Table C.5: Expert statements about "Regulations".

#### C.2.5. Prospect of the future of energy transition

Table C.6 lists all the statements regarding the prospect of the future of energy transition. Statements are labeled from SF-1 to SR-24, where *S* stands for *Statement* and *F* stands for *Future of energy transition*.

Table C.6: Expert statements about "Prospect of the future of energy transition".

Category	Label	Statement	
Energy transition	SF-1	Energy demand of industries will change in future, because they impose	
		efficiency measures or electrify their processes.	
	SF-2	In the course of energy transition, the global flow of energy changes.	
		Continued on the next page.	

Category	Label	Statement
	SF-3	In the future, electricity grid is definitely not sufficient. Expansion of
D		grid takes a lot of time while a huge capacity of windfarms are on the way
Power sector		to be installed in the north sea. The distribution grid needs expansion
		of up to 10-11 GW.
	SF-4	Industry needs a lot of electricity for production and heating needs. The
		current electricity production might afford electrification of residential
		heat, but not industry.
	SF-5	4 million Dutch houses cannot be warmed sufficiently with electricity.
		We still need gas for it.
	SF-6	Other solutions for energy storage are: compresed air energy storage
		and hydrogen storage.
	SF-7	In the Netherlands, there is no business case for electrolysers that work
		during surplus hours only.
	SF-8	If demand is created for hydrogen, it would be a better choice for energy
		transition compared to hydrogen-based chemicals.
Hydrogen	SF-9	Hydrogen production is not the most relevant option in Netherlands, it
		could be produced much cheaper in Spain, Greece, Persian Gulf, etc.
		where plenty of solar energy is available.
	SF-10	Electrolysers are currently hand-manufactured! In the near future when
		the processes are automated and mass-production happens, capex is
		reduced.
	SF-11	We have an intensified gas network. We can easily use it for hydrogen
		transmission. In this sense, gas network is used in parallel with electric-
		ity network in the future.
	SF-12	Hydrogen could be seen as a way to warm houses, because heating sys-
		tems have a lifetime of about 15 years, and should be replaced anyway.
		So better to replace it with something suitable for hydrogen!
	SF-13	In the long term, hydrogen is on of the best energy carriers and means
		for energy storage.
	SF-14	Importing green hydrogen from locations that have a high potential for
		renewables might outperform hydrogen production in the Netherlands.
	SF-15	Hydrogen market is a local market, though fossil fuels are traded in a
		global market. Therefore, local initiatives can't solve the global problem
		unless there is a global effort.
	SF-16	In the future, direct hydrogen production with offshore wind will be-
		come less costly than on-grid hydrogen production.
00110	SF-17	Sources of CO <sub>2</sub> will increase in the next 10-15 years, and decrease in the
CCUS		far future. Therefore, if we utilize CO <sub>2</sub> now, we might need other sources
		like DAC to satisfy $CO_2$ demand.
	SF-18	CCS may act as a catalyst to a future of $CO_2$ supply by DAC.
		Continued on the next page.

Table C.6: Expert statements about "Prospect of the future of energy transition" (continued).

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Category	Label	Statement
	SF-19	Electrofuels are promising alternative fuels for aviation and maritime
		sector when these sectors have to switch to carbon-neutral propulsion.
E-fuels	SF-20	Any investment that is placed now in hydrocarbon production with $\ensuremath{\mathrm{CO}_2}$
		utilization, would turn into a worse business case in the near future if
		the energy system transition goes well.
	SF-21	Production of methane instead of extraction, helps the transition.
	SF-22	In the short term, E-fuels are needed but since their production capacity
		is limited, we need other alternatives in the long term.
	SF-23	For shipping, methanol has an advantage as there is little change in the
		propulsion technology.
	SF-24	Even though the supply chain for e-fuel production is complex, it might
		be the only solution to stabilize the power grid.
Transport sector SF-25		The transport sector is going more and more electric. Buses are mostly
		shifting to electrical propulsion. Even heavy duty road transport is going
		electric.

Table C.6: Expert statements about "Prospect of the future of energy transition" (continued).

# D

# Supplementary material: figures and charts

## D.1. Supporting figures for analysis of renewable energy (RE) grid balance

In this section, the supplementary figures that were referenced in section 6.4 are presented.

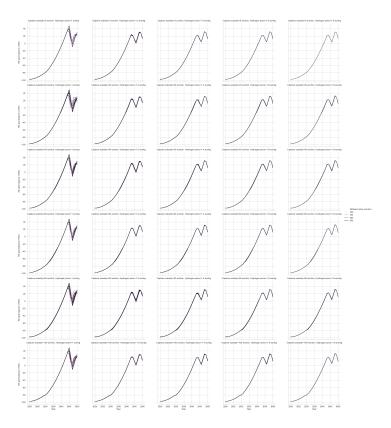


Figure D.1: Different patterns of grid balance for different combinations of hydrogen price and carbon capture subsidy for "Sustainable together" scenario, flexible grid experiments .

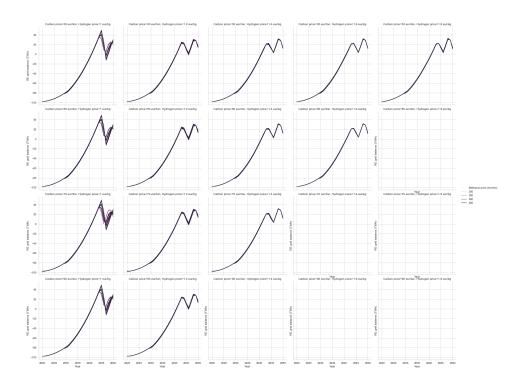


Figure D.2: Different patterns of grid balance for different combinations of hydrogen price and carbon utilization price for "Sustainable together" scenario, flexible grid experiments.

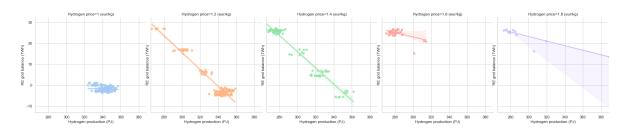


Figure D.3: Grid balance in 2050 versus hydrogen production, low flexibility grid experiment, in "Rapid development" scenario. The solid line shows linear regression estimation of the trend.

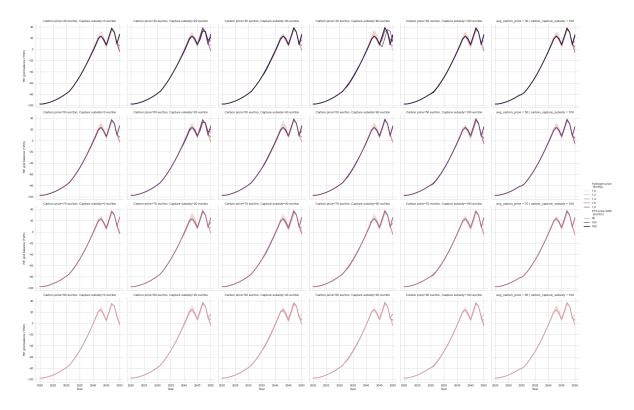


Figure D.4: Different patterns of grid balance in "Rapid development" scenario of low flexibility grid experiments, for different combinations of hydrogen price, carbon utilization price, carbon capture subsidy and ETS price in 2050.

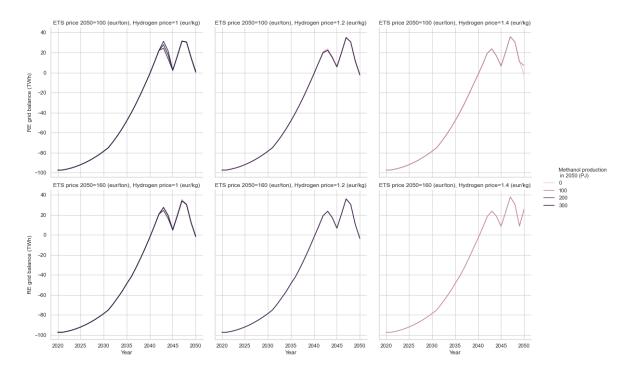


Figure D.5: Different patterns of grid balance in "Rapid development" scenario of low flexibility grid experiments, for different combinations of hydrogen price and ETS price in 2050. Carbon capture subsidy=40 euro/ton and carbon utilization price=70 euro/ton.

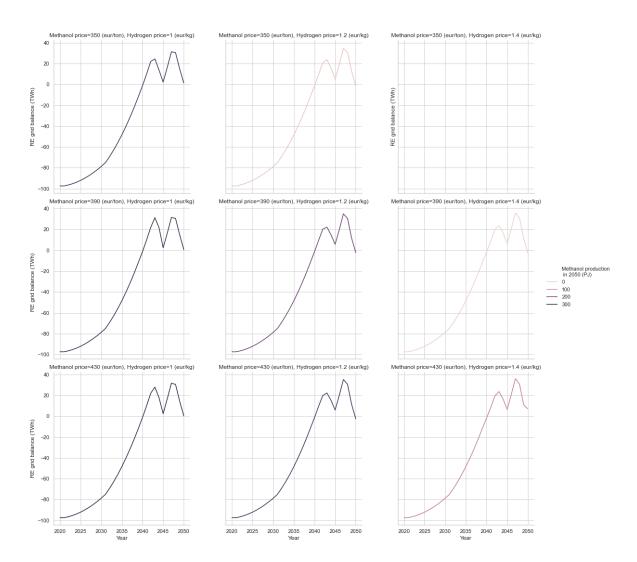


Figure D.6: Different patterns of grid balance in "Rapid development" scenario of low flexibility grid experiments, for different combinations of hydrogen and methanol price. ETS price in 2050=100 euro/ton, carbon capture subsidy=40 euro/ton and carbon utilization price=70 euro/ton.

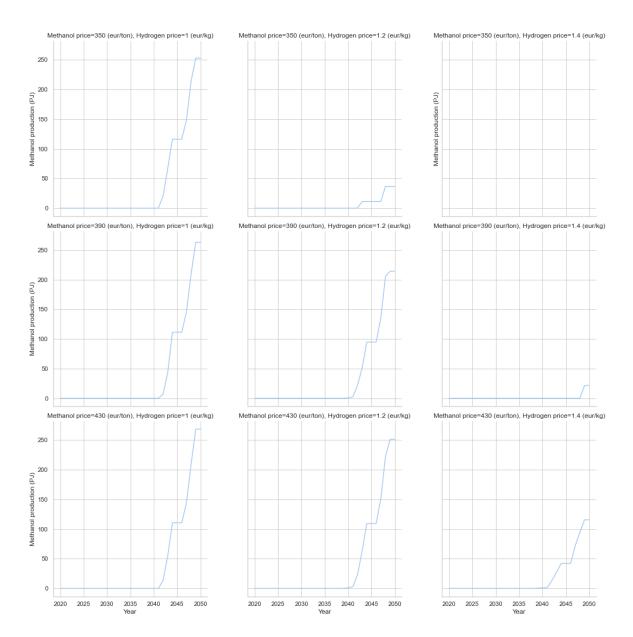


Figure D.7: Different patterns of methanol production in "Rapid development" scenario of low flexibility grid experiments, for different combinations of hydrogen and methanol price. ETS price in 2050=100 euro/ton, carbon capture subsidy=40 euro/ton and carbon utilization price=70 euro/ton.

# D.2. Supporting figures for analysis of CO<sub>2</sub> reduction

In this section, the supplementary figures that were referenced in section 6.5 are presented.

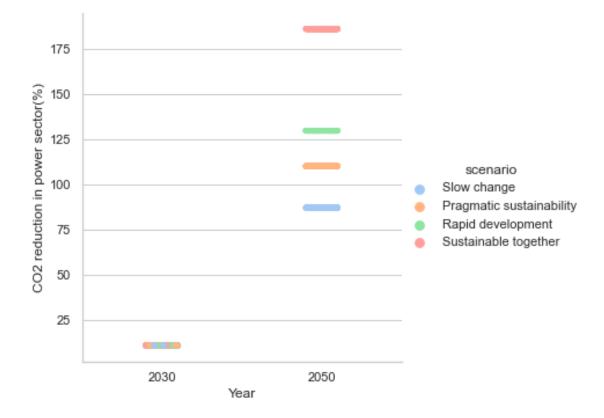


Figure D.8: Percentage of CO<sub>2</sub> reduction in the power sector in 2030 and 2050 in different renewable scenarios, flexible grid.

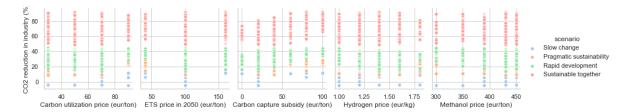


Figure D.9: Percentage of CO<sub>2</sub> reduction in 2050 in the industry versus model inputs, flexible grid.

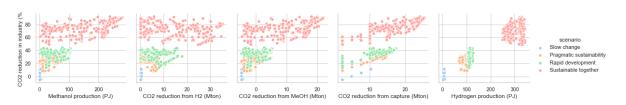


Figure D.10: Percentage of CO<sub>2</sub> reduction in 2050 in the industry versus intermediate variables, flexible grid.

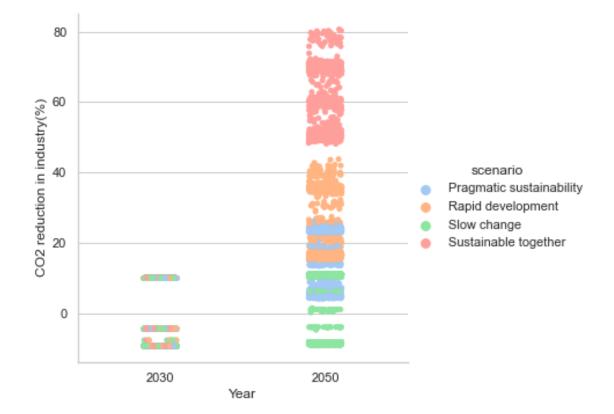


Figure D.11: Percentage of CO<sub>2</sub> reduction in 2030 and 2050 in the industry, when no methanol is produced before 2050, per scenario, flexible grid.

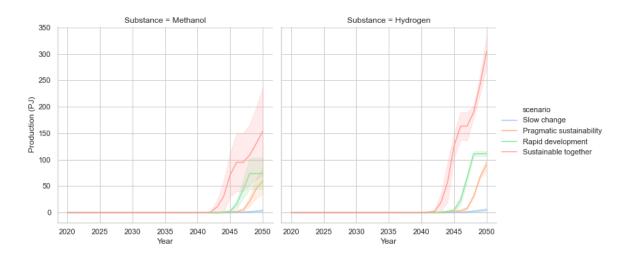


Figure D.12: Methanol and hydrogen production from 2020 to 2050 per scenario, flexible grid.

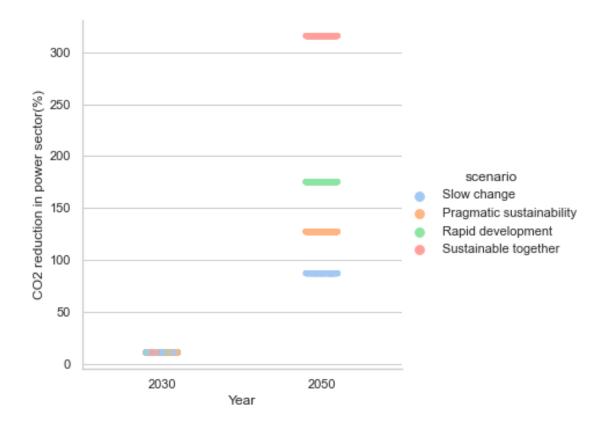


Figure D.13: Percentage of CO2 reduction in the power sector in 2030 and 2050 in different renewable scenarios, low flexibility grid.

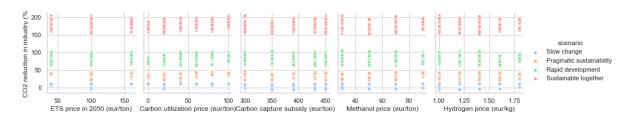


Figure D.14: Percentage of  $CO_2$  reduction in 2050 in the industry versus model inputs, low flexibility grid.

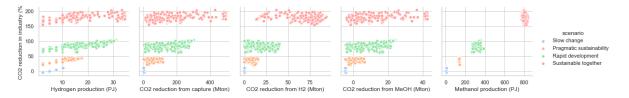


Figure D.15: Percentage of CO<sub>2</sub> reduction in 2050 in the industry versus intermediate variables, low flexibility grid.

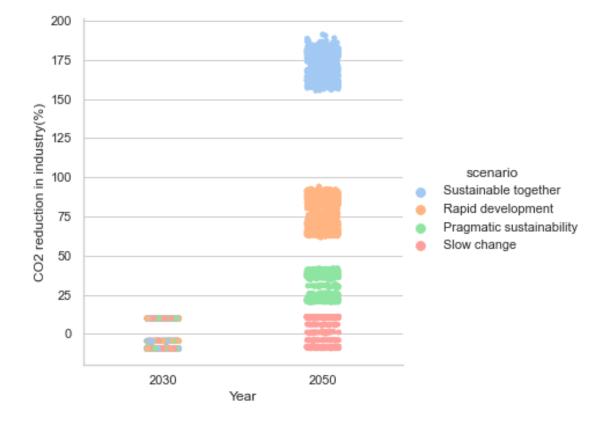


Figure D.16: Percentage of CO<sub>2</sub> reduction in 2030 and 2050 in the industry, when no methanol is produced before 2050, per scenario, low flexibility grid.

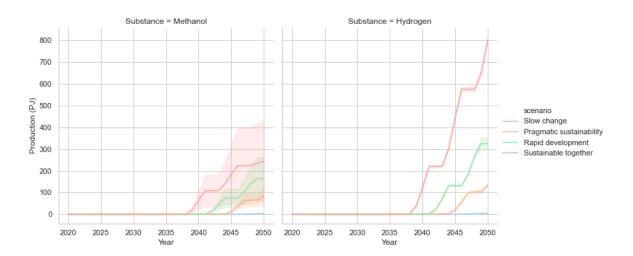


Figure D.17: Methanol and hydrogen production from 2020 to 2050 per scenario, low flexibility grid.