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Techno-economic analysis of hydrogen fuelling supply chains: System integration of mobility sector and power grid including renewable energy generation

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Techno-economic analysis of hydrogen fuelling system supply chains: System integration of mobility sector and power grid including renewable energy generation

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Commissioner for Energy Kadri Simson said: “With 75% of the EU's greenhouse gas emissions coming from energy, we need a paradigm shift to reach our 2030 and 2050 targets. The EU's energy system has to become better integrated, more flexible, and able to accommodate the cleanest and most cost-effective solutions. Hydrogen will play a key role in this, as falling renewable energy prices and continuous innovation make it a viable solution for a climate-neutral economy.”

Executive summary

Ambitious decarbonization targets are introduced to combat climate change. According to the European Commission, sector coupling is required to achieve these targets. This includes the inclusion of renewables into sectors that are difficult to decarbonize, but also using resources more efficient, and introducing new clean fuels. Recent research has examined the increased integration of renewables into the energy system, or the coupling with other sectors, such as the heating industry. However, a paucity of studies investigated the integration of the transportation sector with the power sector based on different configurations of hydrogen supply chains, with hydrogen as a nodal connector. Some studies looked into the decarbonization of the transportation sector but diminished to explore how the coupling based on hydrogen supply chains including hydrogen storage could support the grid by providing balancing services. Therefore, the aim of this study was to examine potential designs for renewable hydrogen supply chains to provide joint applications, which are satisfying a hydrogen mobility demand, as well as providing balancing services to the power grid. However, the interconnection of the hydrogen system within the mobility sector, as well as the functioning power grid, based on the supply chain, poses multiple challenges on different levels. This complex problem requires solving in an integrated manner. In that regard, this thesis proposes a modelling approach for the optimal functioning of hydrogen generation and storage supply chains. Hereby the objective of the function is to maximize the profit of the supply chains through the supply of hydrogen fuel to the mobility sector and the contribution of balancing services to the power grid. The proposed optimization model is employed to perform a techno-economic comparison of two supply chain configurations: a distributed on-site supply chain, in which the hydrogen is generated at the fuelling stations, and a centralized off-site supply chain, where the hydrogen is centrally produced and afterwards transported to the dispersed fuelling stations. Both scenarios are quantitatively studied under two operating conditions, which are only selling to the mobility demand, and providing ancillary services to the power grid concurrently. It was found that both distributed and centralized hydrogen generation and storage supply chains can be used to offer hydrogen fuel to the transportation sector as well as provide different ancillary services to the grid. Furthermore, the numerical findings show that when both supply chains are planned and run concurrently for various ancillary services, the highest improvement in terms of financial parameters can be observed. The results also indicate that the profitability of the distributed and centralized supply chain is comparable under various operating conditions. However, while the distributed supply chain system presents better economic performances than the centralized supply chain system under the performed conditions, the centralized hydrogen supply chain has greater

technological benefits than the distributed supply chain in terms of flexibility. Whereas the decentralized supply chain is more beneficial for smaller demands and a more isolated operation, the centralized supply chain can provide higher values to investors who must deal with larger demands and more interconnected systems. Because the majority of these systems will be operated by larger system operators, and the supply chain, including fuelling stations, will be increasingly connected to the energy sectors rather than operating independently, the centralized alternative is likely to be the most beneficial investment. The analyses reported in this study are useful to interconnected investors or system operators for assessing the technical and economic viability of the widespread deployment of distributed and centralized hydrogen generation and storage supply chains integrated with the power grid. Future research might investigate other system configurations, such as including the hydrogen backbone into the operation or integrating the hydrogen supply chain with diverse industries, such as the heating sector. Different renewable energy sources, such as biomass or hydropower, might also be included. Other research might involve dynamic hydrogen pricing or the engagement of various distribution modalities with global demand points. Finally, for the supply chain systems to be successful, the social aspect must be considered, in which numerous market regulatory and governance impediments must be identified and exploited.

Keywords – Sector integration; Mobility sector, Power grid, Hydrogen generation and storage supply chains; Ancillary services; Multi-objective optimization; Scheduling scheme; Renewable energy sources

Preface

This is the beginning of the thesis 'Techno-economic analysis of hydrogen fuelling supply chains: System integration of mobility sector and power grid including renewable energy generation'. The thesis has been written to fulfil the graduation requirements of the Master Complex System Engineering and Management and in corroboration with Accenture, The Netherlands. From the first of March till the beginning of September I was engaged in conducting and writing the thesis.

Looking back on my academic experience, I can say that I always enjoyed it, even though it was challenging at times. It allowed me to constantly challenge myself which provided me an opportunity to grow in a variety of ways. With this thesis, this desire to challenge myself and my long-standing interest in contributing solutions to energy crises resulted in choosing this research subject. Eventually, this has taught me valuable lessons both professionally and personally.

I would like to thank my supervisors, Dr. Ir. Zofia Lukszo and Dr. Martijn Warnier, from TU Delft, for their excellent guidance and support throughout the process. You provided me with challenges along the way which has increased my learning changes, for which I am thankful. I also want to specially thank Dr. Ir. Paola Ibarra Gonzalez for the excellent weekly supervision. You provided me with constructive, yet critical input, for which I am grateful.

Finally, I would like to thank Accenture and my colleagues for their support. I would also like to thank you, my reader, and wish you a pleasing reading experience.

Joost van Lonkhuyzen

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Abbreviations

VRE - Variable Renewable Energy

LNG - Liquefied Natural Gas

BEVs - Battery Electric Vehicles

FCEVs - Fuel Cell Electric Vehicles

VAR - Volt-Amperes Reactive

DR - Demand Response

OR – Operating Reserve

MILP - Mixed-Integer Linear Programming

MINLP - Mixed-Integer Nonlinear Programming

NLP - Non-Linear Programming

PSO - Particle Swarm Optimization

PV – Photovoltaic

PDF - Probability Distribution Function

MW – Megawatt

MVAr – Mega-volt-ampère reactive

MVA – Mega-volt-ampère

ERC - Equivalent Reactive Compensation

HSCND – Hydrogen Supply Chain Network Design

HFSP – Hydrogen Fuelling Station Planning

RTS - Reliability Test Systems

AC - Alternating Current

DC - Direct Current

PEM - Polymer Electrolyte Membrane

SOECs – Solid Oxide Electrolyzer Cells

AEMs - Anion Exchange Membranes

LOHC - Liquid Organic Hydrogen Carriers

LH_2 - Liquified Hydrogen

pu – Per unit

OC – Operating Capacity

EL – Electric Load

SoC – State-of-Charge

CAPEX - Capital Expenditures

OPEX - Operating Expenditures

GI – Gross Income

NI – Net Income

NPV – Net Present Value

BET – Break Even Time

IRR – Internal Rate of Return

TSOs - Transmission System Operators

SSOs - Storage System Operators

1. Introduction

In December 2019, The European Commission introduced an ambitious set of proposals to help communities share and implement measures to combat climate change (European Commission, 2021a). The initiative commits to ambitious decarbonization goals, including reducing the net greenhouse gas emissions by at least 55 percent by 2030, compared to 1990 levels, and achieving climate neutrality by 2050 (European Commission, 2021b). Each sector, such as industry, construction, energy, agriculture, domestic heating, and transportation, has its own set of science-based targets to achieve the decarbonization goals. For instance, the transportation sector must introduce new policies to increase efficiency, support electrification, and promote the use of low-carbon fuels and vehicles (ICCT, 2021), while the energy sector is also heavily promoting deep carbonization, it has to accelerate the uptake of renewables and cope with the consequences of the increased electrification, such as congestion (European Comission, 2021). However, the study of sectoral transformations considering the existing national determined contributions reveals that the transportation sector is lacking behind the global targets for 2030 and 2050 (REN21, 2020; WWF, 2018). This is because, despite energy efficiency improvements, notably in road transport, the number of cars on the world's roadways has increased, leading to a steady rise in energy demand for transport. Taking into account the fossil fuel dependency of the transportation sector, with only 3.7 percent by far the lowest share of renewable energy usage among end-use sectors, a lot has to be transformed to reach these goals (REN21, 2020). Electrifying the transportation sector is one of the potential solutions. This means using high shares of renewables from the power sector for applications where possible, such as road mobility. Another potential solution is promoting clean fuels, such as hydrogen, biofuels, or biogas (European Commission, 2021c). According to the European Commission, an integrated energy system is required to accomplish these goals. This means bridging the gap between the transport and energy sectors to support universal, efficient, safe, and green mobility. The World Bank stated that utilizing synergies between the transport and energy sector might increase energy efficiency and mitigate the climate impact (Piette, 2021). However, the existing sectors are still based on many parallel and vertical energy value chains with no cross-sectional connections. This means that both sectors have their own value chains, norms, infrastructures, planning, and operation that strictly bind certain energy resources to specific end-use industries, resulting in enormous energy waste (European Commission, 2021c). In these sectors, for example, the energy for the transportation sector provided by the processes is produced from fossil fuels, and even though the energy sector also runs based on fossil fuels, they are usually developed and operated separately. Besides this, the energy sector is ready to be decarbonized but the transportation sector requires a change in the fundamental process setup and transportation modes (Zachmann et al., 2021). In order to achieve cost-effective carbon neutrality by 2050, this has to be changed. This includes factoring the changing expenses of new solutions into the operation of the energy system, whereby new cross-sectoral connections and technology advances must be tested and exploited.

According to IRENA (2019), hydrogen could be the 'nodal' integrator in the energy transition from a technical perspective. This is because hydrogen enables significant volumes of renewable energy from the power grid to be directed into industries, such as the transportation sector, where electrification, and hence decarbonization, is rather challenging (IRENA, 2019). However, this energy sector integration solution is highly dependent on the widespread deployment and development of renewable energy sources, as well as the evolution of the electricity and transportation sector (IRENA, 2019).

In the following sections, a description is given to provide an overview of the situation in the electricity sector including the deployment of renewable generation, as well as the role of hydrogen. Subsequently, the transportation sector is highlighted, whereafter the possible integration of the sectors using hydrogen as a nodal integrator is described.

1.1. Electricity sector and the role of renewable energy and hydrogen

Over the past decades, an increasing amount of renewable energy is used to fulfil part of the demands of the electricity sector. Between 2000 and 2020, global renewable power generating capacity expanded 3.7-fold, from 754 GW to 2799 GW, as costs fell drastically because of continuously improving technology, economies of scale, competitive supply chains, and enhanced developer experience (IRENA, 2021). According to the European Commission, this has to be expanded to achieve net-zero emissions. The European Commission expects that the decarbonization plans are predicated on the widespread adoption of renewable energy technologies, such as wind and solar across all energy sectors (European Commission, 2021b). In 2021, the installed offshore wind capacity in the Netherlands was around 2.5 GW, but according to the coalition and climate agreement it is set to increase to 11 GW in 2030 (Rijksoverheid, n.d., a). Similarly, the installed capacity of solar energy in the Netherlands was set to increase from 3.5 TWh in 2020 to at least 35 TWh in 2030 (Rijksoverheid, n.d., b). From these, the offshore wind capacity is expected to account for approximately 40 percent of the total electricity consumption. As wind and solar energy produce respectively around 11 and 46 g CO_2/kWh of electricity generated, compared to 980 g CO_2/kWh for coals and roughly 465 g CO_2/kWh for natural gas, it can drive down the carbon emissions

(U.S. Department of Energy, 2022). However, to achieve climate neutrality in 2050, the capacity has to be expanded even further.

To increase the capacity, several factors need to be considered, for instance, its inherent intermittency, fluctuation, and difficulty in forecasting on the existing power system (Notton, 2018). More specifically, wind electricity generation is obviously dependent on the weather and, more precisely, wind speeds. Similarly, solar electricity generation depends on the total solar irradiance. This weather dependency poses new challenges in times of high or low wind and solar penetration in the electricity grid. Due to the intermittency of wind and solar power generation, the supply does not always match the electricity demand. The electrification of the energy sector, on the other hand, will significantly increase the overall demand on the electricity grid as well (NREL, 2018). Because both the supply of renewable energy, especially the capacity of wind energy in the Netherlands, and the electricity demand are expected to rise significantly in the future years, the temporal mismatch between power output and consumption is rising. The frequently occurring mismatch requires more flexibility solutions in the energy system, such as demand side flexibility, or storage options.

Hydrogen from renewables could address this challenge. For instance, hydrogen allows to channel significant amounts of renewable energy from the power industry to sectors that would otherwise be difficult to decarbonize through electrification, such as the transportation sector (IRENA, 2019). It has the ability to minimize carbon emissions from trucks, buses, planes, and ships. Additionally, the re-electrification pathway, in which stored hydrogen can be regenerated to electricity, offers a promising long-term solution when substantial proportions of variable renewable energy sources require seasonal storage to balance the seasonality of demand and generation. Alternatively stated, hydrogen might contribute to sector integration between the power system and industry, construction, and transportation, providing increased flexibility while aiding the integration of variable renewable energy (VRE) sources into the power system. This means that hydrogen can be the connector between the electricity sector and the industries, such as the transportation sector. For this, it is important to understand how the demand sectors are developing. Therefore, in the next section, the urge to transform and decarbonize the transportation sector will be highlighted, as well as the future ambitions in this sector. Furthermore, a description on how the energy system may become more efficient and potentially coupled with the electricity sector by using hydrogen as a connector is presented.

1.2. Transportation sector: road mobility

The transportation sector is one of the largest contributors of emissions in Europe. Today, the transportation sector accounts for around 24 percent of the total European Union's greenhouse gases (McKinsey, 2020). In 2020, the transportation sector emitted nearly seven gigatons of carbon emissions. Moreover, the rapidly expanding transportation demand, driven by the economic growth of the world, is likely to result in a considerable increase in transportation emissions in the future decades (The World Bank, 2021).

Within this sector, road mobility is significantly the largest section, contributing to approximately three-quarters of all CO_2 emissions (IEA, 2019; A European strategy for low-emission mobility EU), as depicted in Figure 1. With the global shift towards a low-carbon and circular economy, the European Commission mobility strategy aims to facilitate the transition to a cleaner, greener, and smarter mobility, contributing to the reduction of the transportation sector's emissions of 90 percent by 2030 (European Comission, 2021).

Ambitious measures are crucial to reduce these emissions deeply, such as the alternative fuel infrastructure regulation from the European Commission. This regulation supports the acceleration of the deployment of alternative fuel infrastructure, including binding targets for electric vehicle charging points, the implementation of liquefied natural gas (LNG) networks, or the dispersing of refuelling points for hydrogen. The latter target includes achieving the network, which needs to be accomplished by 2030 and 2035 respectively, with every 150 km one hydrogen refuelling station along with the Trans-European Transport Network (TEN-T) core network, which concerns the establishment and expansion of a European wide network of railway lines, roads, inland waterways, maritime shipping routes, ports, airports and railroad terminal (European Comission, 2021), and in every urban node serving both light-duty vehicles, including passenger cars and heavy-duty vehicles (European Commission, 2021). Another crucial ambition to stay below the two-degree scenario of the Paris Agreement, which establishes a global framework for avoiding severe climate change by maintaining global warming below 2°C and supporting initiatives to limit it to 1.5°C (European Commission, 2021), is to deploy around 160 million low-emission vehicles in the mobility sector, according to IEA (2017). These 160 million low-emission vehicles mainly consist of electric and hydrogen vehicles. In this regard, hydrogen vehicles should be recognized as complementary to battery electric vehicles (BEVs), while they may compete in some market sectors, there is a distinct competitive advantage for either fuel cell electric vehicles (FCEVs) or BEVs in each area. According to IRENA (2019), whereas BEVs are most suitable to smaller and lighter vehicles traveling short distances, FCEVs benefit larger vehicles traveling longer distances, such as trucks or international buses, as well as high usage rate vehicles, such as taxis. Moreover, FCEVs enables combining the flexibility of hydrogen with the efficiency of BEVs, possibly making them the most cost-effective long-term choice.

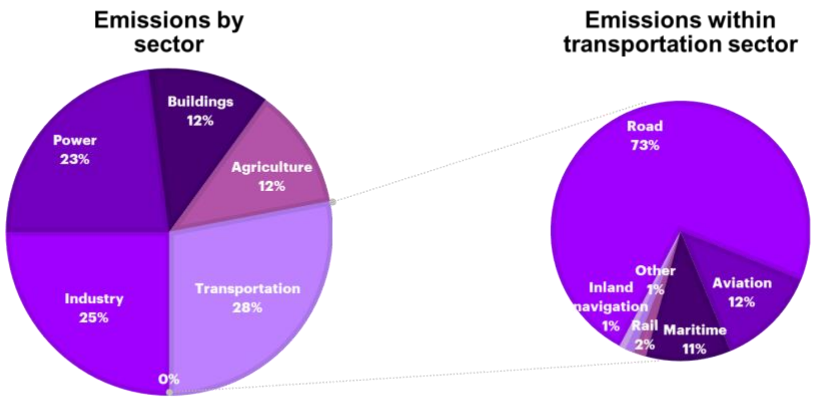

Figure 1. CO_2 emissions by sector and sources of emissions within the transportation sector (Adapted from European Commission (2021c)).

However, the ambitions to include hydrogen solutions in the transportation sector are already highly focused on interconnected value chains between sectors (European Commission, 2021c). It starts with renewable generation, conversion, and distribution to applications, which eventually may result in more flexibility. For this integration, multiple options are expected to be utilized. In the next section, it is described how hydrogen might be a solution, where it can serve as a ‘nodal’ integrator between the energy and transportation sector.

1.3. Mobility and electricity sector integration using renewable hydrogen as ‘nodal’ integrator

According to the European Commission, Europe needs to transform its energy system towards a more efficient and interconnected energy sector. This includes transforming the system of today, which consist of linear and wasteful flows of energy, in one direction only, to an integrated energy system including energy flows between users and producers, reducing wasted resources and money, as depicted in figure 2.

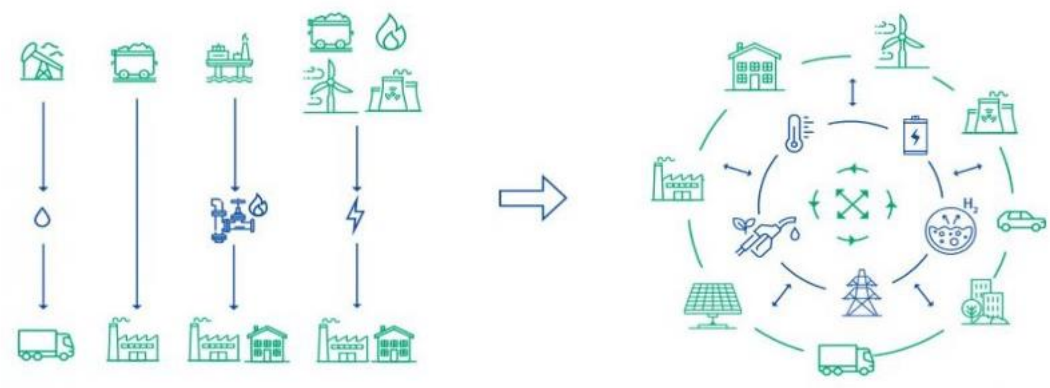

Figure 2. The energy system of today vs the expected energy system of the future (European Commission, 2021).

This transition is dependent on three main pillars: a more ‘circular’ energy system, increased direct electrification, and clean fuels. The more ‘circular’ energy system entails a strategy in which the sectors increase its energy efficiency by using waste energy for other purposes, such as heating of residential areas. Direct electrification means using the high share of renewables from the power sector for applications where possible, such as electric vehicles in transport. The clean fuels section consists of promoting renewable hydrogen, sustainable biofuels, and biogas (European Commission, 2021c).

Within the clean fuel pillar, renewable hydrogen is one of the predicted approaches to achieve sector integration. Renewable hydrogen can be made through water electrolysis, where water is decomposed into oxygen and hydrogen gas by using renewable electricity. After this, it has the potential to be employed as a feedstock, a fuel, an energy carrier, or a storage option in the industry, transportation, power, and construction sectors. It has the important feature of producing no or minimal emissions and pollutants (IEA, 2019). As a result, it provides a way to decarbonize industrial processes and economic sectors that are difficult to electrify by providing storage to balance fluctuating renewable energy flows. This, however, can only be accomplished by concerted public-private action at European level (European Commission, 2021c).

For this, the European Commission introduced targets where renewable hydrogen must be produced from wind and solar energy, or a minimal amount from other resources such as biomass (IEA, 2019). Since there is not enough renewable power capacity available in the near future, it is expected that low-carbon hydrogen is required to cut emissions quickly and enable the transformation into a sustainable market. Hence, the energy market has to undergo major development.

In 2020, hydrogen was only used as raw material for industry and refining of petroleum products. The global consumption in 2020 was around 90 Mt, with more than 70 Mt used as pure hydrogen and less than 20 Mt mixed with carbon-containing gases in methanol production and steel manufacturing. Almost all of this demand is produced from fossil fuels, whereas only around 0.03 percent is produced through water electrolysis, resulting in close to 900 Mt of carbon emissions per year (IEA, 2021). According to the European plans, more electrolyzers will be implemented and more hydrogen will be produced. Along this, the creation of a more developed and sustained hydrogen economy including technologies and applications is increasing. The European Commission has committed to assist the construction of at least 6 GW of renewable hydrogen electrolyzers and the generation of approximately one million tonnes of renewable hydrogen between 2020 and 2024. Between 2025 and 2030, hydrogen must become an integral element of the integrated energy system, including at least 40 GW of electrolyzers and 10 million tonnes of renewable hydrogen generated in the EU. Furthermore, renewable hydrogen technologies should be mature and widely adopted across all hard-to-decarbonize industries between 2030 and 2050 (European Commission, 2020).

This allows hydrogen, produced by renewable electricity, to play a critical role in advancing the development of an integrated energy system, where it can aid the integration of signification amounts of variable renewable energy generation, by offloading power grids during periods of abundant supply and enabling long-term storage. It might also enable local renewable electricity generation to be utilized in a variety of other end-use applications. Renewable hydrogen can, for example, be used in vehicles, whereby it can also be connected to the transport and power sectors, but also buildings, where the refueling points are located. However, the use of hydrogen in this synergetic role, as well as in a cost-effective way, is highly dependent on the entire supply chain (Shabani, 2020). The supply chain comprises, in this sense, the generation of hydrogen, large-scale storage to account for seasonal intermittency of renewable generation, followed by transportation, and distribution from the production facilities to dispersing stations, to end-applications like the mobility sector.

But the interconnection of the hydrogen system within the mobility sector, as well as the functioning power grid, based on the supply chain, poses multiple challenges on different levels. This complex problem requires solving in an integrated manner. Therefore, the analysis of an integrated system including the entire hydrogen supply chain to enable synergies between the electricity sector, with renewable electricity generation, and the mobility sector should be conducted.

To address these concerns, in Chapter 2, a literature review on the recent studies related to hydrogen supply chain applications and current integration among sectors will be presented to identify the existing knowledge gaps, followed by the definition of research questions required to cover these knowledge gaps.

Chapter 3 provides the research approach and methodology implemented to answer the research questions. Then, the hydrogen supply chain system including a detailed description of its components is introduced in Chapter 4. In Chapter 5, the model conceptualization and the mathematical optimization are presented, followed by the model formulation including the experimental designs in Chapter 6. Chapter 7 presents the techno-economic evaluation and analysis of results. Finally, an overall discussion, conclusion, and recommendations for private investors and system operators are given in Chapter 8.

2. State-of-the-Art

In this chapter, a literature review on recent studies and methods on the applications of hydrogen supply chains and integration among sectors is described to identify the existing knowledge gaps. First, the literature on the integration of renewable energy for hydrogen production and the grid is given. Subsequently, studies about the integration of hydrogen for the mobility sector, followed by the integration of renewable energy, hydrogen, the mobility sector, and the grid are described. Lastly, the modelling approaches that have been implemented for the evaluation of hydrogen supply chains including different applications are summarized. From this overview of studies, methods, and modelling approaches, the main research question and sub-questions are defined.

2.1. Literature review

2.1.1. Integration of renewable energy-based systems and role of hydrogen

Several studies have demonstrated the technological and economic viability of renewable energy-based energy systems in various parts of the world, showing that renewable energy resources are sufficient to meet energy demand in the power, heat, and transportation sectors (Hansen, 2019). Most of the studies describe the use of renewable energy for the decarbonization of the power sector (Hansen, 2019). Blanco et al. (2018) and Aghahosseini et al. (2019) displayed that the decarbonization of the power sector costs fairly less effort than decarbonizing other sectors in Europe and America based on renewable electricity generation with energy storage technologies, such as hydrogen. The results highlight that a significant variety of optimal energy system structures are dependent on local climate conditions and renewable energy resource availability. Countries with a lot of solar irradiances are more dependent on solar energy, while coastlines or high attitudes are more in favour of wind energy. These studies were mainly performed for supply-side solutions, such as renewable energy sources integration.

However, the integration of renewable energy sources which are closer to end-users, along with the growing share of renewable energy, have indicated challenges in the energy sectors (Fonseca, 2019). For instance, the emergence of distributed energy systems and the increasing amount of renewable energy requires a transformation on how the power systems are planned, designed, and operated (Adil, 2016). Sdanghi (2019) states that hydrogen can play a significant role in the electricity sector in the near future as a sustainable energy source. Fonseca (2019) showed the trends of distributed energy generation systems using hydrogen as an energy vector. It revealed that the deployment of hydrogen systems in the

energy sector could be valuable in maintaining a secure and stable operation of the distribution network (Fonseca, 2019). Most of these studies analysed the hydrogen impacts at the level of households, small villages, and neighbourhood level, according to power peak demand.
However, a more integrated approach is required including the hydrogen supply chain stages and other sectors to improve efficiency and safety (Fonseca, 2019).

2.1.2. Operation of hydrogen generation and storage systems including renewable energy generation

Furthermore, multiple studies have also investigated the operation of such systems. A methodology for the operation of a hybrid plant including wind generation, hydrogen production, and storage is given in Korpas (2006). In this work, hydrogen is aimed for both the supply of vehicles, as well as fuel cells. A joint operation of hydrogen storage with a wind farm unit in an electricity market was the goal, however, it has been demonstrated how the operating principles could also be applied to isolated hydrogen-based energy systems. Moreover, to manage the overall efficiency of the hydrogen supply chain, it showed that an electrolyzer is only used in cases with large electricity price variations and high balancing costs. Brunotto (2007) provided the optimal sizing of hydrogen storage, which is cooperatively operated with a wind farm to alleviate the challenges caused by the increasing intermittent wind power. The results showed that the cost of the components over the total system costs are crucial for the feasibility considering the net present value (NPV). Similarly, Melo (2014) developed a control method between an offshore wind facility and a hydrogen management system with the goal of reducing the effects of wind generation volatility. The results indicated that the control method increased the flexibility of the wind farm to satisfy grid operations. Trifkovic et al. (2014) proposed an energy management strategy for the integration and control of a hybrid power plant with renewable energy, as well as hydrogen storage units and fuel cells. The power balance between the renewable generation units, energy storage, and the volatile consumers was proposed by the system. The simulation showed an increased efficiency of the system from the control mechanisms. More studies presented these control mechanisms for renewable-based systems with hydrogen storage, but these were all tested on microgrids (Garcia, 2016; Li, 2018). The studies included techno-economic assessments, aiming to maximize the profit of the systems and minimize the degradation causes of the storage units while meeting the constraints of the system.

Hansen (2019) investigated the status and perspective of such 100% renewable energy systems. It mentioned that most of the studies performed have a predominant focus on the electricity sector or other easy-to-electrify sectors. Henceforward, sectors such as industry or transportation, which are non-electric

energy sectors and still operated on fossil fuels, need to be much more coordinated and integrated (Hansen, 2019).
Within the transportation sector, studies were performed using renewable energy to maximize hydrogen production and to evaluate the influential parameters to reduce production costs. Xiao et al. (2011) proposed an optimization algorithm for the hydrogen generation schedule to optimize the production cost of the station. It appeared that the cost of hydrogen was reduced significantly when applying the optimization approach. Garcia-Torres (2016) showed that utilizing lower prices from renewable electricity generation is beneficial for refuelling fuel cell electric vehicles based on a particular demand. Mendis (2015) addressed active power management of a hydrogen-based demand scheme, where the aim was to maximize the hydrogen generation from the intermittent wind energy source. It appeared that the objectives of maximizing the power generation were within the satisfactory limits, which entails lower production costs for the same hydrogen capacity. Hereby these studies showed the opportunities in the power market based on the volatility of electricity prices to produce hydrogen. The hydrogen production and cost were optimized to their full benefit by utilizing the intermittency of renewable energy for a certain hydrogen demand. The benefits were, however, dependent on the interactions within the network, such as the aggregators, local energy market, and energy profile.

The operation of such systems is examined in Chapman (2019), Dawood (2020), Korpas (2006), Bruneto (2007), and Melo (2014). Chapman (2019) investigated case studies with hydrogen as an energy carrier to decarbonize the transport sector, in which hydrogen is stored to channel intermittent renewable energy. It is observed that there is a significant potential for hydrogen adoption and net energetic benefit. Furthermore, using hydrogen for on-road transport in the United Kingdom showed to enable a reduction in rejected energy of nearly 10 percent. Chapman (2019) and Dawood (2020) presented the autonomous operation of hydrogen energy storage to utilize surplus renewable energy. Dawood (2020) mentioned that hydrogen is a promising solution for channelling VRE. It demonstrated the interconnection and interdependency of the four main hydrogen stages: production, storage, safety, and utilization. The pathways to other applications need further investigation and development.

2.1.3. Coupling of energy sector with the transportation sector based on hydrogen

Empasch et al. (2017), for example, conducted a techno-economic analysis for the use of a stationary hydrogen storage unit for an industrial plant. The system provides a design to deliver the necessary energy onsite for the industrial plant, while the authors are evaluating the system's economic benefits for such applications. More studies in the industry focused on the particular use of hydrogen as feedstock for steel, chemicals, and cement, and the potential for direct carbon removal. It appeared that a large-scale deployment of hydrogen for industrial use would entail positive impacts on the energy system. But this can only be assessed if the regional distribution of future hydrogen demand is considered. Its application is also highly dependent on the available technologies.

Hydrogen could also support applications in the mobility sector. For instance, Blasquez (2019) investigated the best design of hydrogen refuelling station in terms of the number of banks and their size, resulting in the most cost-efficient design. The study proposed that the state of charge of a vehicle of 100 percent is not efficient based on costs, since it requires very large high-pressure banks at the stations, which induces higher investment costs. Li (2020) provided a coordinating schedule of a hydrogen supply network considering vehicle demands. It appeared to be effective to coordinate the chain. El-Taweel (2019) showed how emerging technologies offer more economic and efficient mechanisms for hydrogen production. The results showed that the proliferation of hydrogen fuelling stations throughout the transportation network whereby the economic viability is justified is essential to the deployment of fuel cell electric vehicles (FCEVs). Moreover, Zhao (2021) highlighted the state-of-the-art of energy storage systems technologies for power integration support. The control and operation strategies appeared critical to the viability of the systems. So, the configurations and strategies of the system for the transportation sector, as proposed in Blasquez (2019), Li (2020), El-Taweel (2019), and Zhao (2021), where the optimal level of generation and storage units in a network to meet a particular demand is investigated, is required to enhance the efficiency.

2.1.4. Sector integration of transportation sector and energy sector including joint applications

Demand side and system reductions are also vital for transitioning to a fully renewable energy system in all sectors. The energy sectors should be closely coupled to effectively use synergy effects. Recent studies have shown that integrating energy and transport networks can result in energy transition synergies. Alavi et al. (2017), Farahani et al. (2019,) and Park Lee et al. (2015) mention that an integrated approach incorporates both the social and technical aspects of the energy sector, as well as different sectors, such as the transportation sector. An integrated approach is proposed for the Car as a Power Plant concept, to provide hydrogen as an additional solution to the electricity system. The results showed that electric vehicles in the electricity network are technically and economically feasible and can provide flexibility solutions. Furthermore, El-Taweel et al. (2020) investigated how an electrolyzer in a hydrogen fuelling station can be controlled as dispatchable consumer in the electricity market. The results displayed that the provision of ancillary grid services is a win-win situation for both the utility grid and the operator. On the one hand, ancillary services enable grid operators to maintain normal grid conditions, such as volt-amperes reactive (VAR) power control for maintaining voltage limits and balancing generation and demand (IESO, 2018). On the other hand, contributors to ancillary services are encouraged considering their market involvement, resulting in a higher rate of return (El-Taweel, 2019). Several studies have already examined the contribution of energy consumers to the ancillary services market. Valverde (2019) and Christakou (2018) presented a method by which distributed energy sources can provide VAR control to the grid as an ancillary service to improve the quality of the system. Another ancillary service is demand response (DR), which seeks to balance demand and generation in the grid. Leithon (2018) presented a demand response strategy for a nondeferrable load facility including renewable energy generation and storage capacity. The results showed that the costs were minimized over a finite planning horizon. Tumuluru (2018) proposed a methodology for solving the unit commitment problem in the power network taking into account the DR contribution by flexible loads. Kopsidas (2017) presented an optimal DR scheduling to increase transmission system reliability and economic viability. Khani (2020) provided an operation management scheme to schedule hydrogen storage to distribute Operating Reserve (OR) in electricity markets. It unveiled opportunities for these hydrogen storage systems to operate in the operating reserve market. Furtermore, Apostolou (2019) examined the future potential of jointly operated hydrogen fuelling systems with renewable energy sources in the electricity market. It showed that such a fuelling station induces a positive rate of return on investment when participating in the electricity market and mentioned that more fuelling stations could be implemented in the near future. Nasrolahpour (2018) examined the participation of storage systems in energy systems to provide OR services. The study showed that the OR as supplementary service is beneficial and also conclude that using abundant hydrogen storage capacity poses a significant opportunity to provide the OR, VAR control, and DR.

Previous studies have shown that storage systems can participate in the DR, VAR support, or OR market. However, these studies did not develop integrated models for the operation management of the hydrogen generation and storage systems while participating in the ancillary markets, as well as fulfilling a mobility demand. Furthermore, these studies did not include all ancillary services together, but only separately.

2.1.5. Usage of optimization for joint applications between the transportation and energy sector

For operators of hydrogen storage systems, optimization is used to fully implement ancillary services programs. There are two types of optimization algorithms that are used to solve DR optimization problems, which are classic optimization and metaheuristic optimization. While the classic optimization methods are mainly utilized for operation planning using analytical calculations, as it provides a method to find near-optimum solutions, metaheuristic optimization uses computational intelligence algorithms to solve complex problems (Ghaemi, 2022). In most situations, the ON-OFF status of numerous consumers or appliances at various timeslots, which constitute binary decision variables, must be determined. As a result, most DR optimization problems are solved using mixed-integer linear programming (MILP) or mixed-integer nonlinear programming (MINLP) (Jordehi, 2019). MILP presents a flexible and powerful method for solving large, complex problems where some of the decision variables are constrained to be integer values and the problem is linear. MINLP deals with nonlinear problems that have both continuous and integer variables (Sahinidis, 2019).

Parvania (2013) used MILP to optimize resource scheduling of a DR aggregator that participates in the day-ahead wholesale energy market. The goal of a DR aggregator is to employ shares of various DR resources, which means high volumes consumers that are able to curtail or shift load with on-site generation and energy storage (Auba, 2017) while maximizing the revenue. The revenue comprises the income in the wholesale energy market minus the payments to the DR program participants. The impact of the market price and different constraints were examined, which resulted in a positive payoff.

Aghaei (2013) used the Fuzzy method to find a compromised solution in a pareto-front for DR optimization and optimal power flow in microgrids with energy storage systems, including both economic and environmental objectives. The fuzzy method is concerned with approximation of both the sources of uncertainty at the input level and deals with the concept of partial truth to receive output quantities (Messien, 2019). The findings reveal that DR has a considerable impact on peak load reduction, pollution reduction, and operating cost reduction. This has also been used in Mazidi (2014) for unit commitment in microgrids with demand bidding programs while dealing with uncertainties of wind and solar resources.

Nan (2018) used a MILP approach for DR optimization and production scheduling in a community grid with renewable energy generation and energy storage systems. It indicates that EV load can be shifted to off-peak hours.

MINLP has been utilized in Alipour (2017) to optimize the DR in energy hubs and optimal day-ahead scheduling of resources in energy hubs, in which real-time pricing has been used. The outcomes showed that implementation of electric load DR decreases the total cost of the energy hub concerning optimal scheduling without DR.

In the study performed by Nwulu (2017), non-linear programming (NLP) was used where load reduction and paid incentives for each time interval were included in the DR optimization. NLP includes optimization problems where some of the constraints or the objective function are nonlinear. Hereby, the program showed the cost of not supplying 1 kWh of consumption. The results are gathered for PV, wind, and diesel generators. Shafie-Khah (2018) showed how NLP can be used to find the ON-OFF status of a smart home to respond to the market.

Metaheuristic optimization are stochastic search algorithms that utilizes rules or heuristics to accelerate their convergence to a near-optimal solution, with a limited computational burden that can easily handle constrained and discrete optimization problems with a large number of decision variables (Jordehi, 2015; Nesmachnow, 2014). This is seen as suitable for solving DR optimization problems. Particle Swarm Optimization (PSO) or optimization in which the global best is improved iteration by iteration to retrieve the best outcome. This is widely used for solving the DR problems, such as (El-Taweel, 2019). Pedrasa (2009) used PSO for scheduling interruptible loads for a 16-h time horizon to satisfy a scheme of required hourly requirements. Penalty functions have been added to the objective function as constraints. The schedule displayed a required curtailment which was closely followed. In Sepulveda et al. (2010) binary PSO has been used for load control of households, and Wang (2013) has used it for finding the optimal ON-OFF status of the equipment of the manufacturing machines. Combined interior point programming with newton trust, where an algorithm minimizes a nonlinear function subject to nonlinear inequality constraints, has been used for the configuration of tap changers and ON-OFF status of components to deal with voltage unbalances, and DR costs and network losses minimization in Rahman (2018). However, the uncertainties of PV generation and EV have not been considered.

The operators of the storage systems may also mitigate or handle the challenges in implementing a reactive power market. The challenges are system contingencies and load uncertainty due to price volatility and another challenge is unwanted market power in reactive power market. This results in uncertainties in forecasting the load demand. Therefore, load forecasting techniques are utilized to estimate the demand in the system. The general methodology adopted to handle uncertainty in the system is to consider probability distribution function (PDF), including simulation methods to generate different scenarios. PDF relates to the probability that a random variable has a specific, discrete value or falls within a specific range of continuous values (Mathworks, n.d.).

Villa (2012) proposed a Monte Carlo based probabilistic method, where a risk analysis is carried out by replacing a range of values for any factor containing inherent uncertainty, to analyse wind power generation for determining voltage control areas and critical buses in the system. The analysis showed that can help manage uncertainty issues with wind power generation locally, and thus reactive market in other local market areas is less affected by uncertainty in a particular area.

The availability of each reactive power source is determined by the operating conditions of the system. A payment function has been used in Ahmadi (2013) to value the availability of each source while considering the stochastic nature of load and network topologies. As a result, the likelihood of each contingency condition in the system is taken into account when generating a value factor for the reactive power source's availability price bid. In Shargh et al. (2016) and Liang (2015), the correlation between wind speed and load was considered while formulating a probabilistic multi-objective optimal power flow. Instead of the Monte Carlo approach, Mohseni-Bonab et al. (2016) employed the two-point estimation approach, where a 2n calculations of transfer capability to quantify is used, to predict load uncertainty for optimal reactive power dispatch.

A stochastic multi-objective optimal reactive power dispatch problem, in which multiple objectives with a fixed weights were assigned to each objective, was defined in Mohseni-Bonab (2016) to minimize real power loss and voltage stability concerns. The uncertainties in wind power generation are considered in this study. In Biswas et al. (2019), a scenario-based strategy was used to solve stochastic optimal reactive power dispatch issue that took into account uncertainty in solar irradiance, wind speed, and load demand. Other methods that were considered are implementing Information Gap Decision Theory based optimal power flow, in which alternatives were prioritized and choices and decisions made under deep uncertainty, as in Soroudi (2012) and Rabiee (2014) and change constrained alternative current optimal power flow as in Roald (2017).

The cost of reactive power generation is difficult to segregate it out from the active power generation. Furthermore, the price of reactive power support is determined by network parameters, such as active power loading, reactive power loading, contingencies, bus voltage magnitudes. The reactive power price also includes transmission loss, voltage stability, and generator limits. In Choi (1998), a real-time reactive power pricing scheme was considered to maximize the benefit of customers and minimising the real power production cost. It was discovered that reactive power marginal prices are very volatile when reactive power production cost, active power production cost and capacitor capital cost were incorporated in the alternative current optimal power flow while considering load as a constant.

Furthermore, an increased reactive power consumption may result in operating at the point of voltage collapse, hence separate consumption charges for megawatt (MW), mega-volt-ampère reactive (MVAr)

dispatch and MW, MVAr reserve are recommended in Chattopadhyay (2001) to preserve voltage stability margin. The contingency condition was calculated based on mega-volt-ampère (MVA) distance rule.
Equivalent Reactive Compensation (ERC) method can determine a value to a dynamic reactive power source by considering the reactive power requirement in the system alone and not considering the reactive support requirement for real power transport and security. A bi-level optimization problem, where the optimization problem is embedded in another, was used to determine the nodal price for reactive power, with the upper-level issue minimizing active power generation costs and the lower-level problem minimizing transmission losses, as proposed in Dona (2001). An expected payment function, such as in Zhong (2002), can be used to consider the availability of the generating unit, lost opportunity cost, and reactive power loss in the generating unit.
The uniform price auction-based optimal power flow, in which a dynamic pricing model ensures the prices paid based on market demand, was considered in Ahmadi (2013) to calculate the opportunity and availability cost of reactive power cost. The Lagrangian multipliers provide the marginal cost and minimization of power loss in the system was considered for market clearing in Ahmadimanesh (2017). Dynamic pricing was used in Roozbehani (2010). In Kotsan (2005) real and reactive pricing was investigated as a bundled service for cost allocation. The total cost function was solved by modified predictor corrector interior point method in Rider (2004). In Castillo (2020), a method was proposed to determine the participation of reactive power sources such as generators, bus shunts and line shunts on reactive power consumed by loads.

Ghaljehei (2019) advocated simultaneous clearing of energy and reactive power markets with a configurable loading margin and reactive power reserve. The study introduced a stochastic multi-objective framework that used the point estimate method to tackle uncertainty in wind power generation.
Local market areas may be established to account for the localized nature of reactive power markets. This can be accomplished via network partitioning techniques, which divide a large system into smaller subsystems. Contingency analysis, where the power system is modelled to evaluate the effects and calculate overloads, resulting from outages, using the voltage security index was used in Parida (2006) to modify the generated voltage control areas using the electrical distance approach. Song et al. (2006), Kargarian (2011) and Morison (2008) clustered the voltage control areas based on electrical distance, where the internal and external connections between nodes can be identified. Sarsangi (2011) identified the voltage control area using a K-means clustering technique, which is an approach for clustering. Villa (2012) proposed a Monte Carlo simulation-based framework for the identification of the voltage control

area. Satsangi (2011) uses a graph theory, to model pairwise relations between objects. Lastly, Schlueter (2000) used a bifurcation system-based framework, to see changes that causes a change in behaviour. However, the coupling between active and reactive power that are based on such subsystems are not considered in these markets.

In Liao et al. (2011), an energy sensitivity matrix-based strategy for identifying voltage control zones to designate reactive power markets areas was developed. This uses a priority list for deploying resources to correct the voltage using a minimum number of resources. Bahmanifirouzi et al. (2012) partitioned the network into reactive power market areas based on heuristic algorithms, in which problems are solved using shortcuts in each limited time frame to produce almost perfect solutions. Shuffled frog jumping algorithm, which is used for solving combinatorial optimization problems, and PSO for identifying voltage control were also compared in this study. In Islam (2014), a technique based on electrical distance and bus admittance matrix analysis, in which the load data or a power flow study in the buses, was presented for real-time zonal detection of reactive power areas through voltage control areas. In Su (2015), a voltage stability study based on a coupled two-port network analysis was provided utilizing data from the Phasor Measurement Unit (PMU). A PMU is a device utilized in the electricity grid to estimate the magnitude and phase angle of an electrical phasor quantity, such as voltage or current, using a common time source for synchronization. To split the system into voltage stability critical areas, the voltage coupling relative gain approach was applied in Jiang et al. (2016). Jiang et al. (2016) looked at the Volt/Var interaction based on relative gain. These have been shown to be effective in detecting power areas. The dynamic relative gain approach was also utilized to segment the system into voltage sensitive zones in Bai et al. (2016). Cuffe (2015) suggested a 2-D depiction of an electrical network suited for voltage stability investigation.

Moreover, a critical step towards the expansion of hydrogen-based applications is the implementation of the hydrogen infrastructure, namely generation, storage, and distribution (Shabani, 2020). As mentioned before, the integration of sectors is highly dependent on the entire hydrogen supply chain. Two types of supply chain study models are existent, which are hydrogen supply chain network design (HSCND), and hydrogen fuelling station planning (HFSP). The HSCND optimization models are classified as geographically explicit optimization models. Binary and integer decision variables are used to handle facility location, size considerations, selection of appropriate production technologies, and transportation options between facilities. Because continuous constraints are used to describe product flows across the supply chain, these models are typically mixed-integer formulations. For example, De-Leon Almaraz et al. (2015) introduced a multi-objective optimization to deploy a hydrogen supply chain considering the geographic level of implementation. Moreno-Benito (2017) showed a multi-period optimization for hydrogen supply chain infrastructures with the optimization of production technologies, scales, transportation modes, and carbon storage system across time and space. Kim (2008) displayed optimization of hydrogen supply chains under demand uncertainty. Furthermore, Hwangbo (2017) integrated the supply chains with other supply chains, whereby the cost and demand were optimized based on different scenarios.

HFSP concentrate on the location-allocation problem of fuelling stations. There are two primary categories of optimization-based methodologies for arranging fuelling stations, based on the geometric representation of needs, which are models for node-based and flow-based demands (Hosseini, 2015). Under node-based demand models, which view each node as a demand point, a driver would have to go to the facilities to acquire services. The fundamental benefit of utilizing these models is that data, such as demographic and geographical information is very accessible (Hwang et al., 2015). However, modelling demand as network flows, in which the demand is served “on the way”, may be more realistic. For example, Lim (2010) considered limited driving range of vehicles, Hosseini (2017) introduced fuelling capacities, and Wang (2013) took into account the least number of fuelling stations.
As can be observed, a minority of studies include both models and no models include the supply chain with the joint applications of the hydrogen fuelling stations (Eslamdarpour et al., 2015).

As the supply chains can have many configurations, Xiao (2011) and Kurtz (2018) mentioned that centralized on-site deployment of hydrogen supply chains would result in lower capital costs than distributed on-site supply chains. But the distributed on-site production would remove transportation and distribution costs to the station, as well as an opportunity to increase the reliability of the hydrogen availability. Xiao (2011) and Kurtz (2018) also examined the pipelines as transportation method, while El-Taweel (2020) examined the use of the transport of liquefied hydrogen. However, the transportation and distribution methods can be investigated more extensively in this combination. Khani (2020) mention that hydrogen stations are most likely to be distributed as a chain across a broad area and most probably to be owned and operated by a private operator to serve the transportation sector.

Furthermore, these studies have not taken into account the contribution of hydrogen storage stations to the ancillary service market to enhance their profits. The previously methods in the literature do not use the distributed capacity of hydrogen stations as a resource, especially not the storage of hydrogen fuelling systems, supplying ancillary services to the market as an additional source of money for the station owners. As a result, the additional potential that storage can generate by participating in for example the

OR market is not added to the ordinary potential revenue from hydrogen sales to the transportation sector.

Because the operator of the hydrogen generation and storage systems needs to manage the entire supply chain, a supervisory scheduling is required. This scheduling requires information about the level of stored hydrogen in storage tanks, the fuel demand data for the mobility sector at various place around the station network, and signals from the electricity market, to successfully monitor and control the supply chains.
Additionally, in order to open the market for these innovative solutions for the hydrogen mobility sector and accelerate the hydrogen economy, the viability should be justified. Hence, new models should be included to optimally manage the operation of the hydrogen fuelling systems. As seen in literature, the economic viability of the hydrogen supply chains may be increased by using them to their full potential through additional application, such as providing ancillary services to the power grid. This interfacing between sectors and systems will be the aim of the thesis by investigating the profitability of providing joint services.

2.2. Knowledge gaps

In summary, previous research has shown that distributed and centralized systems of hydrogen generation and storage are effective means of hydrogen supply. Some studies examined how renewable energy sources can be integrated into energy systems, as well as how renewable energy can be used for hydrogen production and storage. However, these studies did not develop integrated models for optimal managing the operation of distributed and centralized hydrogen production and storage systems including the specific features and operating characteristics of (i) renewable hydrogen production and hydrogen storage systems, (ii) integrated mobility and electricity power grids, (iii) the configuration of the hydrogen supply chain, and lastly, (iv) the concurrent operation for hydrogen supply chains to serve hydrogen demand and multiple ancillary services to power grids.
To fill the gap between the existing studies and to accelerate the diffusion of hydrogen systems via joint applications, a new approach will be proposed. The aim of this research is to perform a techno-economic analysis of hydrogen supply chains considering system integration of the mobility sector and power grid including renewable energy generation. This is done by proposing an optimization model for both distributed onsite and centralized offsite hydrogen energy systems with multiple compositions. The thesis will include the special features and operation characteristics electrolyzers and hydrogen storage systems, electricity power grids, fuel cell units, and the concurrent operation for the hydrogen systems to serve

hydrogen demand and increase the profit by providing ancillary services to the power grid. Also, different possible delivery options of hydrogen will be considered.

2.3. Research questions

Based on the literature review, existing gaps have been identified. Until now, the literature provides methods to optimize hydrogen systems to deal with the intermittency of renewable energy sources. Also, some studies show a methodology for hydrogen systems to serve a hydrogen demand. Moreover, several researchers state that the profit of hydrogen systems could be increased by providing ancillary services. However, there is a lack of studies that consider the interconnection of hydrogen systems with the power grid, as well as the mobility sector. Some researchers have investigated the interaction with the grid, but most of the studies do not consider the operation of the hydrogen supply chain. Hereby various components can be varied, such as the hydrogen storage systems (onsite/offsite), as well as the transportation methods, to both meet the hydrogen demand, as well as providing ancillary services to the grid to increase the revenue. Therefore, the main research question is formulated as follows:

What are potential designs of hydrogen fuelling supply chains powered by solar and wind energy that can effectively serve the mobility sector demand of a region, as well as providing balancing services to the power grid?

To be able to give answer to the main research question, several sub questions are formulated, as presented as follows:

Sub question 1: *What would a synergetic mobility sector connected with the power grid based on hydrogen and supported by renewable energy look like according to future ambitions of the EU?*

Sub question 2: *What are suitable scenarios and operating conditions to test the system integration of the mobility sector and power grid?*

Sub question 3: *What is the energy profile including generation and demand, and electricity and hydrogen prices?*

Sub question 4: *What are the technical and economic performances of the centralized and distributed supply chain systems under the various scenarios?*

Sub question 5: *What are the potential effects of variations on electricity and hydrogen prices ancillary services price, as well as the expected component cost reductions between now and 2040?*

The findings of this study can enhance academic understanding of energy systems design and the consequences of the increased interfacing between the transportation sector and the power grid, especially in light of providing multiple services as a hydrogen system. In addition, a modelling method can also be useful in assisting decision makers on the design of future energy systems, such as system operator or private investors, by providing a systematic and comprehensive assessment of the benefits obtained by the joint operation of a hydrogen fuelling system.

3. Methodology

In this Chapter, the methodology for conducting this research is elaborated. For this, a modelling approach is selected. A modelling approach's purpose is to answer specific questions, rather than give generic descriptions of systems (Nikolic, 2019). Therefore, before the construction of the model, the modelling problem statement should be defined. In this work, first, the fundamental motivation of the thesis is to design a system and to assess which configuration is more feasible. Based on the outcomes, investment recommendations for decision makers may be given. The main focus is on integrating the mobility sector with the electricity grid, which uses hydrogen as a nodal connector, and powered by renewable energy generation. On the one hand, the hydrogen fuelling system supply chains need to deliver energy to the mobility sector to meet the need and aspirations of the people. On the other hand, the electricity system needs stabilization, and this requires an optimal design. Therefore, this thesis aims to compare different scenarios and evaluate the performances of a jointly operated hydrogen supply chain to reliably and effectively meet the demand of the road mobility and increase the revenue by participating on the electricity market, as well as managing renewable energy flows. As a result, investment recommendations for system operators or private investors may be given.

However, determining the optimal design for the hydrogen fuelling system supply chain is a complex task due to various reasons. First, the operation and interconnection of the hydrogen systems with different sectors result in large scale operation with components on various levels, such as multiple small compliances to the integration of renewable energy plants (Seifi, 2011). Additionally, energy infrastructures are extremely capital demanding, requiring hundreds of millions of euros investments costs (Melese, 2014). Long lifetimes must also be acknowledged, which lead to decision making in the face of uncertainty (Melese, 2014). Lastly, the socio-technical features of the energy system cause that the institutional and economic aspects must be considered next to the technical components (Farrokhifar, 2020). A model can contribute to this investment dilemmas by giving a quantitative tool for discovering the optimal investments in a systematic manner. To address these concerns, a methodological framework is proposed, as presented in Figure 3.

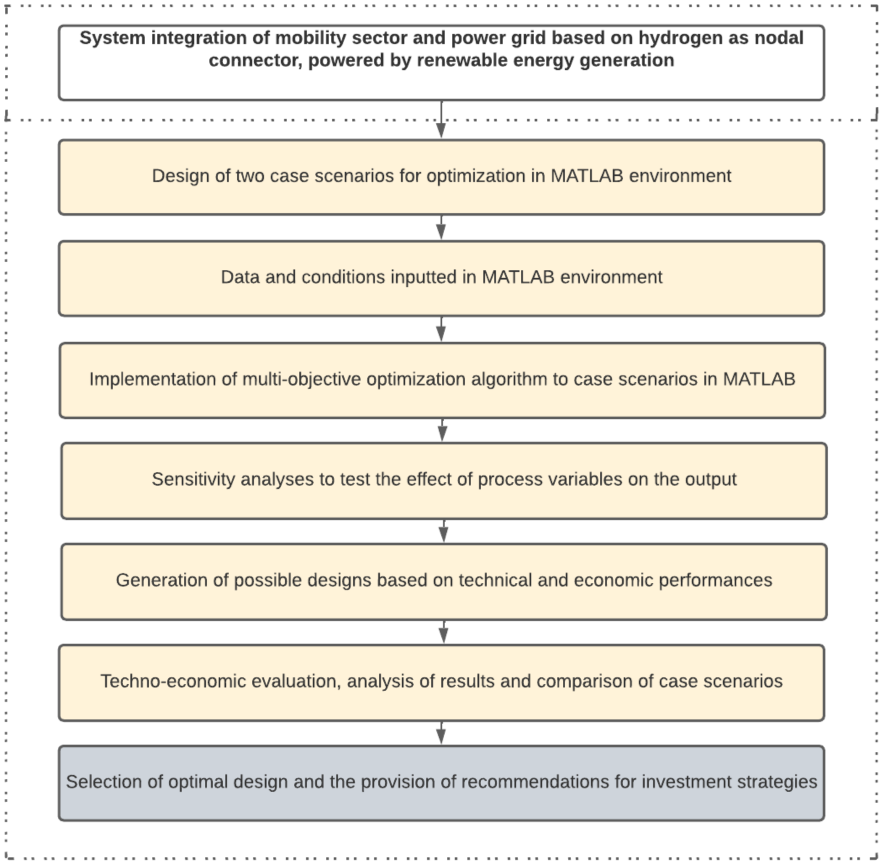

Figure 3. Methodological framework for multi-objective optimization methodology for system integration of mobility and energy sector based on hydrogen supply chains powered by renewable energy.

The methodology for multi-objective optimization for system integration of the mobility and energy sector based on hydrogen supply chains, powered by renewable energy, is focused on optimization. First, two case scenarios have been selected after performing a deep literature review. The first scenario is based on hydrogen supply chains where the hydrogen is produced at local distributed fuelling stations including the generation of hydrogen, its compression, storage, and dispensing, this is further referred as a *distributed on-site hydrogen supply chain*. The second scenario is based on hydrogen supply chains where the hydrogen is produced centrally including hydrogen generation units, compression, and storage, whereafter the hydrogen is distributed to the fuelling station, referred as *centralized off-site hydrogen supply chain*. At the fuelling stations, the hydrogen can be distributed to the hydrogen demand, or it can be used for the stabilization of the electricity network. Following the selection of the scenarios, the data and optimization criteria, including the parameters and decision variables, are selected. This includes the components including the type of technologies, and operating criteria.

Following that, a modelling approach has been selected to enable testing the two scenarios. Because of the multi-objective nature with several objectives for the determination of the optimal design, a multi-objective optimization method is implemented. For its implementation, first, the effectiveness of the proposed scenarios will be simulated through the IEEE Reliability Test Systems (RTS) with Simulink in the MATLAB environment. The IEEE RTS are used to test how the technologies and operational methods are affecting the power system cost and performances. This enables to simulate a wide range of present and future scenarios that the power and mobility sector may encounter (Barrows, 2019). The process simulations provide the operating parameters for both scenarios. Moreover, these simulated scenario models are the starting point for the multi-objective optimization for the determination of the optimal design based on the configuration of the hydrogen supply chain.

The following step is the implementation of the optimization algorithms, as well as a scheduling mechanism, in the MATLAB environment to numerically evaluate the proposed model. The power mismatch makes the proposed optimization problem nonlinear. To solve this, a Newton Trust Region method based on Interior Point techniques will be utilized. This iterative approach will calculate the mismatch in each iteration, whereafter a solution is found when the mismatch is below a certain convergence tolerance. This nonlinear optimization problem will be solved with the optimization toolbox (mathworks.com). The algorithm is performed to search the feasible regions based on the specifications of design parameters and their corresponding search ranges, which allows finding the optimal operating design based on technical and economic evaluation parameters. A sensitivity analysis will be implemented to see the effect of future development of the electricity prices on the outcome. The designs are evaluated and the one which best fits the objective function will be selected. Historical operating data of the hydrogen demand for fuelling stations of fuel cell vehicles and the electricity market data will be used for simulation.

The transport sector and the electricity sector are both included in the model, however, the method can also be used to analyse other energy systems that use hydrogen as a fuel, for example, residential heating. The simulations will produce an energy balance, allowing the cost and performances of several new energy system topologies to be compared.

Following this approach, the present thesis will propose a scheduling strategy for managing the operation of both distributed and centralized hydrogen production and storage systems integrated with the energy grid. The thesis will provide a comparison of two system configurations by assuming that there is a single investor who will own and operate the facilities, and distributed systems are aggregated to provide the same grid services as the centralized form.

Eventually, the model allows for customized research on either the system configurations of the hydrogen generation and storage system which could be used as:

i. a benchmark for assessing the economic viability of both configuration forms to assist private investors in decision making regarding which configuration is more profitable and to enhance the understanding of the benefits of coupling sectors.
ii. A deployment and scheduling of the hydrogen facilities to utilize the full system benefit. This means to effectively use the system for the mobility sector, as well as enhancing the economics of seasonal storage and flexibility to the electricity sector, to maximize the profitability of the system.
iii. A model for comparing technical and economic characteristics of different compositions. More specifically, an off-site centralized system will be compared to a distributed on-site refuelling system. Furthermore, different ways of transporting and distributing the hydrogen for the centralized system will be taken into account, as well as varying the technical side of the components of both systems.

The model will be operated to meet different interconnected services, such as serving a specific hydrogen demand for the mobility sector and the provision of ancillary services to the power grid in order to increase the revenue of the hydrogen system and the grid's flexibility. The model takes into account the physical restrictions of the power grid as well as the system components, such as the hydrogen production and storage units. Furthermore, the composition of the fuel cell units connected to the hydrogen production sites are considered, allowing the system to function as a full energy storage unit, maximizing the benefits of the grid services contributions. The available grid services will be selected based on the specified composition.
In the following chapter, the system description is described. This includes the assumptions considered for the design and modelling of the configurations.

4. System description

In this section, the details of the system, its boundaries and potential scenarios, and the operation framework are described. First, the general description of the system flow including a visualization of the system are given. Subsequently, the system supply chain including the system boundaries and component parameters are specified. Then, the applications of the supply chains are elaborated, as well as the description of markets it can participate in.

4.1. Overall system flow

The network considered in this thesis represents a scenario where hydrogen fuelling stations and its supply chain can fulfil joint applications between the mobility and energy sector. The network consists of solar PV arrays, wind generation units, an AC/DC converter, electrolyzer, compression and transportation, storage, load, power systems, and different load. As mentioned before, the system is operated by one owner, where the network aims to simulate a wide range of present and future scenarios that the power and mobility sector may encounter.

For the sector integration of the mobility sector and the electricity sector based on hydrogen supply chains, two energy carriers play a role, which are electricity and hydrogen. The energy carrier hydrogen is considered to be produced only from electricity from wind turbines and solar PV units. After the hydrogen generation, the hydrogen is compressed to enable storing of the energy carrier. From there, the hydrogen can be dispersed to the road mobility demand, which comprises FCEVs, like medium to large car fleets to large buses. The system must satisfy the mobility demand. Additionally, in times of off-peak demand of road mobility, the hydrogen can be converted back into electricity through a fuel cell, from which it can provide balancing services to the power grid. Overall, four main requirements of the system are considered, which are:

1. Electricity and hydrogen are used as energy carriers.
2. Hydrogen transportation and distribution by trucks or pipelines, in gaseous form and stored in tube trailers.
3. Hydrogen supply chain system division into the mobility sector and electricity network.
4. Hydrogen supply chain system including wind and solar power as energy source to fulfil electricity and mobility demand.

Following this, a representation of the overall system is depicted in Figure 4.

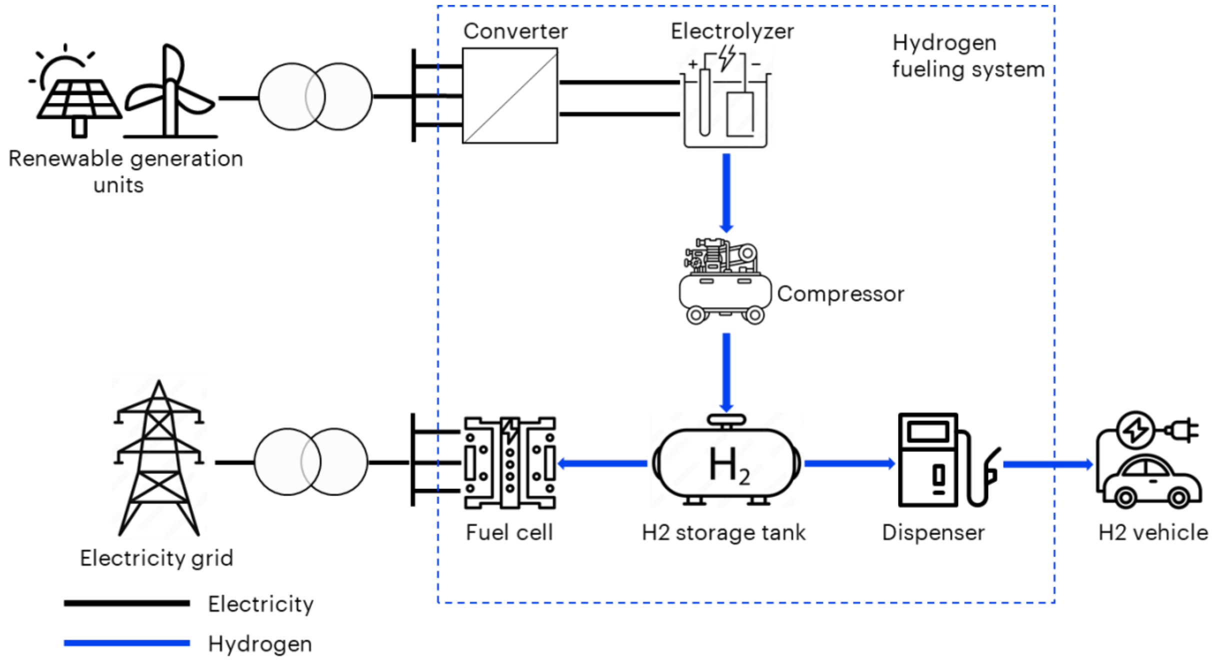

Figure 4. Renewable-based hydrogen supply chain with joint applications in the mobility sector and the electricity grid.

As depicted in Figure 4, the following essential components are present in the supply chain of hydrogen fuelling stations: hydrogen production and supply, hydrogen storage, and hydrogen refueller. The hydrogen refuelling systems can be deployed in two distinct ways:

1. Off-site hydrogen refuelling station consisting only of a dispensing station, and
2. On-site hydrogen refuelling station consisting of a hydrogen storage with reservoir or both a production and dispensing station (Khani, 2020).

As only a dispensing station, the hydrogen is produced centrally with stacked electrolyzers, whereafter the hydrogen is delivered to the site in gaseous form by tube trailers or through pipelines. The on-site hydrogen fuelling systems produce the hydrogen at site by the utilization of electrolysis of water. This supply chain includes the production of hydrogen from renewable sources, hydrogen compression, preservation, and distribution for utilization. While the centralized deployment would result in lower capital costs than distributed onsite, distributed onsite would remove transportation and distribution costs to the stations, which may greatly increase overall costs (Xiao, 2011).
Based on this, different configurations of renewable hydrogen refuelling systems will be considered in this thesis, as depicted in Figure 5 and 6. Figure 5 depicts the hydrogen refuelling system with onsite hydrogen production, whereas Figure 6 visualizes the hydrogen refuelling system with onsite electrolysis.

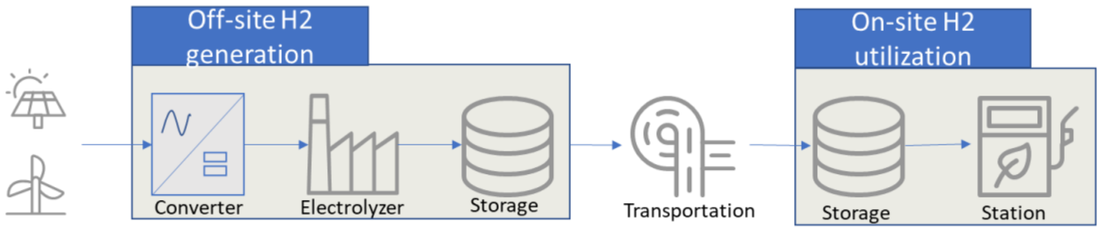

Figure 5. Schematic diagram of centralized off-site refuelling system. Hydrogen is produced through stacked electrolyzers using renewable electricity, thereafter it is transported from the central production center to the refuelling stations. The electrolyzer includes a compressor to enables storage of the hydrogen.

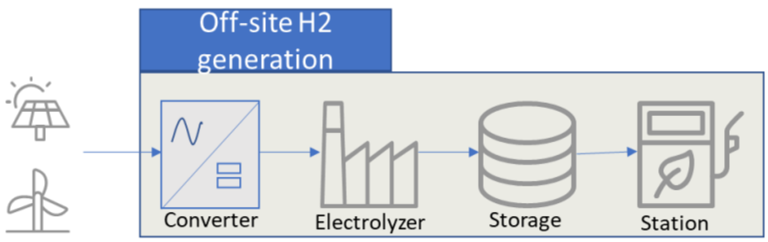

Figure 6. Schematic diagram of distributed on-site refuelling system. Hydrogen is produced through an electrolyzer using renewable electricity. The electrolyzer includes a compressor to enables storage of the hydrogen. The generation and storage system, as well as dispenser are all on-site on site with this configuration.

Overall, the hydrogen fuelling system processes hydrogen by electrolyzing water with direct current, supplied by power from renewable energy sources. First, the converter assists the electrolyzer in obtaining the AC into DC current instead of AC current and the appropriate voltages for the electrolysis reaction. Subsequently, the hydrogen produced is compressed into a high-pressure gas and stored in the storage tank by the compressor. The hydrogen in the storage tank can be further utilized to generate electricity via a fuel cell or directly feed the hydrogen vehicles. A more detailed description of the hydrogen supply chain and integration with the electricity and mobility sector will be presented in the following sections.

4.1. Description of supply chain

Each component in the network, described in the previous section, has its unique technological and economic characteristic. These characteristics, which are given in the next subsections, are crucial for the construction of the system, as well as for modelling its dynamics.

4.1.1. Energy sources

In order to cope with the ambitions of the European Commission, the system is assumed to include renewable energy generation to produce only renewable hydrogen. There are numerous renewable energy sources available in the energy mix, such as geothermal, hydropower, wind, photovoltaics, and

biomass. Nevertheless, the production of energy sources is dependent on multiple conditions, such as climate changes, location, and seasonal variations. According to European and national plans of the Netherlands, wind and solar energy sources are most likely to dominate the energy market in the Netherlands (European Commission, 2022a; Rijksoverheid, n.d., a; Rijksoverheid, n.d., b).
Therefore, in this thesis, wind and PV generation units are be considered to supply electricity to the system. The renewable generation units supply electricity to the system. Due to the flexible characteristics of the hydrogen generation and storage units for multiple applications, the system can be used to channel and proliferate variable renewable energy (VRE) sources. Since the primary function of the supply chain network is to meet the mobility demand, sufficient hydrogen must be produced. For this, wind turbines and solar PV units are required to supply the electricity to produce the required hydrogen.
The standard wind generation units produce alternating current (AC) as output, while electrolyzers require direct current (DC), resulting in the need for converters in the system. Solar PV units, however, produce DC. Hence, the solar generation units are considered to be connected directly to the electrolyzer.

The developers of the wind and solar generation units are required to pay for the connection between the electricity generation units and the power grid or with the electrolyzer. These costs and sizes depend on the capacity of the connection, which is lower when delivering directly to the electrolyzer, reducing the required connection capacity, as well as the investment cost. In this thesis, it is assumed that these costs are not modelled and only the renewable energy generation will be modelled based on fixed data.

For this, wind turbines with a nominal mechanical output power of 5000 W are considered. Furthermore, solar PV characteristics are retrieved from the NREL (NREL, 2021), where the solar panels are tested in four areas: grid integration, technology validation, solar resource assessment, and balance of system development. As a result, Suntech STP260-24/Vb solar panels are used since these are applicable for grid-connected systems. These PV arrays consist of Npar strings of modules connected in parallel, whereas each string consist of Nser modules connected in series. According to this, the component characteristics are summarized in Table 1. Moreover, historic electricity market price data of the Netherlands from 2018 will be used.

Table 1. Wind and solar PV characteristics.

Wind and solar PV characteristics	
Wind nominal power output	5000 W
Wind speed (m/s)	12

Electrical efficiency (%, LHV)	71
Number of solar cells per module	72
Number of series-connected modules per string	2
Number of parallel strings	50

Following this, the next section describes how the electricity from renewable energy sources can be transformed to hydrogen.

4.1.2. Power to hydrogen

As mentioned before, hydrogen can be produced from electricity by the electrolysis of water, which is a simple process that can be carried out with relatively high efficiency (Breeze, 2018). As depicted in Figure 7, during this process, water reacts at the anode to produce oxygen and protons. The electrons flow through an external circuit, while hydrogen ions selectively migrate across the membrane to the cathode. At the cathode, hydrogen ions mix with electrons from the external circuit to generate hydrogen gas (U.S. Department of Energy, n.d.). This process generates carbon-free hydrogen when using renewable energy sources such as wind and solar, or nuclear energy, but the process can also entail high emissions by using high carbon-intensive electricity sources. (IEA, 2021). As mentioned before, in this thesis, solar and wind energy will be considered as electricity sources.

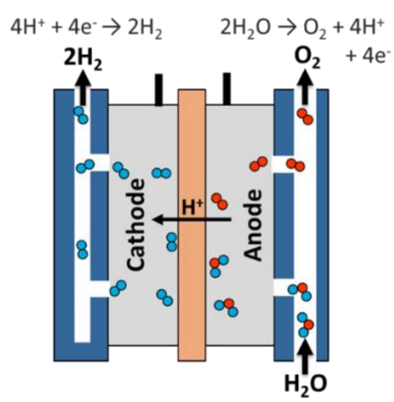

Figure 7. Electrolyzer process (U.S. Department of Energy, n.d.).

There are four electrolyzer designs available, which are alkaline and polymer electrolyte membrane (PEM) electrolyzers, solid oxide electrolyzer cells (SOECs), and anion exchange membranes (AEMs). Alkaline and PEM electrolyzers are already commercially available, whilst SOECs are at precommercial stage, and AEMs at the start of development. The most mature electrolysis technology are the alkaline electrolyzers, which have histrorically dominated the market. This is because of the widespread deployment of these electrolyzers in industrial operations, such as the chlor-alkali industry. However, in the last three years, PEM designs are more adopted than alkaline electrolyzers for the dedicated hydrogen production.

Nonetheless, as technology advances, it is unknown which design will dominate the market. While the alkaline technology is more mature and have lower cost, PEM electrolyzers are becoming more affordable, are less carbon intensive, and can supply hydrogen at high pressures, such as 30 to 60 bar, compared to 1 to 30 bar for alkaline technology. Furthermore, spill over technical learning gains from the development of PEM fuel cells might aid PEM electrolyzers. Therefore, in this thesis, PEM electrolyzers will be considered. The techno-economic characteristics of the PEM electrolyzer are summarized in Table 2.

Table 2. Techno-economic characteristics of the PEM electrolyzer (IEA, 2019).

PEM Electrolyzer characteristics	
Electrical efficiency (%, LHV)	71
Energy per kg (kWh/ kg H2)…P2H conversion factor (m^3/MWh)	55.5…360
Operating pressure (bar)	30-60
Stack lifetime (years...hours)	20...80000
Cold-start time (min)	<20
Gas purity (%)	99.99
CAPEX (incl. power supply and installation cost) (€/kW)	700
OPEX (% of the CAPEX/year)	2.7
Min power generation…Max power generation (m^3/h)	0…257

Furthermore, the water which is used as feed-in product should be of high purity. This to extend the lifetime of the electrolyzer (Oldenbroek et al., 2017). In this thesis it is assumed that the water is treated outside the system boundaries and received with required quality for the electrolyzer.

After the generation of the hydrogen, the hydrogen must be compressed, stored, and transported and distributed. This is elaborated in the next section.

4.1.3. Hydrogen compression, transportation, and storage

As depicted in Figure 4, after the generation of hydrogen, the hydrogen must be compressed, transported, and stored, before distribution into the applications. Various technologies are available for transporting and distributing the generated hydrogen (ENTSOG, 2021). These technologies enable transport of hydrogen, as well as storage. The straightest way is hydrogen in compressed form. This compression can be applied to pure hydrogen or hydrogen mixes with other gases. After the compression, the hydrogen can be stored in stationary tube systems or trailers. For the selection of the most appropriate system, several aspects have been considered and are presented as follows;

A compression stage is required for compressed hydrogen storage in a tube trailer. When the storage is connected to a fuelling station, two more compression stages are necessary. Following that, the compressed hydrogen must be stored, for example, in hydrogen tanks. Hydrogen tanks has its advantage because it offers high discharge rates and efficiency of approximately 99 per cent, making it ideal for smaller-scale applications, such as the fuelling stations, where a local supply of fuel is required. At 700 bar pressure, the energy density of compressed hydrogen is 15 per cent of the density of gasoline, resulting in a need for a seven times larger storage space compared to gasoline (IEA, 2019). The hydrogen can also be stored on a trailer, whereas it has the potential to sell or move it to other utilities in times of high abundancy of hydrogen, such as when more hydrogen is produced than sold. Two types can be deployed to store hydrogen on trailers, which are a tube trailer and a container, at pressures of respectively 200-250 and 500 bar. The hydrogen tube trailer of 200 kg cost approximately 146.000 euros.

The pressure in stationary tube systems is typically between 200 and 350 bar (Klell, 2010). For storage in the tube trailer, the initial compression stage is from 30 to 250 bar pressure and consumes 1.5 kWh/kg H2 (DOE, 2009). To dispense hydrogen at 350 bar at the filling station, the hydrogen must first be compressed to 440 bar, which consumes 2.23 kWh/kg H2 when starting at 30 bar (DOE, 2009). Similarly, to distribute at 700 bar, hydrogen must be compressed to 880 bar, which consumes 3.2 kWh/kg H2 when starting at 30 bar (DOE, 2009). In reality, the hydrogen for the fuelling at 350 and 700 bar is compressed using hydrogen from the tube trailer at 250 bar, which reduces the required energy for the second compression phase. Because the step from 30 to 880 bar, as well as 30 to 250 bar, consumes the same energy, it is assumed that the hydrogen refuelling at 700 bar costs 3.2 kWh/kg.

The most suitable solution is depending on the required amount of seasonal hydrogen storage. Because of the flexible characteristics, and its adaptability and ability to store relatively small volumes of hydrogen, tube trailers will be considered in this thesis. A tube trailer has an initial cost of 730 €/kg H2, annual operating expenses of 2 percent, and a lifespan of 30 years (Oldenbroek, 2019).

Gaseous hydrogen at 700 bar is the most practical storage technology for on-board hydrogen storage in automotive applications (Edwards, 2014).

Hydrogen can also be stored in liquid organic hydrogen carriers (LOHC). This is a technique that allows for the safe and efficient storage of high-density hydrogen in an easy-to-handle organic liquid, eliminating the need for pressurized storage and transportation tanks. Another way is hydrogen in liquefied form. The hydrogen liquefies at minus 253 degrees Celsius. Liquefication raises the density of hydrogen by around 800 times, resulting in a reduction of storage volume (Adolf, 2017). Once it has liquefied, it can be preserved as a liquid in compressed and thermally insulated containers. There is, however, relatively low experience using liquefied hydrogen (LH_2) in a distributed energy system.
An additional technology is synthetic gas, whereby hydrogen is mixed with CO_2 to produce methane through a chemical process. This produces synthetic gas, consisting mostly of methane, the primary component of natural gas, which can be conveniently transported and stored using the existing gas infrastructure without modification. Hydrogen can also be combined with nitrogen to produce ammonia, allowing for transport and storage of energy in liquid form around minus 30 degrees Celsius. Similarly, the combination of hydrogen with CO_2 to produce methanol enables the transportation and storage of energy in liquid form.

However, the cost-effectiveness of the various alternatives is determined by the distance that hydrogen is distributed, as well as the scale and final usage. For distances below 1500 km, transporting hydrogen in gaseous form via pipelines is most often the cheapest method. On the other hand, for delivery above 1500 km, shipping hydrogen as ammonia or as LOHC are the more realistic option (IEA, 2019). Furthermore, conversion losses can have a considerable effect on the business cases. For example, during the LOHC dehydration, up to 28 percent, around 11 kWh/kg, of the delivered energy might be consumed (GmbH, 2020).

Besides the distance, the most appropriate storage and transportation method also depend on the volume, time, required speed of discharge, and geographic availability. Because the distances between the fuelling stations in the network of this thesis are considered to be below 1500 km, and a hydride and refrigerated storage add to the complexity and energy losses, gaseous storage and transportation by pipelines and trucks will be considered in this thesis. The transportation is only considered for the centralized supply chain. This is because the hydrogen production facilities are in the vicinity of the fuelling stations, and therefore, the hydrogen requires transportation to the refuelling stations. For the decentralized form, the hydrogen is produced and stored at the stations, and therefore, no transportation is required.

Eventually, the cost of hydrogen transportation from the production site to distribution facilities comes down to around 12 €/m^3.

The other characteristics of the compression, storage, and transportation sections are summarized in Table 3.

Table 3. Transportation, storage, and compression characteristics.

Transportation, storage, compression characteristics	
Hydrogen transportation from production to distribution facilities (€/m^3)	12
Pressure in storage tubes (bar)	200-350
Tube trailer cost (€/kg H2)	730
Compression energy consumption at 700 bar (kWh/kg H2)	3.2
Min SoC tube trailers…Max SoC tube trailers (m^3)	60…600
Min SoC hydrogen tank fuelling station…Max SoC hydrogen tank fuelling station (m^3)	2000…5000
Hydrogen tank efficiency (%)	99
Discharge rate (%)	99
Hydrogen storage energy dissipation rate (%/h)	0

Following this, the next section describes how the hydrogen can be dispensed by fuelling stations.

4.1.4. Refuelling station

Hydrogen refuelling stations are designed for storage of hydrogen and dispersing it to applications, such as to road mobility demand. The system may include equipment for the supply, compression, storage, and dispensing of fuel. Furthermore, two refueller systems are available: the cascade storage fill system, and the booster compressor fill system (Clean Hydrogen Partnership, n.d.). A cascade filling system is a high-pressure gas cylinder storage system that allows smaller compressed gas cylinders to be refuelled. A booster system passes air through additional stage to augment or magnify the air pressure produced by an existing compression system. This allows an increase of the current air pressure from between 0.6 and 10 bar to 138 bar (Clean Hydrogen Partnership, n.d.).

The investment costs of a hydrogen fuelling station is determined by the delivery pressure of the hydrogen, a system with 700 bar is expected to cost between 0.6 and 2 million dollars, while 350 bar will cost between 0.15 and 1.6 million dollars. The compressor and storage tanks are the most expensive components. Since hydrogen booster stations provides sage and clean hydrogen compression which is in the range of the required pressure needed in the vehicles, it is considered in this thesis. Such a fast fill station with a single 700 bar dispenser cost 1.2 million euros according to the IEA (2019). The operational cost and the lifetime are respectively 1%/year and 15 years (Oldenbroek et al., 2017). Because two dispensers, one at 700 bar and one at 350 bar are included in this thesis, it accounts for 1.5 million euros investment cost. These two dispensers are chosen since the road mobility refuel at 350 or 700 bar. The expenditures of the compressor, as well as the storage at 440 bar and 880 bar are considered in this estimate. According to this, the characteristics of the fuelling station considered in this thesis are summarized in Table 4.

Table 4. Refuelling station characteristics.

Fuelling station characteristics	
CAPEX at 700 bar (€/station)	1.2 million
OPEX (% of the CAPEX/year)	1
Lifetime (years)	15
Air pressure (psig)	9/150-2000

4.1.5.Hydrogen to electricity

The abovementioned section describes how easily hydrogen can be formed through electrolysis, and how it can be separated and stored. However, the hydrogen can also be converted back into electricity through heat engines, or more efficiently, via fuel cells (Steilen, 2015). A fuel cell consists of two electrodes, an anode and a cathode, with an electrolyte in the between. The anode receives a fuel, like hydrogen, while the cathode receives air. In a PEM fuel cell, a catalyst splits hydrogen atoms into protons and electrons, which take distinct pathways to the cathode. This process is conversely to the electrolyzer process which was depicted in Figure 7.

Although all different types of fuel cells perform the same basic functions, numerous types have been designed to take advantage of differing electrolytes and satisfy varied application demands. The fuel and the charged species that migrate through the electrolyte are different, but the concept remains the same (Steilen, 2015), as shown in Figure 8 depicts the processes of the fuel cell. Since hydrogen is typically used as the fuel in PEM fuel cells, this type of fuel cells will be considered in this thesis. These cells function at low temperatures and can react quickly on changing power needs. PEM fuel cells are the most suitable technique for powering vehicles. They are also suitable for the generation of stationary electricity (U.S. Department of Energy, n.d.). The electrons flow through an external circuit, causing an electricity pathway. The protons move through the electrolyte to the cathode, in which they react with oxygen and electrons to form water and heat.

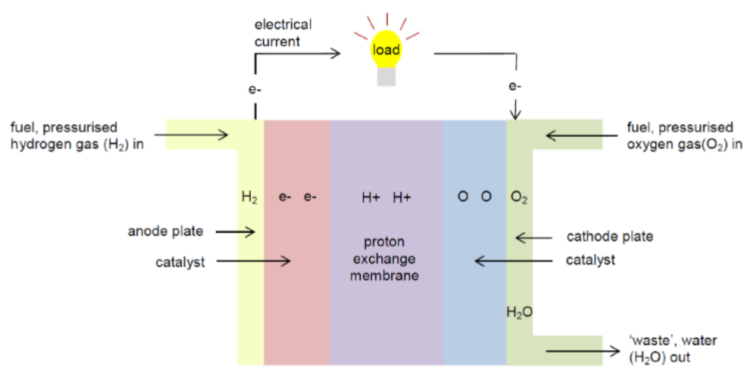

Figure 8. Fuel cell: hydrogen conversion to electricity (Fulcher, 2019).

The capital expenditure of PEM fuel cells is 700 €/KW. The operational cost is 1.6 percent of the total capital cost per year. The characteristics are summarized in Table 5.

Table 5. Fuel cell characteristics.

Fuel cell characteristics	
CAPEX (€/KW)	700
OPEX (%/year)	1.6
Efficiency (%)	70
Hydrogen to power conversion factor (MWh/m^3)	1/360
Lifetime (years…hours)	20...80000

4.1.6. Applications: mobility sector demand and balancing services to power grid

The network has to deal with a diversity of mobility and electricity demand patterns, and balancing authorities that operate in or near locations. The hydrogen fuelling stations should serve hydrogen fuel to road mobility, but the storage capacity would not always be entirely utilized for transportation purposes. The energy stored in the fuelling stations, for example, would not be used effectively during off-peak demand by hydrogen powered cars. Given the possibility of several hydrogen storage systems distributed across a wide area, a considerable percentage of storage capacity would be underutilized by the transportation sector during off-peak hours. At this moment, a potential arrives to utilize the available storage capacity in these stations to provide balancing services for the power sector. This concept is considered in this thesis based on a 24-hour forecast at hourly resolution and an actual load profile. In the next section, a description of the hydrogen fuelling system concept will be given, as well as an energy market background to elaborate in which market the system can operate.

Mobility sector demand

One of the applications for the hydrogen supply chain is selling hydrogen for transportation purposes, such as the mobility fleet. There are a variety of refuelling infrastructure alternatives available, ranging from single car refuelling to large-scale refuelling facilities capable of refuelling a vehicle fleet on a continuous basis. In this thesis, a fixed hydrogen demand, generated by the NREL will be considered (NREL, 2021), which will further be delineated in Chapter 5.

When considering renewable hydrogen for the transportation fleet, fuel cell electric vehicles (FCEVs) offer a low-carbon transportation solution with the driving range and refuelling time of conventional vehicles. FCEVs has the potential to expand the market for electric mobility to heavy duty cycle categories, such as long-range or high utilization rate vehicles, e.g., trucks, trains, buses, taxis, ferry boats, cruise ships, aviation, and forklifts, where batteries are currently limited. FCEVs should therefore be considered as complementary to BEVs; while they may compete in some market segments, either FCEVs or BEVs have a clear competitive advantage in each segment.

According to IRENA, possible future segmentation of the FCEVs consists of medium to large cars, fleets and taxis, and buses to trucks and trains (IRENA, 2018). In this thesis, only road mobility will be considered, which means all fuel cell electric vehicles from medium cars to large trucks. The average sale price of hydrogen in the transportation sector is expected to be respectively 0.3525 €/m^3, or 6.02 €/kg (IRENA, 2019; NREL, 2019; H2Council, 2019; El-Taweel, 2019. Furthermore, according to the NREL, the average fuelling amount is 1.4 kg of hydrogen, which comprises 17.07 m^3 hydrogen (NREL, 2019).

Balancing services to power grid

The other application of the hydrogen supply chain is offering a re-electrification pathway, in which the hydrogen can be converted back to electricity to balance the power grid. In the next section, background information is described to give an overview of the energy market.

Electricity market background

In the electricity market, an intraday market opens after the day-ahead and the reserve market. In this thesis, two different electricity markets are considered, which are the day-ahead and the secondary reserve market. The intra-day market is excluded because the hydrogen fuelling system does not participate in this market. Finally, the market for the imbalance settlement is also considered.

Participants in the day-ahead market submit 24-hour power sale and purchase bids for the next day. A market operator handles the electrical transactions, followed by a clearing price which is announced after the bids.

The secondary reserve market provides ancillary service to preserve the difference between the generation and demand of electricity during the power delivery process. This market applies a strategy where participants submit their available upward and downward reserves. When needed, the committed reserve is called upon to bridge the gap between anticipated and the actual power.

At the end of each day, the differences between the actual power generation of the market participants and the cleared energy in the day-ahead market are determined. Participants are compensated if the actual power generation exceeds the cleared energy. Conversely, when the cleared energy exceeds the actual power generation, the participants are required to pay.

Figure 9 depicts the sequence of event in the electrical markets. Until 12:00 in day D-1, the bids of all the hours in day D should be submitted to the day-ahead market. At 12:00, the day-ahead market shuts down. Before 13:00, the clearing price is publicized. After the day-ahead market closes, the reserve market for day D starts. Before 14:00, the hydrogen fuelling system operator can send the reserve offer for day D to the reserve market, whereafter the clearing price is publicized at 15:00. The power imbalances are computed, and the imbalance prices are published in day D+1 after the actual power is supplied on day D (Wu, 2021).

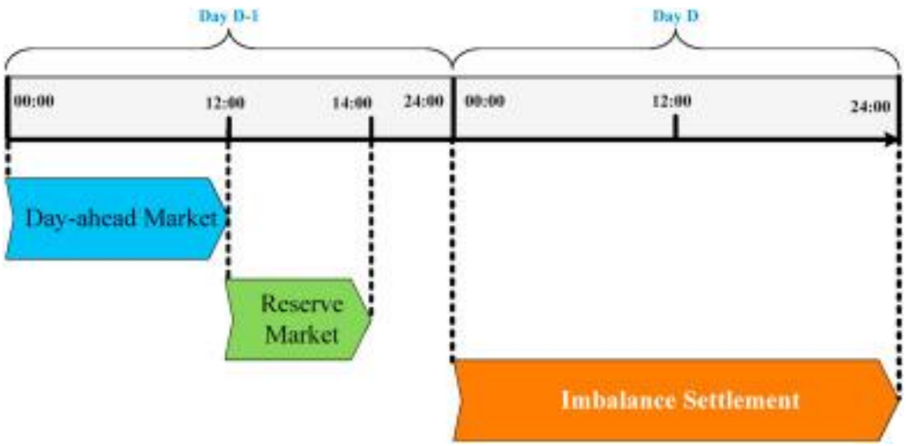

Figure 9. Sequence of electricity markets (Wu, 2021).

In the next subsections, the three most important imbalance services will be elaborated. Moreover, a general calculation approach is given.

Ancillary services

For the safe and secure functioning of power systems, system operators have indicated ancillary services, which primarily comprise energy scheduling and dispatch (Jay 2021). Rescheduling and dispatching are required to remain the frequency, voltage, and power load within certain limits. This happens on continuous basis. To avoid loss of generality, three different system services are deployed in this thesis, which are VAR support, DR, and OR (Next Kraftwerke, n.d.). Therefore, in this section, the VAR support mechanism will be elaborated. Subsequently, the DR approach is specified, followed by an explanation of OR.

VAR support

In any AC power system, reactive power management is an integral part of the control process related to voltage level (Avenston, 2016). This is required due to the reactive, inductive or capacitive, nature of electrical loads and transmission and distribution networks. Reactive power support must equalize this reactive power demand locally, as well as maintaining system-wide voltages within the permissible limits (Jay, 2021). When there is a deficit in load, the system produces reactive power that should be absorbed. On the contrary, during abundancy of load, the system consumes a large amount of reactive energy that requires compensation. This is because reactive power results in excess currents that flow back into the power supply system, which are not only destructive but also costly in terms of money. These currents in both electricity transmission lines and solar power station, wind turbine and hydrogen generation equipment cause financial losses. This is due to the conversion of electric energy to thermal energy, which include lowering the generation amount and thus decreasing the profit of the system, and increase asset degradation, resulting in non-failure operating time and an increased maintenance expenditure (Avenston, 2016).

Furthermore, generating reactive energy into a national grid incurs penalty charges, resulting in direct financial losses. As a result, controlling and compensating reactive power is an apparent way to increase the profitability of a power station (Jay, 2021).

The reactive power can be determined by averaging the voltage and current product with a running average window across one cycle of the fundamental frequency, with the powers being assessed at fundamental frequency (MathWorks, n.d.). For instance, a current that flows into the reductor-inductor branch, which are passive circuit components such as resistors and inductors connected to a current or voltage source within a circuit (Linquip Technews, 2021), produces positive active and reactive powers.

Because the block employs a running window, one simulation cycle has to be conducted before the output provides the correct active and reactive powers.

Reactive power balancing can be supported by local reactive power sources connected to the power grid, such as a hydrogen supply chain integrated with the power grid. The system can either absorb reactive power, preventing voltage boost in the connection point or create it, preventing voltage spikes. Hereby, the reactive power consumption or production may be altered, allowing the voltage to be controlled within certain operating limits (Jay, 2021).

According to the IEC, voltage fluctuations are cyclical variations of the voltage envelope, or a series of random voltage shifts up to around ten percent of the nominal, this means 0.9 to 1.1 per unite (pu) as defined by ANSI C84.1-1982 (ESIG, 2021). Therefore, in this thesis, the following characteristics are used, as given in Table 6. The reactive power service price is also specified, which is 37.50 €/MVAr.h according to El-Taweel (2019). This is the average from up and down prices that are paid when operators provide ancillary services.

Table 6. VAR support characteristics.

VAR support characteristics	
Reactive power service price (€/MVAr.h)	37.50
Min voltage of power system buses of distribution network (pu)…Max voltage of power system buses of distribution network (pu)	0.95…1.05

Min voltage of power system buses of transmission network (pu)…Max voltage of power system buses of transmission network (pu)	0.9-1.1

DR

The transformation of the electricity system to enable net zero trajectories is exerting pressure on both supply and demand, necessitating increased flexibility, which may increasingly be provided through demand-side resources, such as demand response mechanisms (IEA, 2021).

On the one side, the share of renewables in total output expands, driving the need for additional system flexibility. On the other side, also the share of electricity in final energy demand expands. As a result, the role of demand response grows rapidly in advance economies. These demand response mechanisms can be deployed to manage the correlating power system problems, such as high generation costs, high peak to average ratio of demand, reliability difficulties, and congestion in generation, transmission, and distribution networks. Their primary purpose is to help power systems during peak demand periods as well as during emergencies (Jordehi, 2019).

To appropriately determine the amount of load reduction, the customer's baseline load must be known. A few days prior to the event, the base load can be monitored. To compute the load deduction, all grid purchases made during the demand response event are deducted from this baseline (Francklyn, 2019).

So, if a utility forecasts an exceptionally high peak in the next few hours or days, demand response customers will receive a notification. It will typically include information such as when and how long the DR event is anticipated to occur. Customers, such as the operators of hydrogen supply chains, can subsequently plan to reduce their grid purchases during those hours. This can be achieved by lowering their consumption during that time period, shifting consumption to either before or after the demand response event or temporarily relying on on-site energy production rather than using power from the grid. For each kW saved, the end-user will be rewarded with a pre-determined amount (Jordehi, 2019).

This pre-determined amount is in this thesis defined as 37.50 €/MWh. This is the average from up and down prices that are paid when operators provide ancillary services.

OR

OR refers to excess operating capacity (OC) that can quickly respond to a sudden rise in electric load or a sudden fall in renewable power generation. OR provides a safety margin that aids in assuring consistent power supply despite fluctuations in electric load and renewable power supply.

Because electric load is volatile, power systems must constantly offer some level of OR. In absent of OR, the load would occasionally surpass the OC of the system, resulting in power outages. Renewable energy systems including, for example, wind and solar energy sources, require additional OR to protect against unpredictable drops in the renewable power supply.

The OR equals the OC subtracted by the electric load (EL), given as

$$Capacity\ OR = OC - EL \qquad (1).$$

Where the OC is the total available and operational electrical production capacity at a specific time moment. It refers to the maximum amount of electrical load that the system could serve at any given moment. In this thesis, the model will keep track of the OC, and hence the OR, separately for the AC and DC buses. When the OR at one bus is required to compensate load at the other bus, it evaluates the efficiency and capacity of the converters. For instance, a diesel-storage-inverter system that serves an AC load has a capacity of 5 kW. If the storage is offloading 1 kW, it can offer 4 kW of DC OR. When the inverters efficiency of 90% is considered and the capacity is within the operating limits, 3.6 kW of AC OR can be served.

The required OR is the minimum volume of OR that the system must be able to provide. This reserve state-of-charge (SOC) for contribution to OR market is 15% times the maximum SOC of hydrogen (m^3). The OR service availability price is 37.50 €/MWh. This is the average from up and down prices that are paid when operators provide ancillary services.

A summary of the simulation parameters considered in the model are given in Table 7.

Table 7. Simulation parameters.

Simulation parameters	**Value**
DR service price ($\frac{€}{MWh}$)	37.50
VAR service price ($\frac{€}{MVAr.h}$)	37.50

OR reserve service availability price ($\frac{€}{MWh}$)	37.50
Electrolyzer capital cost (CC) ($\frac{€}{MW}$)	700
Fuel cell unit capital cost (CC) ($\frac{€}{MW}$)	700
OPEX of electrolyzer ($\frac{€}{m^3}$)	3.02 % * $\frac{CC^{elz}}{8760}$
OPEX of fuel cell unit ($\frac{€}{MWh}$)	3.02 % * $\frac{CC^{FC}}{8760}$
Cost of hydrogen transportation from production to distribution facilities ($\frac{€}{m^3}$)	12
Power to hydrogen conversion factor ($\frac{m^3}{MWh}$)	360
Efficiency of the electrolyzer (%)	71
Minimum power of electrolyzer (MW)	0
Maximum power of electrolyzer (MW)	257
Hydrogen to power conversion factor ($\frac{MWh}{m^3}$)	1/360
Efficiency of fuel cell unit (%)	70
Volumetric storage density ($\frac{m^3}{m^3}$)	1/630
Minimum hydrogen flow of fuel cell unit (m^3)	257
Maximum hydrogen flow of fuel cell unit (m^3)	0
Minimum hydrogen SoC tube trailers (m^3)	60
Maximum hydrogen SoC tube trailers (m^3)	600
Maximum SoC hydrogen tank fuelling station (m^3)	5000
Minimum SoC hydrogen tank fuelling station (m^3)	2000
Maximum power at power system branches (MW)	9
Minimum voltage at power system buses (pu)	0.9
Maximum voltage at power system buses (pu)	1.10
Admittance magnitude between buses (pu)	Admittance matrix
Reserve SoC for contribution to OR market (m^3)	15% *SoC_h^{max}

5. Model conceptualization and optimization

In this chapter, the system described in the previous chapter is transformed into a computer model. This model can be used to evaluate the different configurations of the hydrogen generation and supply chains. In the first subsection, the modelling approach is presented. Then, the characteristics of each component in the models are described, as well as the input data. Subsequently, the decision variables, optimization problem and constraints are specified. Following that, the model testing including the verification, validation of the model is presented, as well as the sensitivity analysis. Lastly, the economic evaluation parameters are formulated.

5.1. Modelling approach

To convert the system of Chapter 4 into a computer model, a suitable modelling approach must be considered. Energy models can be implemented for the efficient forecasting, planning, design, operation, and optimization of future energy systems (Kaldellis, 2010). Depending on the implementations and uses of the problem, the model paradigm can be encountered as simulation or optimization, and top-down or bottom-up. A simulation model provides the performance of a system over a predetermined period and a certain set of conditions. An optimization model proposes the decision variables that generates the optimal design corresponding to a set of assumptions and constraints. While bottom-up models are based on technological features to balance supply and demand in a system, top-down models show the economic linkages among various sections of a national or regional system (Willmann, 2019). As this thesis examines the optimal design for hydrogen generation and storage supply chains systems for the coupling between the transportation sector and the power grid including renewable power generation, where achieving an energy balance is required, a bottom-up optimization model is considered.

For the establishing of the model, the context and positioning, as well as the type of optimization criteria, that may be utilized in different future energy systems should be defined (Ostergaard, 2009). The context and positioning include different aspects, such as the represented energy carriers, the evolution over time, the computation logic, the studied approach, and the choice of dynamics. As mentioned before in Chapter 4, the system uses electricity and hydrogen as energy carriers. Furthermore, the model uses fixed and evolving parameters, such as economic and technical parameters described in the previous chapter. Additionally, an optimization logic is used to find the optimal system design for hydrogen generation and storage supply chain systems operators. Lastly, operational planning decisions are considered to investigate the optimal design for hydrogen generation and storage supply chains.

Besides the context and positioning, the criteria should represent the economic functions, such as net present value (NPV), total cost, and profit, or alternatively a well-defined performance measure depending on the operation of the energy system, or even the consideration of sustainability issues (Ostergaard, 2009). In this thesis, different economic functions, such as the gross income, net income, net present value, breakeven time, internal rate of return, and profitability are considered to compare different designs, while satisfying different operational boundaries of the system. Furthermore, the model should also incorporate the physical, technological and resource constraints of the system under consideration. Figure 10 visualizes the approach to generate the model including the input and output flows, to obtain the optimal design for hydrogen generation and supply chains.

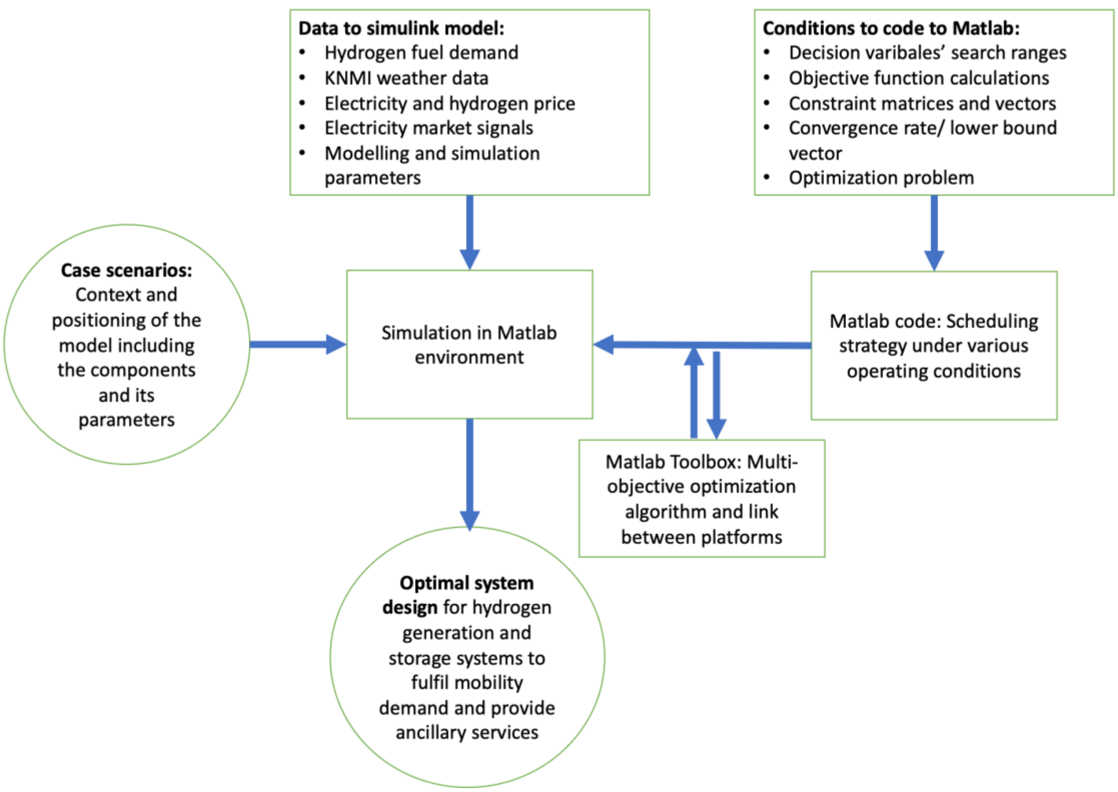

Figure 10. Flowchart of optimization model.

As depicted in Figure 10, first, two case scenarios are designed based on the reviewed literature. This includes the framework for exploring the context and positioning of the model based on future energy perspectives, including various combinations of technology options and their implications, as described in

Chapter 4. Other input parameters to the Simulink model, such as demand and generation patterns are considered in this step, which are described in this chapter.
Another component of the generation of the optimization model is the determination of conditions into the MATLAB environment, such as the decision variables, which are the quantities that can be controlled and changed subjected to the optimization problem. Regarding this optimization problem, objective functions are utilized to describe the target variables whose optimal value is searched by the model and also the direction of the search which is conducted by the model. Finally, the optimization model searches the solution space by means of mathematical formulations. Therefore, a scheduling scheme, as well as constraints are formulated to describe the relationships between the real system and the model. From this, the model including its constraints describe the feasible solution in the model by means of optimization algorithms, so that the optimal solution can be found. After the optimization process, the designs will be numerically evaluated.

Following the flowchart, in the next section, the model systems that will be numerically evaluated are described, including the elaboration on how the model components are modelled.

5.2. Model characteristics

For the optimization, different RTS bus power systems are considered: the IEEE 33-distribution and IEEE 30-transmission systems. The IEEE 33 bus system is meant for testing the efficacy of the distributed hydrogen supply chain system whereas the IEEE 30 bus system is meant for evaluating the centralized hydrogen supply chain system, as depicted in Figures 11 and 12. Both supply chain systems are supported by wind turbines and solar PV panels. As depicted in Figure 11, the IEEE 33 bus system is equipped with six numbers of hydrogen production and preservation facilities. For local electricity production, each hydrogen generation and storage system are allocated with FC unit, electrolyzer, and hydrogen storage tank. As depicted in Figure 12, the centralized based hydrogen generation and storage system is connected to a bulk transmission system. The system includes one centralized hydrogen generation and storage facility including stacked electrolyzers, fuel cell units, and hydrogen tanks. The hydrogen will after the generation be stored at the central facility where it can be distributed to the applications.

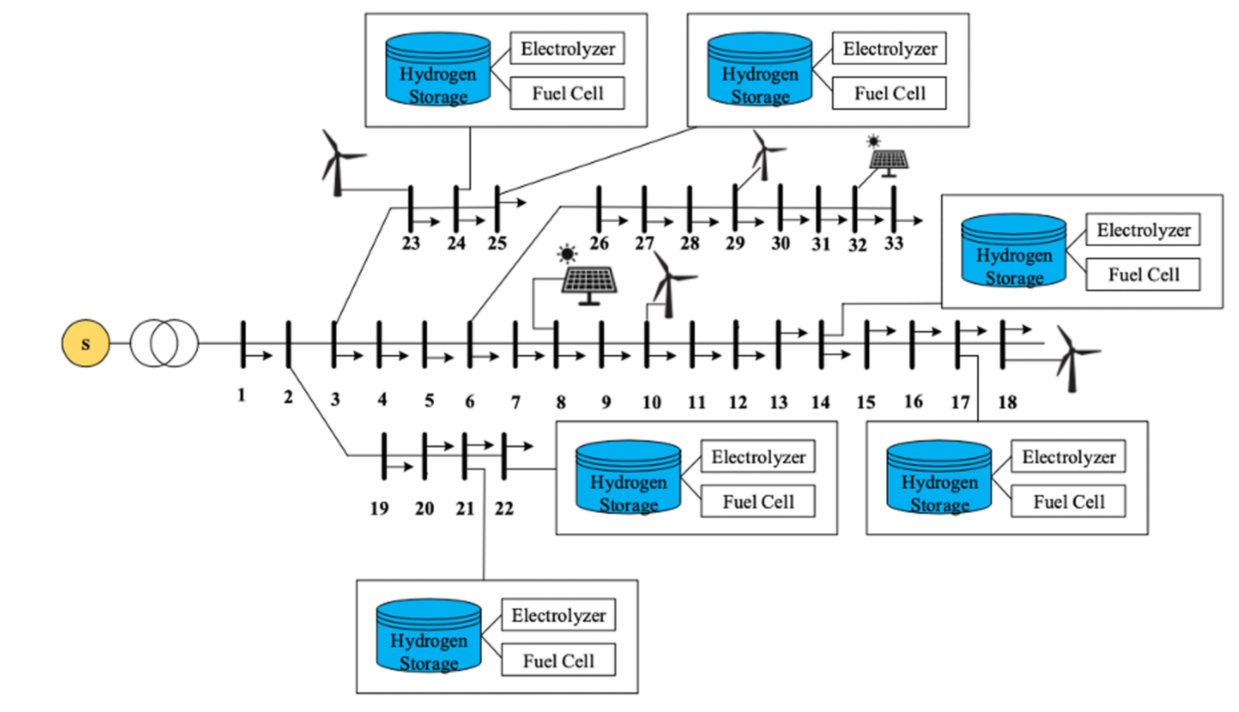

Figure 11. IEEE 33 bus system: Distributed hydrogen generation and storage supply chain system.

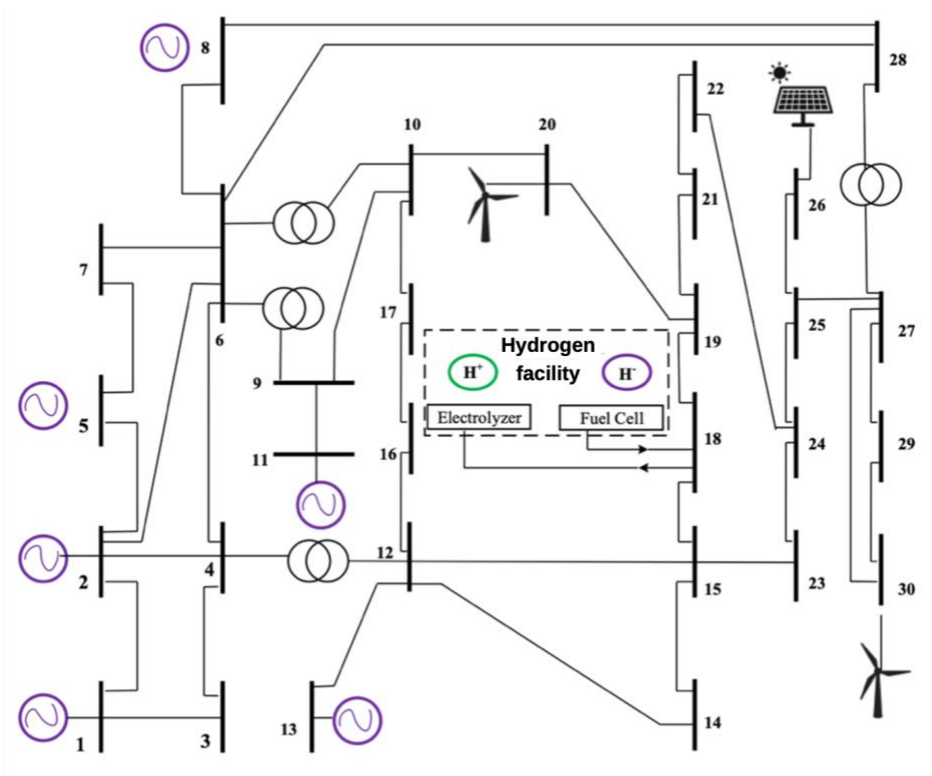

Figure 12. IEEE 30 bus system: Centralized hydrogen generation and storage supply chain system. The central facility include a stacked electrolyzer, fuel cells, and a storage tank.

The next subsections describe how the components of the model system, from production to end-user, are modelled. This includes the description of input data in the model, such as the energy sources, and the mobility demand.

5.2.1. Energy sources

To account for the fluctuation in renewable energy production, the scheduling setpoints are iteratively altered by revising the optimization problem at each time interval (Haijmiragha, 2015). For this, a block is implemented to simulate a variable pitch wind turbine model. The performance of the wind turbine is decided by the performance coefficient Cp, given as: "the mechanical output power of the turbine divided by wind power and a function of wind speed, rotational speed, and pitch angle (beta)" (Mathworks). When the pitch angle is zero, Cp achieves its maximum value. Three wind turbine power characteristics at a desired pitch angle are inputted in the model to obtain the output characteristics. The first input is the generator speed of the generator base speed, expressed in per unit (PU). The basic speed of the generator is synchronous speed. The second vector is the angle of the blade pitch (beta) in degrees, the third input is the wind speed in m/s (12 m/s). The output is the torque exerted on the generator shaft of the generator ratings, measured in PU, as depicted in Figure 13. Also, the inertia of the turbine must be added to the inertia of the generator.

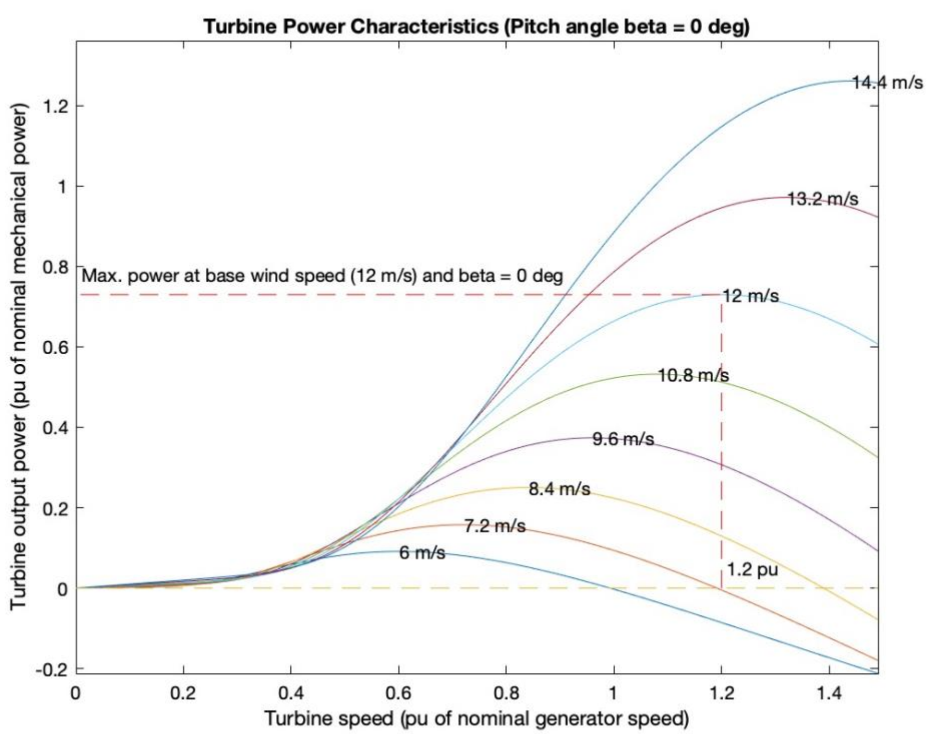

Figure 13. Wind generation characteristics (Adapted from MATLAB).

Besides the wind turbines, the solar characteristics are modelled as well to deliver electricity. For this, a solar PV block is simulated to implement an array of PV modules with different specifications, corresponding to the Suntech STP260-24/Vb panels. The characteristics are retrieved from the system advisor model of the NREL (2018). Five input parameters are used indicate the irradiance and temperature-dependent I-V characteristics of the modules to the PV array block, which are a light-generated current source (I_L), diode, series resistance (Rs), and shunt resistance (Mathworks, n.d.). The following equations define the diode I-V characteristics of a single module:

$$I_d = I_0 \, [\exp\left(\frac{V_d}{V_T}\right) - 1] \quad (2)$$

$$V_T = \frac{kT}{q} * nI * Ncell \quad (3)$$

where I_d is the diode current (A), V_d is the diode voltage (V), I_0 is the diode saturation current (A), nI is the diode ideality factor close to 1.0, k is the Boltzman constant (1.3806e-23 $J.K^{-1}$), q the electron charge ($1.6022e^{-19}$ C), T the cell temperature (K), and Ncell the number of cells connected in series in a module. The power output, including the current (Imp) and voltage at maximum power (Vmp), is visualized in Figure 15.

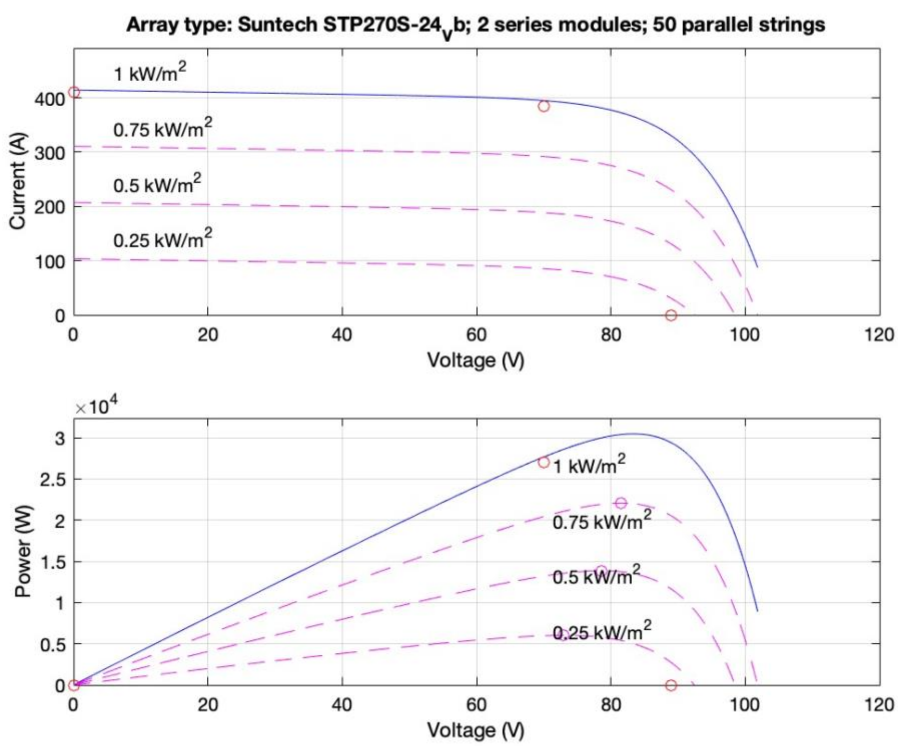

Figure 14. Power output of solar PV panels (Adapted from MATLAB).

Furthermore, historical electricity market data is used from the Entsoe Transparency platform, as depicted in Figure 16. 2018 is considered as reference year. This is to avoid using invalid data due to the Covid pandemic, as well as the influence of the Ukraine war on the prices.

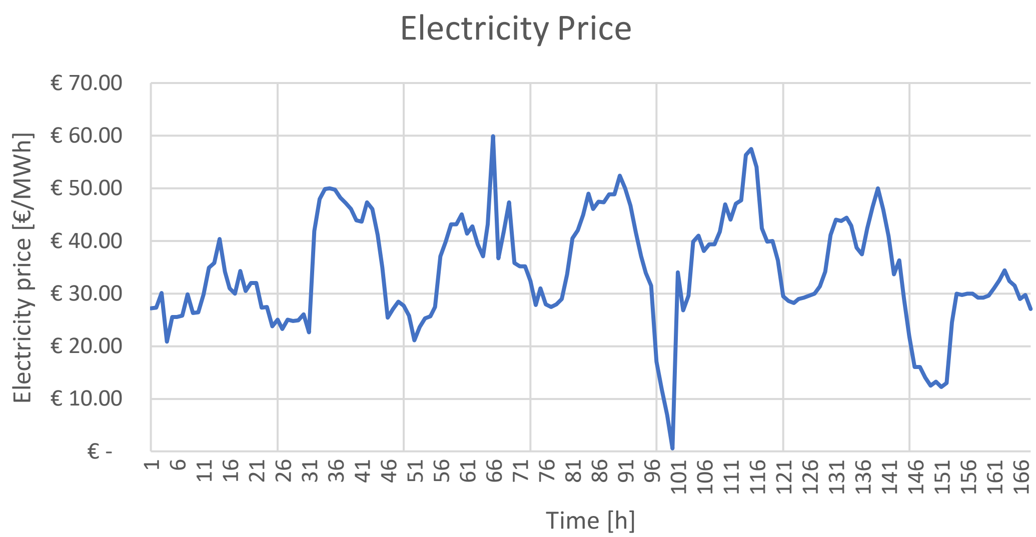

Figure 15. Electricity price (€/MWh) for one week in 2018 (Adapted from Entsoe Transparency Platform).

5.2.2. Hydrogen production

A Simscape block is utilized to simulate the PEM power to hydrogen interface with the power grid and its power circuit control structure (Mathworks, n.d.). The concept of the PEM interface is to split water molecules into hydrogen and oxygen by supplying DC across two electrodes submerged in water. The configuration of the electrolyzer demands a high level of DC current at a low voltage supply (Torok, 2017). As a result, an AC-DC converter must be used to rectify and control the AC power (Naidu, 2018). The control system is primarily composed of the power to hydrogen flow rate and pressure control (Gyawali, 2010), with the steady state equations demonstrating the power to hydrogen flow rate, as follows:

$$P_{h,t}^{PtH} = \frac{F_{h,t}^{PtH}}{PtH\ conversion\ rate * \eta PtH} \quad (4)$$

$$Conversionrate_{h,t}^{PtH} = \frac{\eta^F}{2 * F * \ v^{PtH}} \quad (5)$$

$$\eta^{PtH} = \frac{F_{h,t}^{PtH} * LHV_{H2} * \lambda_{H2}}{P_{h,t}^{PtH}} \quad (6)$$

where $P_{h,t}^{PtH}$ is the input power of the electrolyzer (MW), $F_{h,t}^{PtH}$is the hydrogen outflow of electrolyzer (m^3/h), ηPtH the efficiency of the electrolyzer (%), η^F is the Faradays efficiency, F is the Faradays constant

(MAh/m³), input voltage v^{PtH} (V). Furthermore, LHV_{H2} is the lower heat value of hydrogen (MWh/kg), λ_{H2} is the hydrogen density (kg/m³).

The control system creates switching signals for the converter, which regulate the power to hydrogen input power flow and, as a result, the generated hydrogen. A feedback controller is used in the system to change the pressure in the storage tank (Gyawali, 2010). Using this, the pressure regulation generates a reference signal for the input power of the compressor (Pcmp), based on received feedback on the electrolyzer and hydrogen pressures. Corresponding to this, the steady state equation of the pressure controller is delineated as follows:

$$P_{h,t}^{Cmp} = \frac{F_{h,t}^{PtH}}{\eta^{Cmp}} * \frac{k*R*T^{PtH}}{k-1} [rhotsto/rhotpth], \quad (7)$$

where k, R, and Tpth represent respectively the polytropic coefficient, gas constant, and PtH temperature.

The electrolyzer units use market prices to decrease the cost of purchasing while maximizing the system profit. The hydrogen demand at the stations affects the operational setpoints. At each time period, the system must function within the wide minimum and maximum bus voltages in the test system. If the wide voltage of the system operates within the boundaries at each period, the functioning of the entire system would be satisfactory.

5.2.3. Conditioning and storage

As mentioned before, a feedback controller is used to regulate the SOC of the hydrogen storage, as well as the pressure. The polytropic compression model describes the relationship between the hydrogen molar flow rate and the compressor power, given as:

$$M_{H2,out} = \frac{\alpha com}{w} P_{comp} \quad (8)$$

$$w = \frac{kRT_{elz}}{k-1} [\left(\frac{P_{tank}}{P_{elz}}\right)^{\frac{k-1}{k}} - 1] \quad (9)$$

where w is the polytropic work, $\alpha com$the compression efficiency, k the polytropic coefficient, and $P_{tank}$the pressure of the storage tank. In this regard, the pressure of the stored hydrogen is formulated as:

$$\frac{V_{tank}}{RT_{tank}} \frac{d}{dt} P_{tank} = M_{H2,out} - M_{H2,in} \quad (10)$$

where T_{tank} and V_{tank} are respectively the temperature and volume of the hydrogen inside the tank, $M_{H2,in}$ the hydrogen inflow.

The storage works as a dispensing system for the mobility demand. However, when a signal for ancillary services is provided, capacity is supplied to follow the signal, while maintaining the constraint of always satisfying the demand for mobility. As a result, depending on the ideal setpoints determined by the optimization problem, each storage is able to react differently to the signal. Yet, the total SoC of all storage is considered to indicate the revenue, as well as the technical performance of the system. The optimization issue also determines the price of hydrogen at each station.

5.2.4. Transportation

The transportation from the centralized electrolyzer facilities to the dispensing facilities is determined by the length and the diameter of the pipelines, as well as the initial pressure regulated by the control system. The exchange of hydrogen fuel via pipeline I from zone x-y, which is the pipeline from the centralized production facilities to the fuelling stations, is divided into two parts: hydrogen delivering and flowing out. For the hydrogen delivery it is assumed to be 12 €/m^3, as mentioned in section 4.1.3, to deliver the hydrogen over the 50 km range from the production facility to the dispensing facilities. However, this depends on the flowing out of hydrogen. For this a block is implemented to check the gas properties, which checks the bearable appropriate pressure, volume, and temperature, according to the ideal gas law, as given as:

$$p = Z\rho RT \qquad (12)$$

Where p is the pressure, Z is the compressibility factor (1.00060 for hydrogen), R the specific gas constant (0.98506 kcal/kg K), and T the temperature.

For this process, the system is divided in zones (Z), and when a signal is issued by the fuelling stations, the bearable hydrogen capacity can be sent.

5.2.5. Fuelling stations

The fuelling stations supply hydrogen fuel to the mobility demand. This requires bidirectional communication to collect data, including receiving the control signals to the stations. A Crossing block is implemented to detect the hydrogen demand of the transportation sector, the hydrogen tank SoC, electricity prices, and signals for ancillary services from the energy market operator and generate signals corresponding to these events. The tank releases the hydrogen corresponding to the hydrogen fuel demand. This works along the proposed optimization algorithm aims to optimize the joint operation of the hydrogen fuelling stations by use of the central controller. The controller analyses the received data and determines the appropriate electrolyzer unit setpoints for each hydrogen fuelling stations. Furthermore, the central controller determines the hydrogen sale prices. It is also worth mentioning that the scheduling model meets the limits of the electricity system.

5.2.6. Load

Hydrogen demand data for fuelling station of FCEVs is adopted from the National renewable energy laboratory (NREL) report for numerical studies (NREL, 2019), as depicted in Figure 17. According to the NREL, Hydrogen fuel electric vehicles provide a similar driving and fuelling experience to traditional gasoline-powered vehicles. The NREL compared usage data for hydrogen vehicles driving and fuelling events for both time of day and day of the week in comparison to typical NHTS gasoline-powered-car consumption data (NHTS, 2009) and to a profile of a typical gasoline station created using Chevron consumption data (Chen, 2008). Hereby similar patterns are distinguished for fuelling events by time of day and by day of the week. The hydrogen vehicles fleet resulted in 18,568 fuelling events, whereas 75% of the events occurred between 6 a.m. and 6 p.m. The fleets generally fuelled more during weekdays and less during weekends. Furthermore, the vehicles fuelled more frequently at the start of the workday and less during working hours. From this, an average filling amount of 1.4 kg per fuelling moment is observed. The data is retrieved by using empirical fuelling data sets, whereby it has been validated over a range of fuelling conditions to match common light-duty fill profiles.

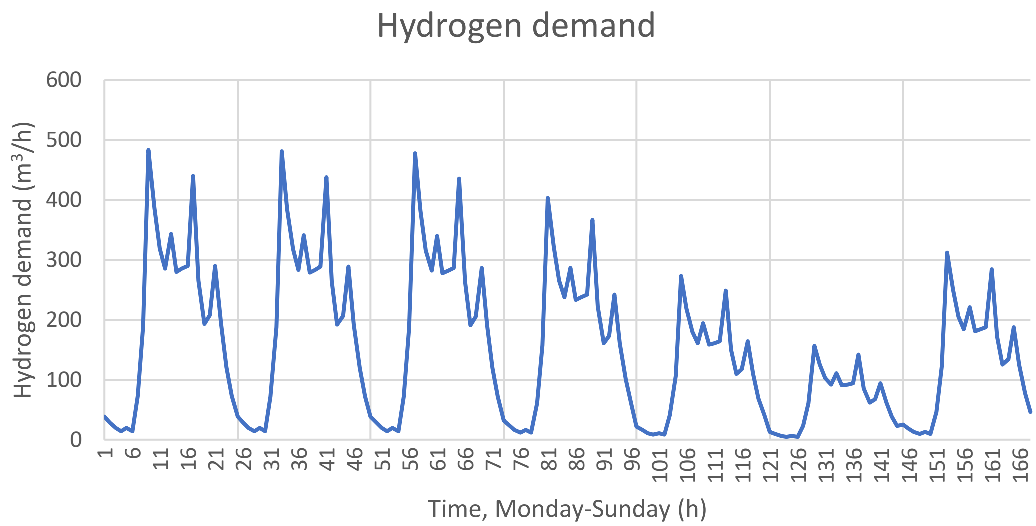

Figure 16. Hydrogen demand per hour (m³/h) from Monday-Sunday (Adapted from NREL).

Ancillary services signals

Hydrogen refuelling stations are dispatchable and can easily respond to ancillary services signals provided by the market. It can assist reduced power demand during a certain time period, allowing it to compensate a deficit of hydrogen during peak power periods.

For the modelling of the ancillary services signals, it is worth noting that once the signals are provided, the model prioritizes the contribution to the hydrogen generation. This process is accommodated in the objective function by slack variables, which will be discussed more in the constraints section. The highest emphasis is given to the mobility demand in order to guarantee that the fuelling stations can meet their commitments and increase their profit margins, as ancillary services revenue could often be larger than the fuel supply to the mobility demand. By executing the optimization process at each time step, the scheduling setpoints are adjusted iteratively. The thesis uses data from the IESO to replicate the ancillary service programs. This means that the average ancillary services signals are observed, whereafter the signalled capacity and moments can be replicated (IESO, 2018), as depicted in Figure 18-10.

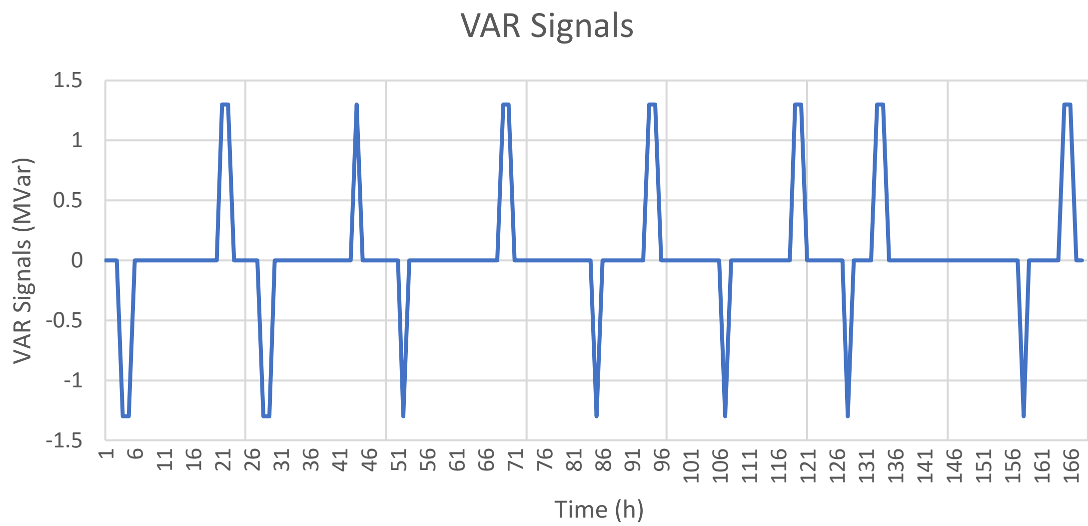

Figure 17. Replicated VAR Signals (Adapted from IESO).

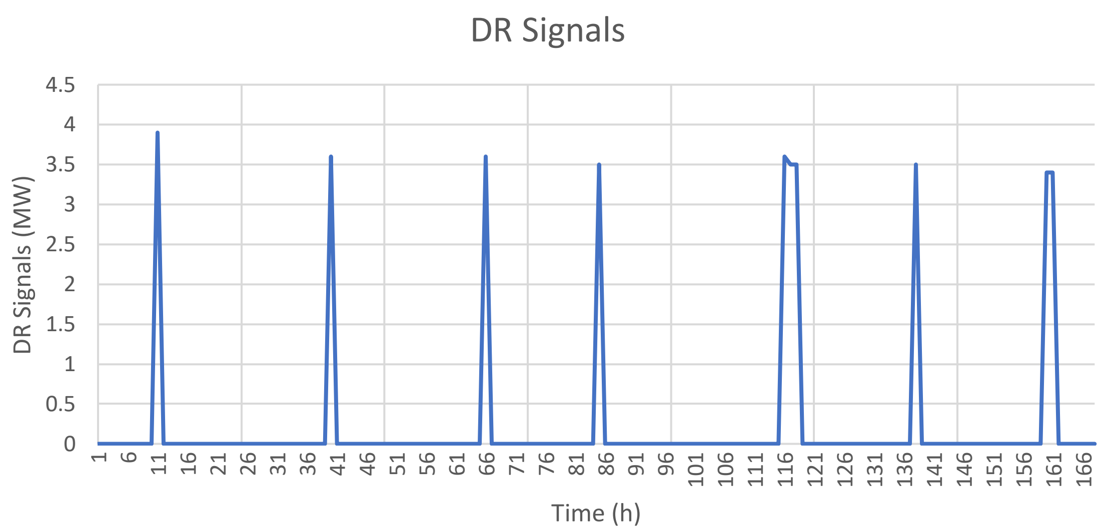

Figure 18. Replicated DR Signals (Adapted from IESO).

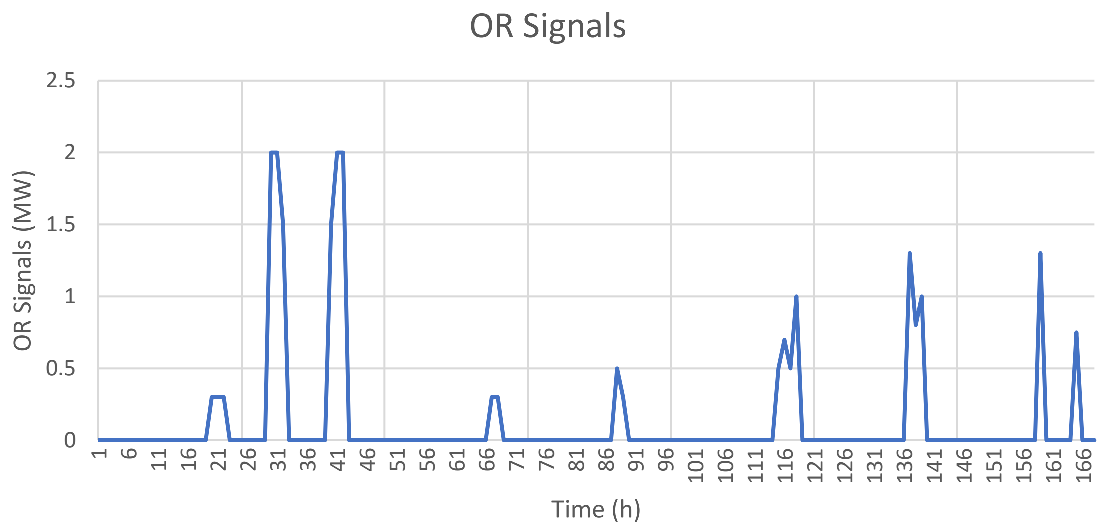

Figure 19. Replicated OR signals (Adapted from IESO).

In this section, the model components, as well as the optimization model is described. Following this, in the next section, this model is translated into a mathematical formulation, including its decision variables and scheduling scheme.

5.3. Mathematical model

Previous sections are used to explain the modelling approach, and the model characteristics. This section presents translates the optimization model into the mathematical formulation. The decision variables and parameters description are described in the Nomenclature. In the following sections, first, the decision variables are described. Then the optimization problem is elaborated, and lastly, the constraints, which connect the model to the reality are identified.

The formulated model is categorized as a nonlinear optimization model. To solve the nonlinear problem aroused by the power grid power imbalances, united numerical and nonlinear optimization methods are utilized. For this, the Newton Trust Region (NTR) and Interior Point Nonlinear Programming (IP-NLP) algorithms are utilized. In every iteration, the power imbalances are estimated by iterative methods as delineated by power constraints equations. The suggested method is programmed and optimized in the MATLAB environment using Simulink, whereas the convergence tolerance and the maximum number of iterations are considered as respectively 10^{-6} and 500. The parameters and decision variables are embedded in data frames and matrices. The optimization window considers intervals of 15 minutes for a year. Based on the predicted demand for those same hours, the look-ahead optimization problem determines the scheduling setpoints for upcoming hours. According to this, storage will be set up to meet the anticipated demand from the transportation sector. Data from the NREL is utilized for acquiring the hydrogen demand of the mobility sector. Furthermore, Dutch electricity market data from the Entsoe transparency platform are used for the optimization. This propelled work is operated by the model using a scheduling scheme, where the decision variables are the underlying optimizer of the model, as delineated in the next section.

5.3.1. Operation management scheme and decision variables

Figure 20 visualizes the operation management model for the system described in the previous sections to serve the hydrogen mobility demand, as well as providing ancillary services to the electricity grid. Both case supply chain scenarios are included, which are the distributed and centralized hydrogen supply chain. As illustrated, the corresponding operating parameters are inputted in the model, including grid constraints, hydrogen supply chain specifications, hydrogen demand, and electricity and hydrogen pricing are inputs for the operation. The model also includes ancillary service signals for the provisioning of VAR, DR, and OR, which are provided.

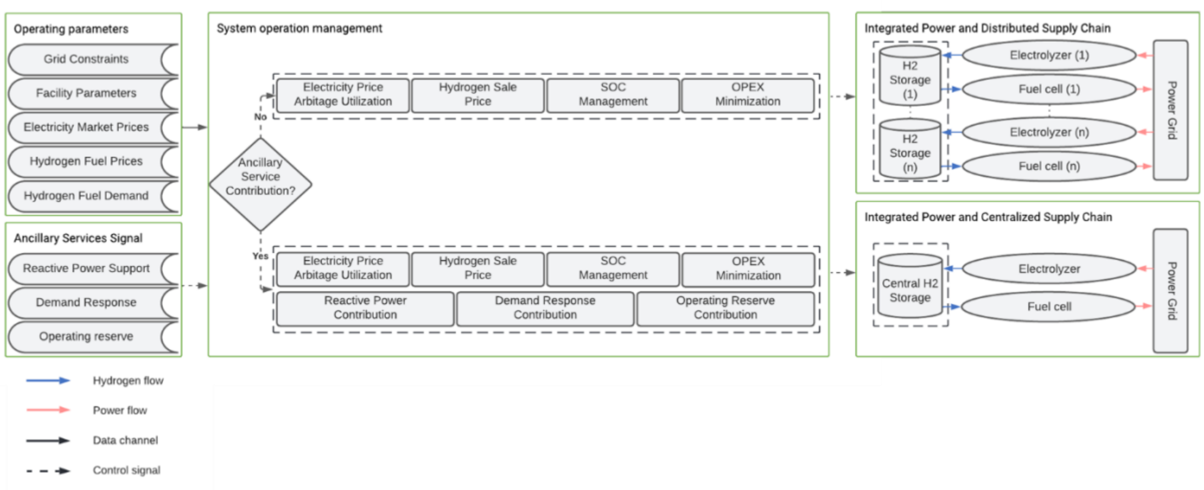

Figure 20. The operating management model of the hydrogen supply chain to serve hydrogen mobility demand, as well as provide ancillary services to the electricity grid.

The model includes two operation manners: with and without the participation of ancillary services. The former manner uses price arbitrage, ensuring fuel supply to the road mobility demand while minimizing the operating expenditure (OPEX), and managing the SoC reserve of hydrogen storage, as well as the participation of different ancillary services. The latter manner does not consider SoC reserve management for ancillary services. Control signals are included in the hydrogen supply chain, which includes the electrolyzer, fuel cell units, and storage, where the energy carrier's hydrogen and electricity are produced for different hydrogen demands and grid ancillary services.

The operation management model determines the optimal values of the decision variables during the optimization process. The main decision variables of the model are the sizes of the model components, such as the size and locations of the wind generation and solar generation units, size of the electrolyzers and fuel cell units, as well as the converter and storage, but above all the dispatch strategy, which includes the hydrogen sold to the mobility demand, as well as the power supplied to the power grid, and the aggregated penalty factors of the ancillary services. The size and location of the components are determined by the mobility demand and the criteria for grid participation.

In the next section, the optimization problem is described, as well as the constraints.

5.3.2. Optimization problem

This section contains the mathematical formulation of the optimization problem. The objective of the optimization problem is to maximize the hydrogen supply chain operational revenue over a predetermined time horizon. The objective function has two key terms, which are revenue and penalty, formulated as:

$$\text{Maximize:} \quad \sum_{t\in\xi} \left(REV_t - \phi_t^{Pen}\right) * \Delta t, \tag{13}$$

where REV_t is the revenue of the hydrogen consumption in the system ($\frac{m^3}{h}$), ϕ_t^{Pen} is the aggregated value of penalty factors (€), and Δt is the time over a period of length. From the optimization model, optimal system configurations will be selected and further evaluated in terms of economic and technical parameters.

The revenue includes (i) the power arbitrage term, established by the volatility of the electricity prices over time, (ii) the hydrogen profit and cost terms derived from selling to the mobility demand, and supply to the fuel cell unit, and (iii) the terms for including external ancillary services into the optimization issue, such as VAR support, DR, and OR signals. The equation including these three terms is specified hereunder.

$$REV_t = \sum_{h\in H} \left(F_{h,t}^{Dmd} - F_{h,t}^{FC}\right) * \Gamma_{h,t}^{H2} + \sum_{h\in\psi} F_{h,t}^{FC} * \Gamma_t^{Elc} + \Gamma^{DR} * \left(P_t^{DR} - P_t^{DR,Slk}\right) + \Gamma^{VAR} * \left|\sum_{h\in\psi} Q_{h,t}^{Elz}\right| + \sum_{h\in H} SoC_t^{OR} * \Gamma^{OR} - \sum_{h\in\psi} P_{h,t}^{Elz,Adj} * \Gamma_t^{Elc} \quad \forall t \in \xi, \tag{14}$$

where $F_{h,t}^{Dmd}$ is the hydrogen demand in mobility sector $\frac{m^3}{h}$, $F_{h,t}^{FC}$ is the hydrogen consumption of the fuel cell unit, and $\Gamma_{h,t}^{H2}$ the hydrogen sale price in the mobility sector $\frac{€}{m^3}$. $F_{h,t}^{FC}$ is the power production of the fuel cell unit (MW), Γ_t^{Elc} is the electricity market price $\frac{€}{m^3}$, Γ^{DR} is the DR service price $\frac{€}{m^3}$, P_t^{DR} the ancillary service DR signal (MW) and $P_t^{DR,Slk}$ the slack variable for DR management (MW), Γ^{VAR} the VAR service price ($\frac{€}{MVAr.h}$), $Q_{h,t}^{Elz}$ the VAR services signal ($MVAr.h$), SoC_t^{OR} the SoC reserve margin for OR support to grid (m^3), Γ^{OR} the OR reserve service availability price ($\frac{€}{MWh}$), $P_{h,t}^{Elz,Adj}$ the adjusted power consumption of the electrolyzer (MW), and Γ_t^{Elc} the electricity market price ($\frac{€}{MWh}$).

The net power utilized by the hydrogen supply chain at each time instant t is provided as:

$$P_{h,t}^{Elz,Adj} = \sum_{h \in \psi} P_{h,t}^{Elz,Adj} + B * P_t^{H+} \; \forall t \in \xi, \qquad (15)$$

where B is a binary variable for the distributed fuel supply (B=0) and centralized supply (B=1), and P_t^{H+} is the additional power required by the supply chain.

The OPEX of the hydrogen supply chain, including the electrolyzer units, transportation, and fuel cell facility is provided as follows:

$$OPEX_t = \left(OP^{Elz} + B * OP^{H+} + B * OP^{H-} + B * OP^{Trp}\right) * \sum_{h \in \psi} F_{h,t}^{Elz} + OP^{FC} * \sum_{h \in \psi} F_{h,t}^{FC} \quad \forall t \in \xi \qquad (16)$$

where the OPEX of the electricity to hydrogen conversion process, $OP^{Elz} * \sum_{h \in \psi} F_{h,t}^{Elz}$ ($\frac{€}{m^3}$), hydrogen first compression, $OP^{H+} * \sum_{h \in \psi}$ in ($\frac{€}{mH2^3}$), hydrogen second compression, $OP^{H-} * \sum_{h \in \psi}$ in ($\frac{€}{mH2^3}$), the transportation from the central facility to hydrogen stations, $OP^{Trp} * \sum_{h \in \psi} F_{h,t}^{Elz}$, and the fuel cell operation, $OP^{FC} * \sum_{h \in \psi} F_{h,t}^{FC}$, are taken into consideration, B is a binary variable for the distributed fuel supply (B=0) and centralized supply (B=1).

The following equation is related to the penalty factor term for ancillary participation management:

$$\phi_t^{Pen} = \phi^{VAR} * \left(Q_t^{VAR,Slk} + Q_t^{VAR,Slk'}\right) + \phi^{DR} * P_t^{DR,Slk} + \phi^{OR} * P_t^{OR,Slk} \; \forall t \in \xi \qquad (17)$$

where ϕ^{VAR} is the penalty factor for VAR service ($\frac{€}{MVAr.h}$), $Q_t^{VAR,Slk}$ the slack variable for management of electrolyzer VAR ($MVAr$), $Q_t^{VAR,Slk'}$ the slack variable for management of electrolyzer VAR ($MVAr$), ϕ^{DR} the penalty factor for DR service ($\frac{€}{MWh}$), $P_t^{DR,Slk}$ the slack variable for DR management (MW), ϕ^{OR} the penalty factor for OR service ($\frac{€}{MWh}$), $P_t^{OR,Slk}$ the slack variable for management of OR signal (MW).

The penalty factors in Equation 5 would penalize non-zero values of the slack variables in the objective function, ensuring that they only assume non-zero values when needed to alter the ancillary services signals. Slack variables with non-zero values lead to higher cost of the optimization problem. Because the objective function strives to maximize profit, slack variables are assigned zero values until they need to be adjusted.

5.3.3.Constraints

This section presents the constraints of the optimization problem. The constraints are divided per component of the system, which are the electrolyzer, fuel cell, storage, power grid ancillary services, and power grid.

5.3.3.1. Electrolyzer constraints

The generation of hydrogen by the PEM electrolyzer include a fast response rate, an increased efficiency between 65 and 75 percent, and a low minimum loading capability between 0 and 10 percent. This process uses 571.6 kJ to produce two moles, this reaction is specified below:

$$2H_2O \rightarrow 2H_2 + O_2 \Delta H = +571.6\, kJ. \quad (18)$$

The following equations show the hydrogen generation flow in the electrolyzer unit as a function of its power input and power constraints:

$$F_{h,t}^{Elz} = \xi^{Elz} * \eta^{Elz} * P_{h,t}^{Elz} \quad \forall t \in T \wedge \forall h \in H \quad (19)$$

$$P_h^{min} \leq P_{h,t}^{Elz} \leq P_h^{max} \quad \forall t \in T \wedge \forall h \in H \quad (20)$$

where ξ^{Elz} is the power-to-hydrogen conversion factor ($\frac{m^3}{MWh}$), and η^{Elz} resembles the efficiency of the electrolyzer (%). P_h^{min} and P_h^{max} are the minimum and maximum power of the electrolyzer (MW).

5.3.3.2. Fuel cell constraints

The power generation of the fuel cell depends on the amount of hydrogen which flows in, as enumerated by:

$$P_{h,t}^{FC} = \xi^{FC} * \eta^{FC} * P_{h,t}^{FC} * \frac{\eta^{H-,H+}}{\xi^{H}} \; \forall t \in \xi \wedge \forall h \in \mathcal{H} \quad (21)$$

$$P_{h}^{min} \leq P_{h,t}^{FC} \leq P_{h}^{max} \; \forall t \in \xi \wedge \forall h \in \mathcal{H} \quad (22)$$

Where $\frac{\eta^{H-,H+}}{\xi^{H}}$ is relevant for the compression and transportation. ξ^{FC} is the hydrogen-to-power conversion factor ($\frac{m^3}{MWh}$), and η^{Elz} the efficiency of the fuel cell unit (%). P_{h}^{min} and P_{h}^{max} are the minimum and maximum power of the fuel cell unit (MW).

5.3.3.3. Storage constraints

The energy balance of the hydrogen storage SoC is required, which is given in:

$$SoC_{h,t} = SoC_{h,(t-1)} + \left(P_{h,t}^{Elz} - P_{h,t}^{Dmd} - F_{h,t}^{FC} - \eta^{Dsp} * SoC_{h,t}\right) * \Delta t \; \forall t \in \xi \wedge \forall h \in \mathcal{H} \quad (23)$$

$$SoC_{h,t} = SoC_{h,(t-1)} + (\xi^{H+} * \eta^{H+} * F_{h,t}^{Elz} - F_{h,t}^{Dmd} - \frac{\xi^{H-}}{\eta^{H-}} * F_{h,t}^{FC} - \eta^{Dsp} * SoC_{h,t}) * \Delta t \; \forall t \in \xi \wedge \forall h \in \mathcal{H} \quad (24)$$

where the electrolyzer usage, compression and transportation consumption, fuel cell usage, and energy losses are taken into account. Furthermore, the parameters $\xi^{H+} * \eta^{H+}$ and $\frac{\xi^{H-}}{\eta^{H-}}$ account for the compression and transportation processes, with compression occurring at local sites, such as the refuelling stations for the mobility sector.

The SoC of the storage and its constraint is given as:

$$\sum_{h\in\psi} SoC_{h}^{min} + (1 - M_{t}^{VAR}) * SoC_{t}^{Var} + (1 - M_{t}^{DR}) * SoC_{t}^{DR} + (1 - M_{t}^{OR}) * SoC_{t}^{OR} \leq \sum_{h\in\psi} SoC_{h,t} \leq \sum_{h\in\psi} SoC_{h}^{max} \; \forall t \in \xi \quad (25)$$

where the reserve capacity for providing VAR, DR, and OR support is included in the lower bound. When the market issues an ancillary service signal for the provisioning of ancillary services, sufficient reserve capacity is provided for the contribution for that service.

5.3.3.4. Hydrogen compression and transportation constraints

Hydrogen transportation through pipelines and trucks is considered in this thesis. In this section, the constraints involved for the hydrogen transportation via pipelines and trucks is described. The exchange of hydrogen fuel via pipeline I from zone x-y, which indicate the different pipelines from the centralized hydrogen production facility to the dispersing facilities, is divided into two parts: hydrogen delivery ($H_{x\rightarrow y,i,T}^{Pip-}$) and outflow ($H_{x\rightarrow y,i,T}^{Pip+}$), given as:

$$H_{x\rightarrow y,i,T}^{Pip+} = H_{x\rightarrow y,i,T}^{Pip+} - H_{x\rightarrow y,i,T}^{Pip-} \;\; \forall x \rightarrow y \in \; p, i \;\wedge\; i, T \in \; t \qquad (26)$$

where the operation limitations are limited by the hydrogen produced from the electrolyzer, as well as the operating pressures for the hydrogen mobility demand, given as:

$$0 \leq \; H_{h,t}^{fill} \leq C^{pip}, 0 \leq \; H_{h,t}^{unfill} \;\; \forall x \rightarrow y \in \; p, i \;\wedge\; i, T \in \; t \qquad (27)$$

where $H_{h,t}^{fill}$ and $H_{h,t}^{unfill}$ are the amount of hydrogen retrieved and supplied by pipelines at zone x with respect to the capacity of the pipelines C^{pip} to the refuelling stations.

5.3.3.5. Power grid ancillary services

The following constraint is used to conduct and control the contribution to the VAR market as an additional service to the grid:

$$\sum_{h\in\psi} Q_{h,t}^{Elz} = \; Q_t^{VAR} + \; Q_t^{VAR,Slk} - \; Q_t^{VAR,Slk'} \;\forall\; M_t^{VAR} = 1 \;\forall t \in \; \xi \qquad (28)$$

where

$$0 \; \leq \; Q_t^{VAR,Slk}, Q_t^{VAR,Slk'} \; \leq \; Q_t^{VAR} \;\; \wedge \; \forall t \in \; \xi \qquad (29)$$

The slack variables $Q_t^{VAR,Slk'}$ and $Q_t^{VAR,Slk}$ generates soft constraints to ensure VAR contribution according to the propounded optimization issue. While $Q_t^{VAR,Slk}$ enables a larger contribution to VAR signals, $Q_t^{VAR,Slk'}$ would permit a reduction of VAR contributions. The slack variables, as depicted in equation 23, would reproduce fictional VAR support signals and implement the signal to guarantee the viability and convergence of the optimization problem.

In addition to the VAR signals, the facility is controlled to contribute to the DR program according to the following constraints:

$$\sum_{h \in \psi} Q_{h,t}^{Elz,Addj} \leq P_t^{DR} + P_t^{DR,Slk} + P_t^{DR,Slk'} \; \forall \, M_t^{DR} = 1 \; \forall t \in \xi \qquad (30)$$

where

$$0 \leq P_t^{DR,Slk} \leq P_{max}^{Elz} - P_t^{DR} \;\wedge\; \forall t \in \xi \qquad (31)$$

The DR signal sent by the market limits the absorbed power by the electrolyzer unit in equation 18. Furthermore, the slack variable which works as a fictional DR signal, enables for the control of DR provisioning and the viability of the optimization problem by introducing soft constraints.

The contribution of fuel cell units to the OR market is determined using the given constraints:

$$\sum_{h \in \psi} P_t^{FC} = P_t^{OR} - P_t^{OR,Slk} \;\wedge\; M_t^{OR} = 1 \; \forall t \in \xi \qquad (32)$$

$$P_t^{OR,Slk} \leq P_t^{OR} \;\wedge\; \forall t \in \xi \qquad (33)$$

where the slack variable is a fictional OR signal that is used to regulate the OR contribution of the fuel cell units and allow the optimization problem to converge if the facility is unable to completely follow the market signal.

5.3.3.6. Power grid constraints

The power system model is limited by the flow through the lines, as well as the voltage limits of the buses, and the active and reactive power imbalance equations, given as:

$$P_{b,t} \leq P_{b,max} \;\; \forall t \in \xi \wedge \forall b \in \beta \qquad (34)$$

$$V_{b,min} \leq V_{b,t} \leq V_{b,max} \;\; \forall t \in \xi \wedge \forall b \in \beta \qquad (35)$$

$$P_{b,t} = V_{b,t} \sum_{b' \in \mathfrak{H}} (V_{b',t} * Y_{bb'} * Cos(\delta_b - \delta_{b'} - \theta_{bb'})) \;\; \forall t \in \xi \wedge \forall b \in \beta \qquad (36)$$

$$Q_{b,t} = V_{b,t} \sum_{b' \in \mathfrak{H}} (V_{b',t} * Y_{bb'} * Sin(\delta_b - \delta_{b'} - \theta_{bb'})) \;\; \forall t \in \xi \wedge \forall b \in \beta \qquad (37)$$

where $P_{b,t}$ is the active power injected to power system buses (MW), $P_{b,max}$ the maximum power at the power system branches (MW), $V_{b,min}$ the voltage of the power system buses (pu), $V_{b,t}$the minimum voltage at power system buses (pu), $V_{b,max}$ the maximum voltage at power system buses (pu), $Y_{bb'}$the admittance magnitude between buses (pu), δ_b the voltage angle at power system buses (Rad), and $Q_{b,t}$ the reactive power injected to power system buses (MVAr).

The power grid model is taken into account when performing the optimization algorithm by either a power grid operator or a private owner to carry out the techno-economic and grid impact analysis, while assuring the fulfilment of the grid limitations. Despite of the fact that the model is simulated in real time, the hydrogen supply chain operator (owner of the storage and fuelling station) simply receives ancillary service signals from the grid operator, hence the grid constraints in the optimization model are not considered.

5.4. Model testing

After describing the model, the model should be addressed through verification and validation to test the accuracy and credibility of the model. In the first subsection, the verification process will be presented. The second subsection describes the validation of the model. Subsequently, the sensitivity analysis variations are presented to describe the effect of the new information or changes on the model outcomes.

5.4.1. Verification

In this subsection, the verification process is elaborated. During this process, the model approach is tested to ensure that the process is conducted correctly regarding the conceptual model. This means that the specifications and assumptions are in accordance with the given objective. There are several methods to verify a model, such as using the expertise of experts, the creation of logic flow diagrams, the use an interactive debugger, or the investigation of the model output for reasonableness under various input parameters values (Banks, 2010). The latter is utilized in this thesis to verify the expected outcomes, as delineated below:

- If the investment costs or operating costs in the system increases, the breakeven time also increases.
- If the efficiencies of the components are increased, the power consumption decreases.
- The breakeven time is reduced due to extra financial profit.
- Hydrogen consumption is increased when more ancillary services contributions are provided.
- If the hydrogen consumption is higher, the power consumption of the electrolyzer increases.
- The hydrogen storage SoC get depleted faster when the system is providing ancillary services to the mobility demand and to the power grid.

- If the electricity prices are higher, the cost of the system are higher, which leads to a lower profitability.
- If the electrolyzer uses power, the hydrogen storage SoC get higher.
- If the electricity prices are lower, the electrolyzer produces more hydrogen.
- If there is abundant capacity in the hydrogen storage, VAR Signals can be supported.
- If there is abundant capacity in the hydrogen storage, DR Signals can be supported.
- If there is abundant capacity in the hydrogen storage, OR Signals can be supported.
- Comparing the electrical power losses under the various cases, the operation of only the grid has the lowest losses, then the operation of the grid and the electrolyzer, and lastly, the losses are the highest when joint applications, serving the mobility demand and providing ancillary services, are added.

5.4.2. Validation

Besides the verification, in which the optimization model is correctly translated into computer languages, the model should also represent the reality and the purposes of the thesis. Therefore, in this section, the validation process is described in which the model results are compared to real energy systems or other studies. However, since the research is relatively new and not introduced in real systems yet, the results are mostly compared to similar studies from literature.

5.4.3. Sensitivity analysis

The experimental designs are implemented to investigate the effect of process variables on the process output, as well as the relationships between those variables. As mentioned before, the viability of hydrogen generation and storage facilities depends on electricity prices. This is because the electricity prices determine the actual hydrogen generation price, and thus, the hydrogen selling price. Therefore, the electricity prices will be varied. Three scenarios will be considered, a low electricity price scenario, in which the price is set at 50%, a mid-electricity price scenario where the original price pattern is used, and a high electricity price scenario, in which the price is set at 150%, as depicted in Figure 21.

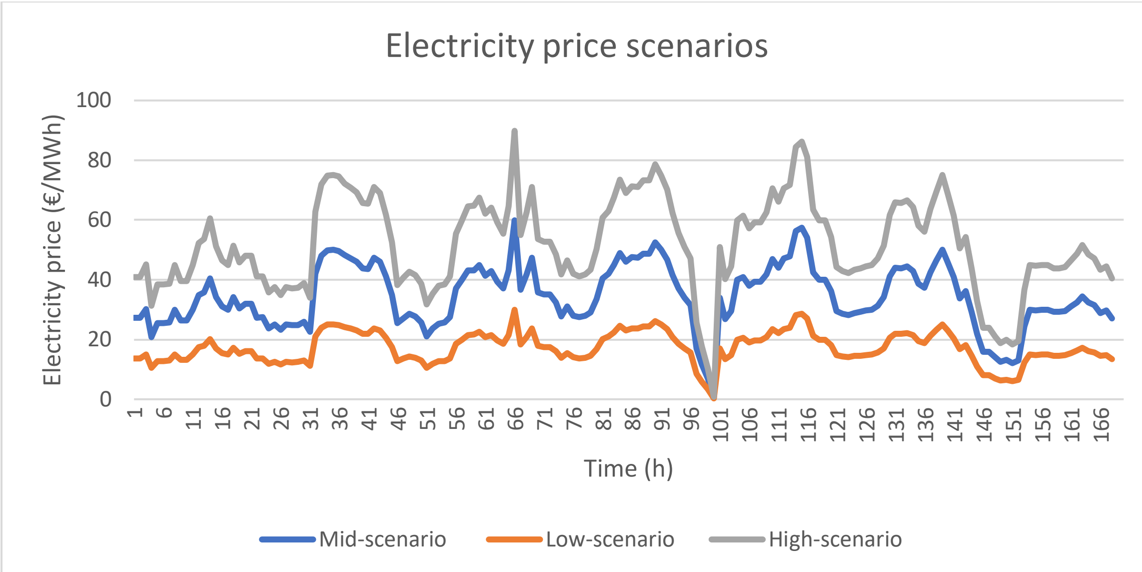

Figure 21. Electricity price scenarios: Low-scenario (50%), Mid-scenario (100%), High-scenario (150%).

Furthermore, the hydrogen sales price influences the profitability of selling the hydrogen to the transportation market and possibly also changes the operation management of the system. Similarly to the hydrogen sales price, the aggregated value of penalty factors of the ancillary services also influence the total revenue and the operation of the system. Because of this, the aggregated value of penalty factors, and the fixed price of the ancillary services, as well as the capacity of the ancillary service signals, are varied to see the influence on the operation and the viability of the system. For the aggregated value of the penalty factors and the price of the ancillary services, similar price scenario variations as the electricity prices are considered, which means that the values of the penalty factors are set to 50%, 100% and 150%. For the capacity of the ancillary services, a 30% decrease, a 15% decrease, a 15% increase, and 30% increase variations are taken into account.

Lastly, the costs of the components are likely to reduce significantly. This will influence the viability of hydrogen systems. Therefore, different cost scenarios are considered in this thesis. The scenarios are subtracted from the cost's expectations from five big different research organizations, which are H2Counsil, E3/UCI, IRENA, BNEF, and energy government (DOE, 2020). From this, the average costs for 2025 and 2040 from these organizations are given into the model.

5.5. Economic evaluation

To economically evaluate the different case scenarios, several parameters have been selected. These parameters include gross income (GI), net income (NI), net present value (NPV), break even time (BET), internal rate of return (IRR) and profitability are used to compare the scenarios. These parameters are described as follows:

Gross income (G) is the total income of the system, given as:

$$Gross\ income = Total\ sales\ (revenue) - Total\ cost\ of goods, \qquad (38)$$

net income (NI) is the total revenue of the system minus the expenses of the system, given as:

$$Net\ income = \ Total\ revenue - Total\ expenses, \qquad (39)$$

Net Present Value (NPV) is a term used to analyse the profitability of a project by expressing the difference between the present value of cash inflows and outflows over a certain time horizon, which is defined as:

$$NPV = \ \sum_{t=o}^{n} \frac{CF_t}{(1+r)^t}, \qquad (40)$$

where t is the time of the cash flow, I the discount rate of x, CF_t the net cash flow, which is calculated by subtracting the outbound cash from inbound cash. The **break-even time (**BET), which is the time required to equalize the cash flows to its initial cost of the project, formulated as:

$$Break\ even\ time = \frac{Fixed\ costs}{Total\ sales\ revenue - Cost\ to\ supply\ product}, \qquad (41)$$

the **internal rate of return** (IRR) is a metric to evaluate the profitability of investments, given as:

$$IRR = \ \sum_{t-1}^{t} \frac{C_t}{(1+r)^t} - C_0\ (\text{al.}, 2017), \qquad (42)$$

where C_t is the net cash inflow during the period, r the discount rate of x, t the number of time periods, and C_0 the total initial investment cost. Lastly, the **profitability**, where it is a measure of attractiveness for the investor of the project, given as:

$$Profitability = \frac{Present\ Value\ of\ future\ cash\ flows}{Initial\ investment}. \qquad (43)$$

6. Results

In this chapter, the experimental results are presented for both scenarios under various operating conditions. The first section delineates the results from the operation of the distributed and centralized supply chain systems without ancillary support to the power grid, in Section 6.2, the operation of the distributed and centralized supply chain systems with ancillary service support to the power grid are elaborated. Subsequently, the economic evaluation of both scenarios is described, followed by the system losses for both scenarios. Lastly, the results of the sensitivity analysis are presented.

6.1. Operation of both supply chains without ancillary support to power grid

This section illustrates the results for the distributed and centralized hydrogen generation and storage supply chain systems obtained from the operating manner when the power grid involves no ancillary services signals provisioning. This operation utilizes lower market prices for hydrogen generation in order to meet the projected hydrogen demand. First, the results from the operation of the distributed hydrogen supply chain system without ancillary service support to the power grid will be presented. Then, the operation of the centralized hydrogen supply chain system without ancillary services support will be highlighted, whereafter a comparison of the results for both scenarios is given.

6.1.1. Distributed hydrogen supply chain

This subsection delineates the results of the distributed hydrogen supply chain system under the operating manner when the power grid involves no ancillary services signals provisioning. Figure 22 display the electrolyzer consumption and the electricity market prices for the same week of the year. As depicted in the figure, the electrolyzer is operated more power during lower electricity prices, which indicates that the system uses the price volatility to increase the revenue while meeting the projected hydrogen demand. Figure 23 depicts the power consumption of the electrolyzer and the SoC of hydrogen storage. The results indicate the proposed model is capable of optimally managing the SoC of hydrogen storage in a way that avoids operating the electrolyzer during periods of higher power prices while satisfying the demand of the hydrogen fuelling stations.

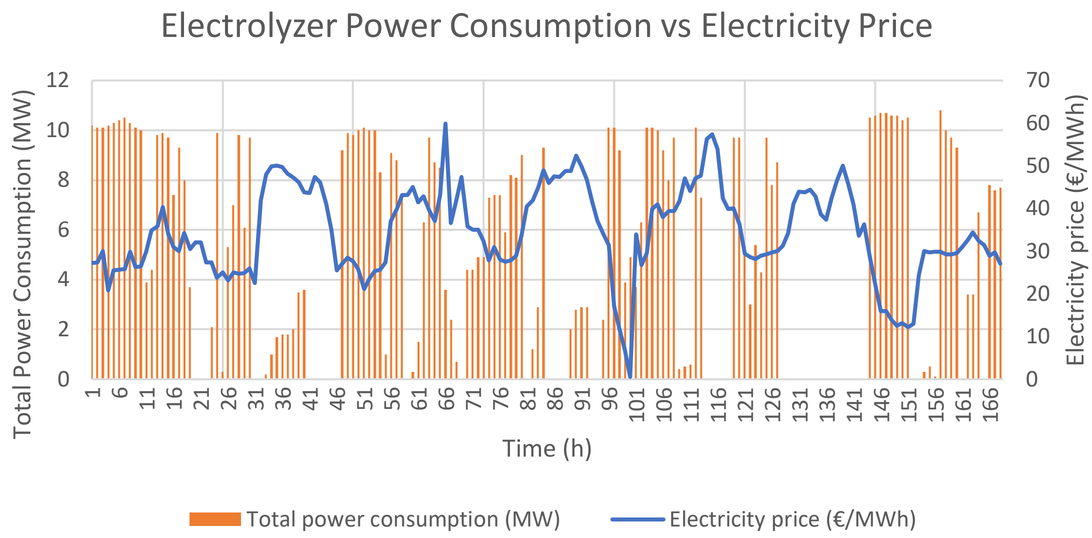

Figure 22. Total Power Consumption and Electricity prices vs Time.

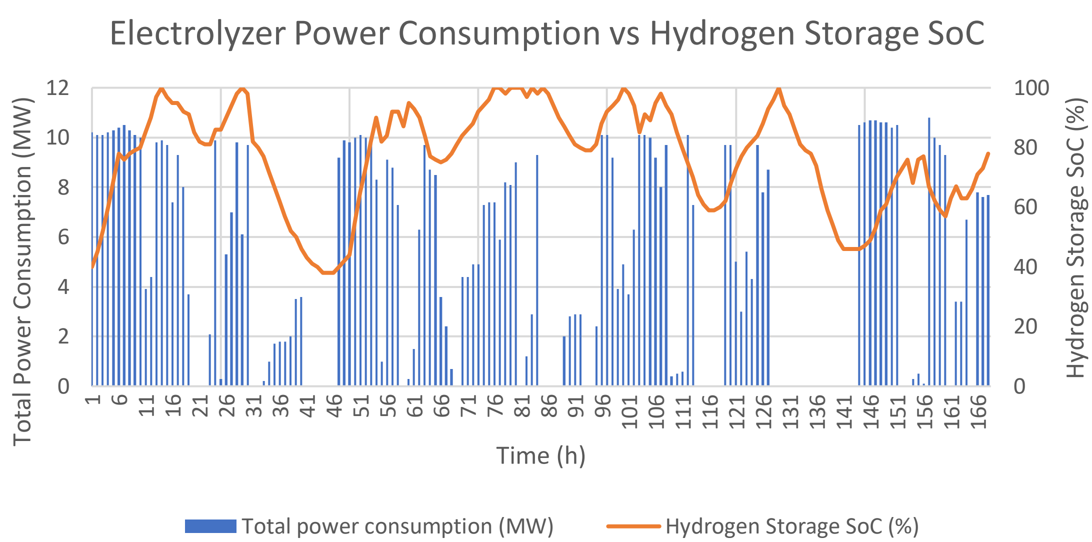

Figure 23. Total Power Consumption and Hydrogen Storage SoC vs Time.

6.1.2. Centralized hydrogen supply chain

Figure 24 and 25 demonstrates the optimal operation of the hydrogen generation and storage systems based on the hydrogen demand, electricity price profiles and hydrogen storage SoC. As indicated in figure 24, the electrolyzer uses lower electricity prices for the generation of hydrogen for the supply to the mobility demand. Furthermore, Figure 25 displays that the hydrogen storage SoC can be controlled in a way that it can satisfy the future demand of the mobility sector.

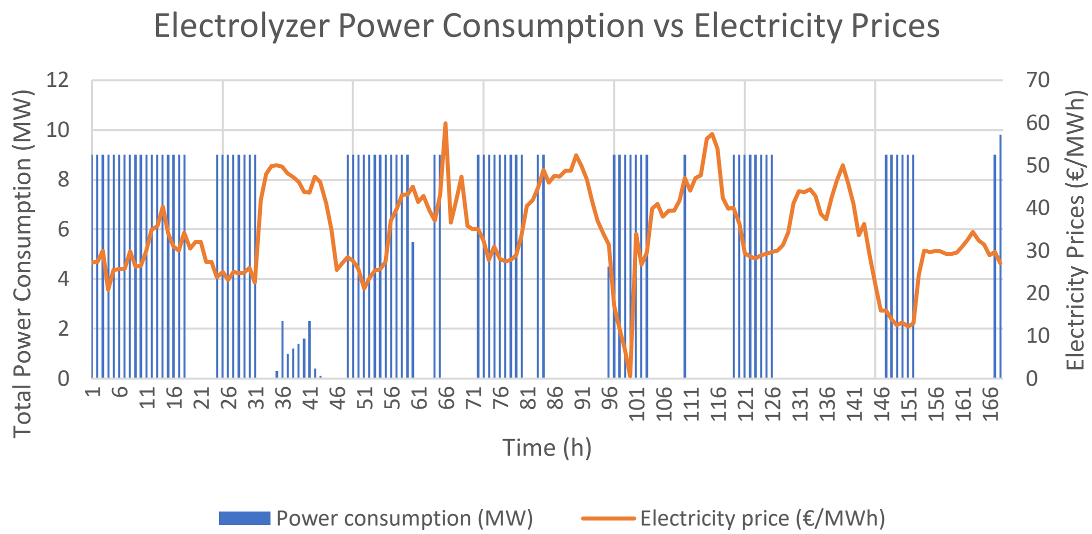

Figure 24. Electrolyzer Power Consumption and Electricity Prices vs Time.

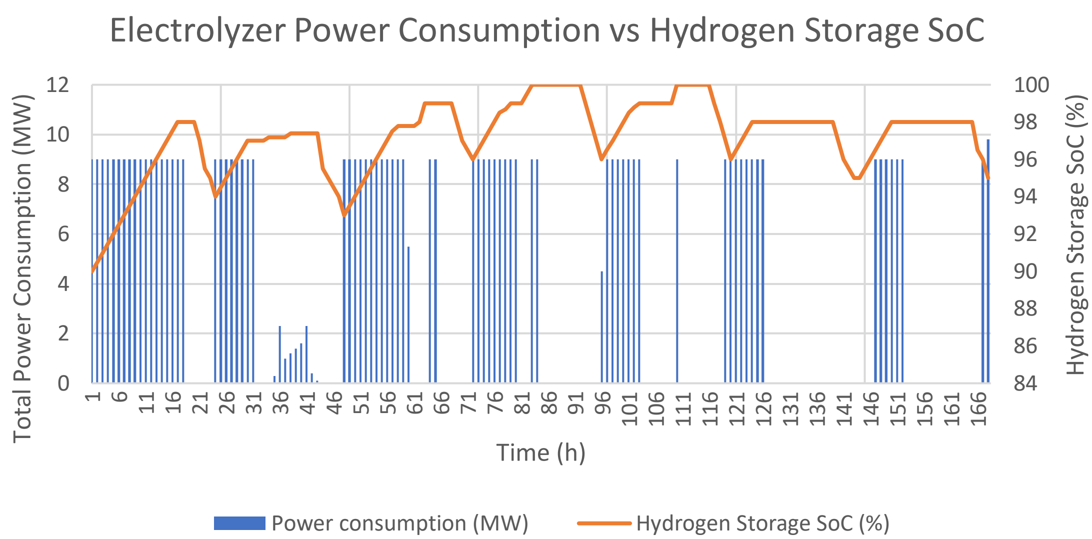

Figure 25. Electrolyzer Power Consumption and Hydrogen Storage SoC vs Time.

6.1.3. Comparison between distributed and centralized supply chain

This subsection evaluates the results of the distributed and centralized supply chain systems under the operation condition without ancillary services support. It is observed that both systems are able to satisfy the mobility demand while using the volatility of the electricity price. However, the main difference between both scenarios is that the electrolyzer power consumption of the distributed supply chain system is more volatile than the power consumption of the centralized supply chain system. Similarly, the hydrogen storage SoC pattern of the distributed supply chain system is more volatile than the centralized supply chain system. This is due to the ability to react on the hydrogen demand: where the centralized supply chain system has to regulate the supply to the mobility sector with one centralized stacked electrolyzer, the distributed supply chain system can react with six smaller electrolyzers. Furthermore, it is observed that the total electrolyzer power consumption for the centralized supply chain is lower than the power consumption of the distributed supply chain system. This indicates that the centralized supply chain system uses less power to satisfy the mobility demand.

6.2. Operation of both supply chains with ancillary service support to power grid

This section presents the results of the distributed and centralized hydrogen generation and storage supply chain systems where the hydrogen production and storage facilities provide ancillary services while also meeting the demand of the mobility sector. The ancillary service signals are created with respect to a 15 minutes-based time interval from the general operation criteria of the ancillary services patterns from the IESO. However, the primary function is to satisfy the mobility demand, whereas the supply chain systems can generate more revenue by providing ancillary services. First, the results from the operation of the distributed hydrogen supply chain system with ancillary service support to the power grid will be presented. Then, the operation of the centralized hydrogen supply chain system with ancillary services support will be highlighted, whereafter a comparison of the results of both scenarios is given.

6.2.1. Distributed hydrogen supply chain

This subsection delineates the results of the distributed hydrogen supply chain system under the operating manner when the power grid involves ancillary services signals provisioning. Figure 26 visualizes the power grid with VAR signal support, which characterizes the electrolyzer electric demand, as well as the VAR signals directed to the distributed hydrogen supply chain by the power grid operator. The results show that the power consumption gets depleted faster when the supply chain runs near optimal to its estimated value while aiding the electric grid by offering sufficient VAR signals. After the clearance of VAR signals, the electrolyzer power utilization is recommended at former levels or higher levels.

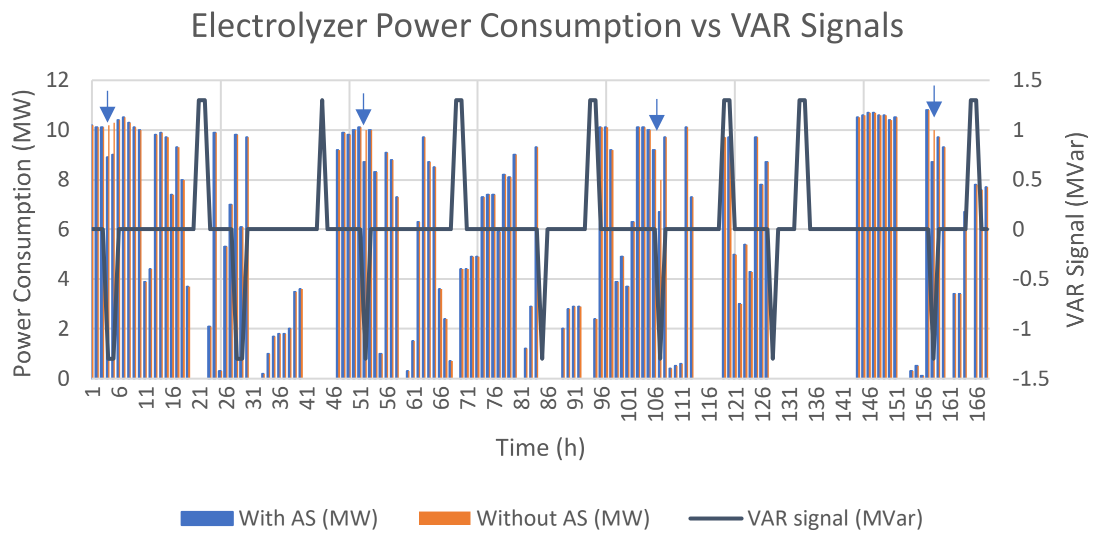

Figure 26. Electrolyzer Power Consumption and VAR Signals vs Time.

The power consumption of fuel cells during adopting the ancillary service OR are depicted in Figure 27. The results indicate that the distributed hydrogen supply chain can completely support the OR signals. This means that sufficient storage capacity was available, and additionally, it was beneficial for the system to provide OR instead of providing other services. It also indicates that the cost of delivering OR is lower than the potential benefits of providing ancillary services.

Figure 28 displays the results from the contributions to the DR response signals and the effect on the electrolyzer power consumption. As the results show, the model alternates the demand for power with respect to the DR signals. This indicates that it is economically beneficial to decrease the overall power consumption of the hydrogen generation and storage system in times of peak moments.

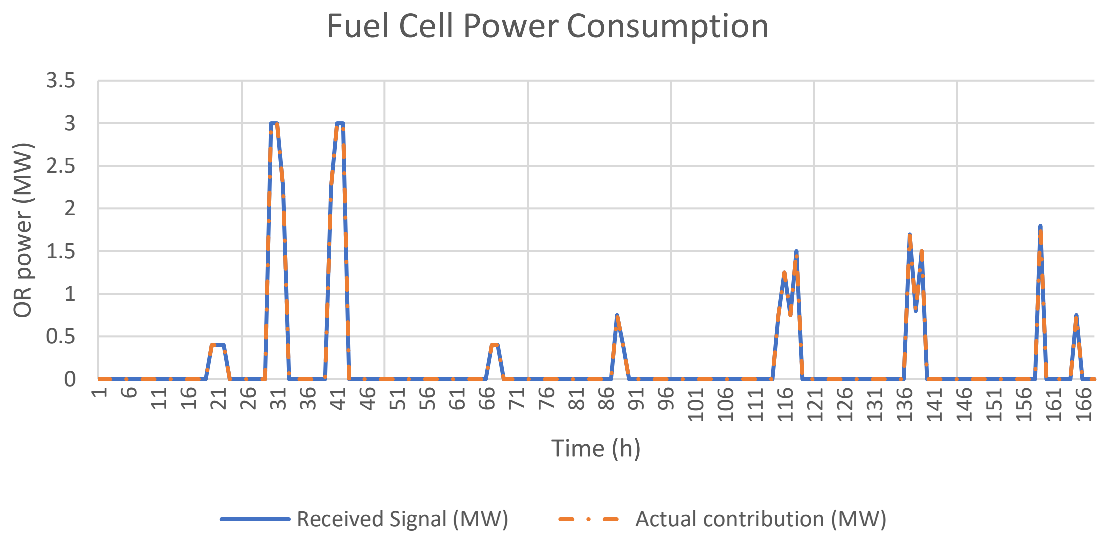

Figure 27. Received OR Signals and Actual Contribution vs Time.

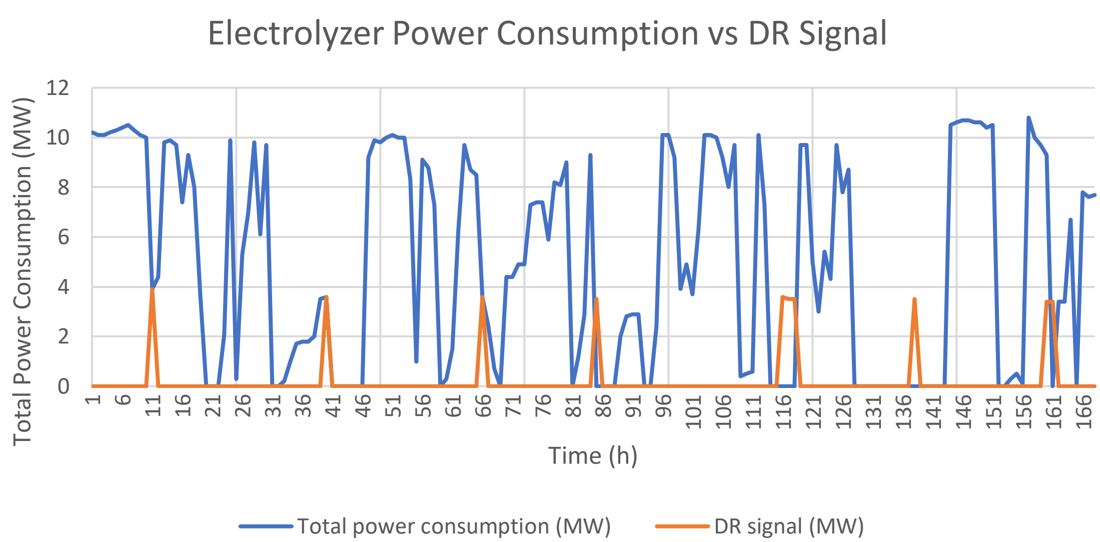

Figure 28. Electrolyzer Power Consumption and DR Signal vs Time.

Figure 29 demonstrates that the stored hydrogen gets depleted faster when ancillary services are provided. This is due to the higher hydrogen demand, which could, in turn, cause a higher power consumption trend to produce more hydrogen, as shown in Figure 30. This indicates that the optimal operation of the supply chain including balancing services can offer more economical benefits without considering lower electricity price tracks. It can therefore also be concluded that more potential can be observed, which may be constrained by the limiting capacities of the system.

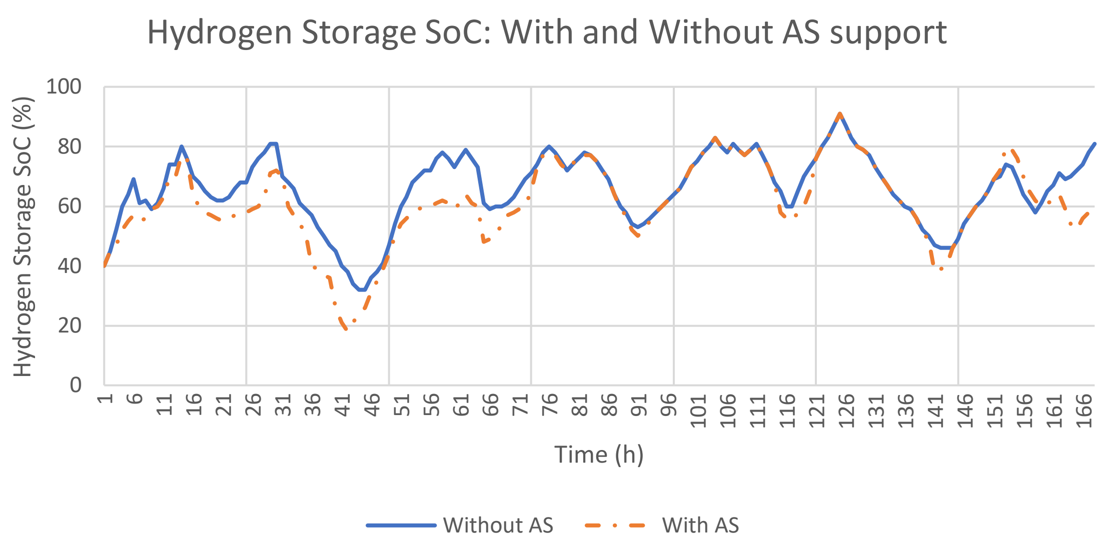

Figure 29. Hydrogen Storage SoC under various operating conditions vs Time.

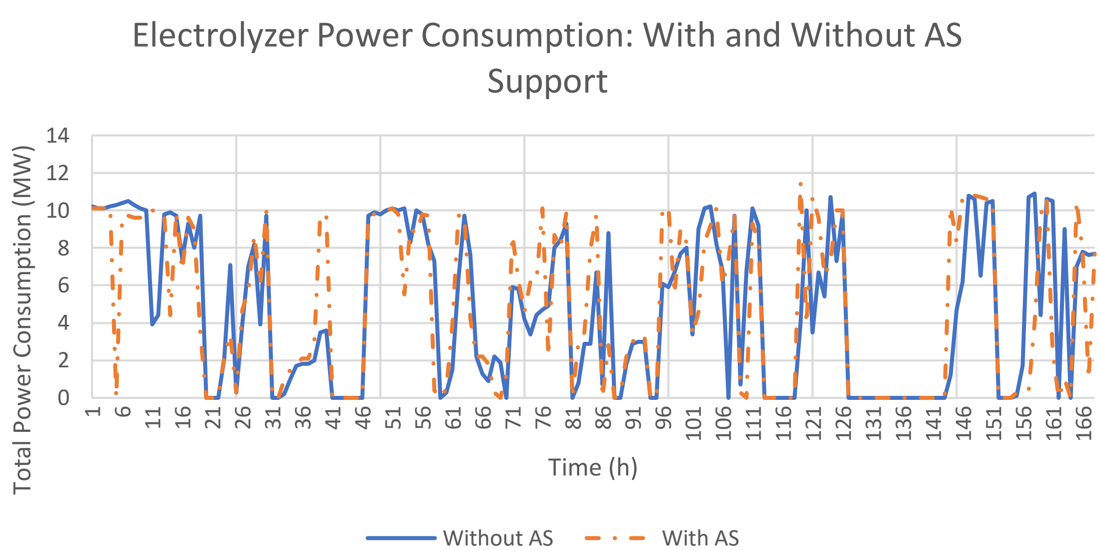

Figure 30. Electrolyzer Power Consumption under various operating conditions vs Time.

6.2.2. Centralized hydrogen supply chain

This section shows the model results of the centralized supply chain system, in which the model is planned for multiple ancillary services in conjunction with the use of lower power market pricing to satisfy hydrogen demand. The ancillary service signal provided by the energy grid operator is similar to the signals issued in section 6.1.2, whereas the magnitudes are altered corresponding to the centralized supply chain system ratings. Figure 31 and 32 demonstrates the electrolyzer power consumption based on VAR and DR ancillary services signals. The figures show that the optimal operation of the electrolyzer power changes when varying the operation requirements as a result of the provided ancillary service signals. From this, it can be observed that the provisioning of ancillary services to the VAR and DR market can be beneficial based on the respective costs and other potential revenues.

Figure 33 illustrates the fuel cell consumption based on the OR signals. The results indicate that the centralized hydrogen generation and storage system can satisfy all the OR signals of the grid.

Furthermore, Figure 34 and 35 displays how the hydrogen storage SoC and power consumption of the electrolyzer alter when the centralized hydrogen generation and storage supply chain system is used to provide multiple ancillary services rather than only producing hydrogen fuel for the mobility demand. The figure indicates a similar trend to the services of the distributed supply chain system, resulting in the hydrogen storage depleting quicker because of the ancillary service provisioning to the grid. This causes an increase in hydrogen generation to counterbalance these lower levels. Moreover, this indicates that the provisioning of the ancillary services has a positive effect on the systems consumption. The pattern of the storage SoC also indicates that sufficient hydrogen is available at any times.

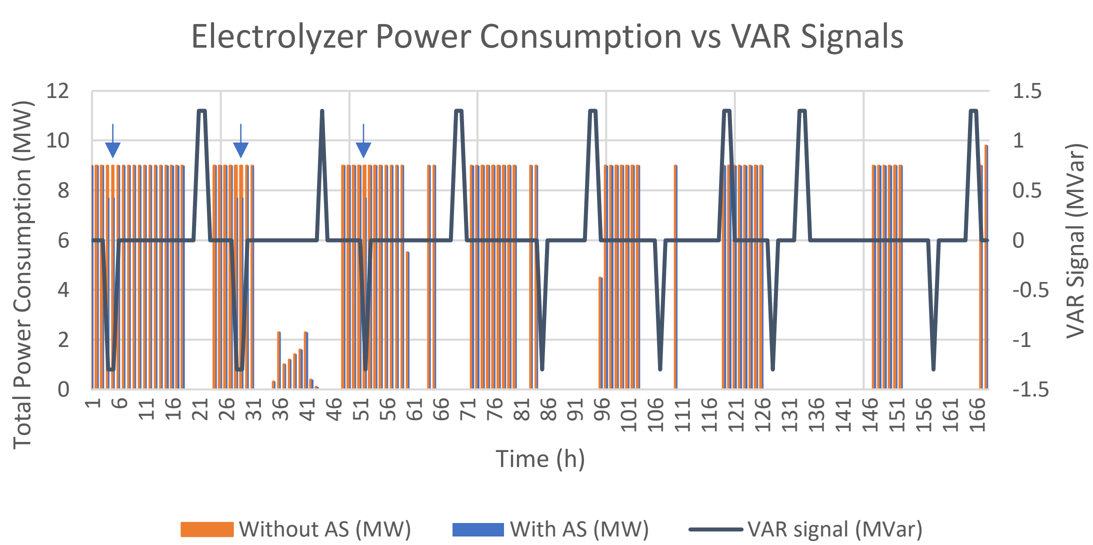

Figure 31.Electrolyzer Power Consumption and VAR Signals vs Time.

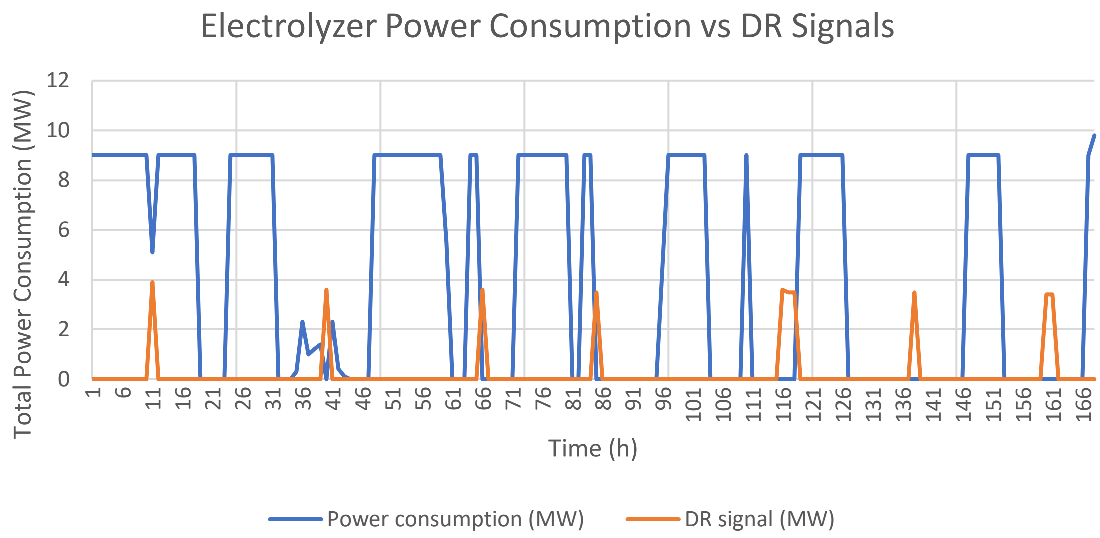

Figure 32. Electrolyzer Power Consumption and DR Signals vs Time.

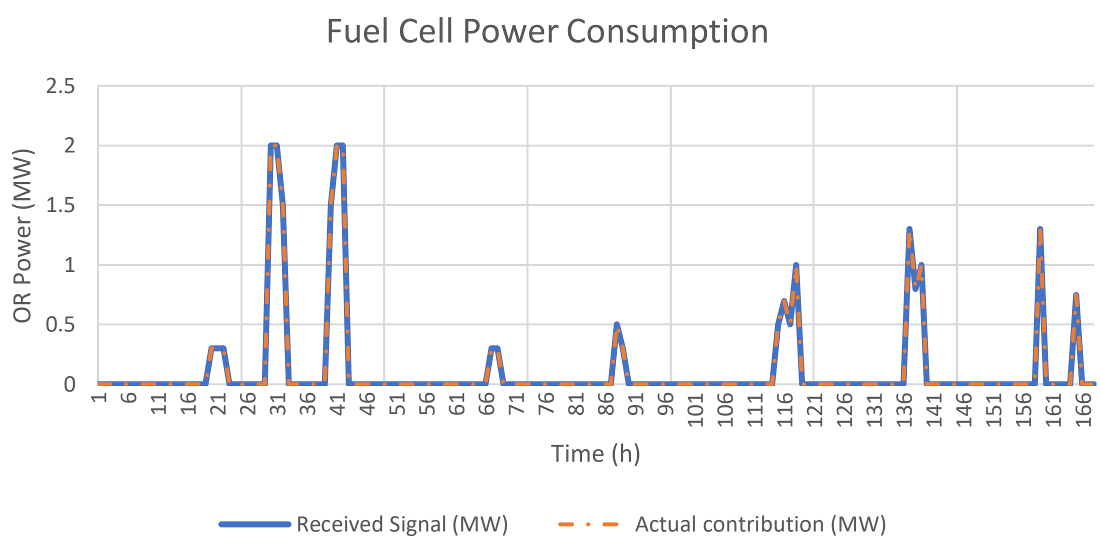

Figure 33. Received OR Signals and Actual Contribution vs Time.

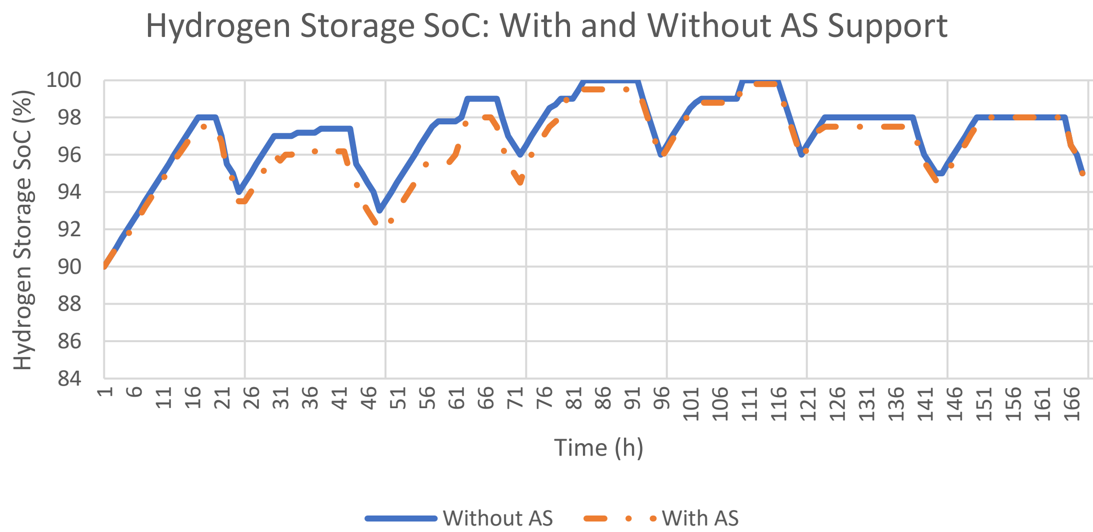

Figure 34. Hydrogen Storage SoC under various operating conditions vs Time.

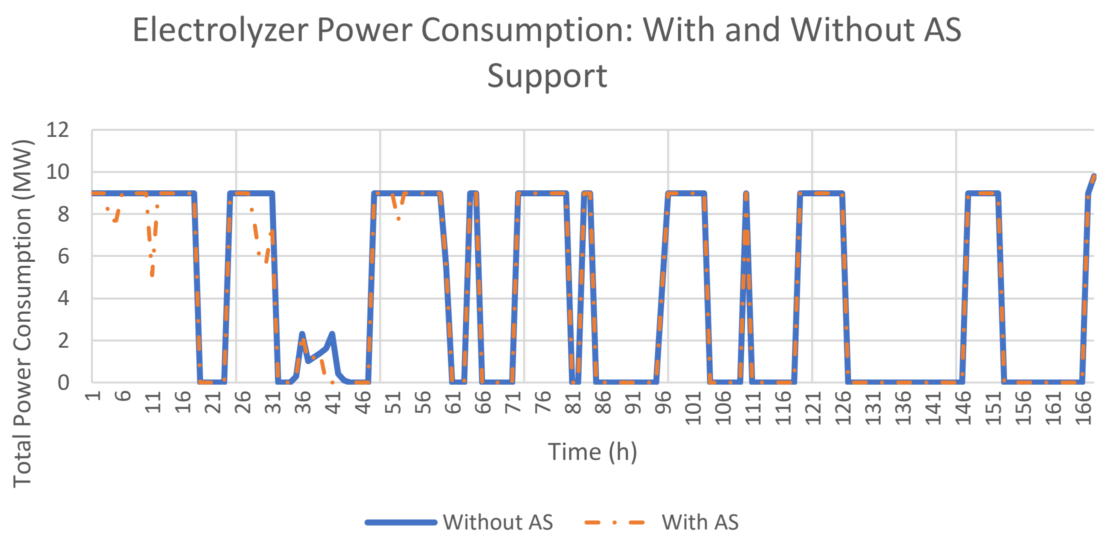

Figure 35. Electrolyzer Power Consumption under various operating conditions vs Time.

6.2.3. Comparison between decentralized and centralized hydrogen supply chains

This subsection evaluates the results of the distributed and centralized supply chain systems under the operation condition where the system provides ancillary service support to the power grid. Both supply chain systems indicate similar trends based on the contribution to the power grid. It is observed the provisioning of ancillary services is more beneficial for the system than providing other services at certain moments. This is because the ancillary services provide better economic performances for the system through providing ancillary service support to the grid. However, some differences exist for given week. The first difference is that the distributed supply chain can abide five of the provided the VAR signals in the given week, while the centralized system is only able to abide three of the provided VAR signals. Similarly, the distributed supply chain system can follow the DR signals for four times in the given week, while the centralized supply chain can follow the signals for only two times. This is due to the electrolyzer power consumption regarding the mobility demand. However, since the demand patterns are slightly modified each week model the anticipated demand of the future for all fuelling stations, it is more likely to be a coincidence. Considering the OR signals, the contribution trend is similar for the distributed and centralized supply chain systems.

Furthermore, the comparison of the electrolyzer power consumption and Hydrogen Storage SoC considering support to the power grid and without for both centralized and distributed supply chains indicate that the stored hydrogen gets depleted faster when the supply chain provides ancillary service signals to the grid. Hence, a similar trend exists regarding the production of more hydrogen. Moreover, it is observed that the optimal management of the operation results does not coincide with times of lower electricity prices, given that the contribution of ancillary services is more beneficial. However, a similar pattern as in Section 6.1.3 of the electrolyzer power consumption and hydrogen storage SoC is observed, whereas the power consumption and hydrogen storage SoC centralized supply chain is less volatile than for the distributed supply chain. This indicates that the capacity of the distributed hydrogen production and storage supply chain including the feeder of the power distribution systems are severely limiting the power consumption of the distributed supply chain system. Since the centralized system is connected to the bulk transmission grid, the corresponding problems are avoided.

6.3. Economic evaluation of both supply chains

Table 9 and 10 present the annual economic parameters, as described in Section 5.7, for the distributed and centralized hydrogen supply chain systems. It can be observed that the participation of ancillary services to the power grid enhances the economic values of both systems. This leads, in turn, to a lower breakeven time, as the profit increases with the participation of the ancillary services signals. Whereas providing DR and VAR support to the electricity grid enhances the profitability rate, the OR ancillary services immensely augment the profitability rate. This because it ensures two different payment options based on usance and availableness. The former compensates for the reserve provision during a specific period, while the latter pays for the actual energy delivered to the grid in response to an OR signal. Yet, the concurrent incorporation of all ancillary services results in the highest profitability ratio, as well as the most beneficial economic values.

When comparing both supply chain systems, the distributed supply chain outperforms the centralized supply chain in terms of the economics under the given operating conditions. Furthermore, the operational costs of the centralized system are higher due to the higher transportation costs. However, the NPV of the centralized system whereby it provides all services together is higher than the NPV of the distributed system. This is due to the higher capacity and ability to provide more flexibility services.

Table 8. Yearly economic parameters of the distributed hydrogen supply chain system based on diverse operating manners.

Ancillary services	GI	NI	NPV	BET	IRR	Profitability
None	€ 1.96 M	€ 0.96 M	€ 9.52 M	7.55 Year	10.06%	67.15%
VAR	€ 2.06 M	€ 1.06 M	€ 10.73 M	7.19 Year	10.92%	70.48%
DR	€ 2.01 M	€ 1.01 M	€ 10.17 M	7.35 Year	10.33%	68.96%
OR	€ 2.91 M	€ 1.60 M	€ 16.83 M	6.62 Year	12.43%	76.49%
All ancillary services together	€ 3.09 M	€ 1.87 M	€ 18.85 M	6.27 Year	13.49%	80.78%

Table 9. Annual economic parameters of the centralized hydrogen supply chain based on diverse operating manners.

Ancillary services	GI	NI	NPV	BET	IRR	Profitability
None	€ 1.90 M	€ 0.81 M	€ 7.35 M	8.51 Year	8.01%	59.03%
VAR	€ 2.08 M	€ 1.01 M	€ 9.54 M	7.80 Year	9.48%	62.92%
DR	€ 1.96 M	€ 0.90 M	€ 8.05 M	8.29 Year	8.48%	61.19%
OR	€ 2.08 M	€ 1.59 M	€ 16.22 M	6.94 Year	11.54%	72.88%
All ancillary services together	€ 3.21 M	€ 1.82 M	€ 19.08 M	6.45 Year	12.94%	78.48%

6.4. System losses for both scenarios

Table 11 summarizes the power system losses for both the distributed and centralized supply chain systems under the various operating cases, which are only the operation of the electric grid without hydrogen stations, the electric grid with the hydrogen stations and mobility demand, and the system including electric grid, hydrogen stations and the provisioning of ancillary services.

The results show that the inclusion of the hydrogen supply chain systems including the delivery of hydrogen to the mobility demand causes higher system power losses. This relates to the operation of the electrolyzer in the distribution system, which strains the system. Furthermore, the results indicate that the system losses are higher for the distributed supply chain than for the centralized supply chain. This is because the higher capacity of the centralized transmission system allows a more robust power supply to the hydrogen production and storage supply chain. Moreover, from the results it can be observed that the provisioning of the ancillary services has no significant effect on the system losses in both scenarios. Additionally, the functioning of the centralized supply chain in the transmission grid can lead to greater values for the investor. This is due to the higher output potential, as can be seen from the system losses, of the centralized supply chain and the greater capacity of the power line corridor, which generally allows larger contributions to the ancillary services market.

Table 10. Yearly system power losses for both scenarios under various operating manners.

Scenarios	Transmission (centralized) grid	Distribution (distributed) grid
Only operation of electric grid	283.400 GWh	100 MWh
Electric grid + operation of electrolyzers	297.723 GWh	1925 MWh
Electric grid + operation of electrolyzers + provisioning of all ancillary services	297.778 GWh	2095 MWh

6.5. Sensitivity Analysis

In this section, the results of the sensitivity analysis are presented. The sensitivity analysis highlights the importance of the costs of the variables in future energy systems. The results display that the profitability of the different operating cases highly depends on the range of the electricity prices, as described in Table 12 and 13. Lower electricity prices reduce both end-use costs for hydrogen, as well as redispatch costs, resulting in a higher profitability and lower breakeven time. Controversially, higher electricity prices increase the end-use costs for hydrogen, as well as redispatch costs, resulting in a lower profitability and higher breakeven time. However, the profitability trend remains similar, which indicates that the system is relatively robust against electricity prices.

Table 11. The effect of different energy price scenarios (Low: 50%; Mid: 100%; high: 150%) on the economic results for the centralized supply chain system.

Ancillary services	GI	NI	NPV	BET	IRR	Profitability	Mid-scenario
None	€ 1.90 M	€ 0.81 M	€ 7.35 M	8.51 Year	8.01%	59.03%	
VAR	€ 2.08 M	€ 1.01 M	€ 9.54 M	7.80 Year	9.48%	62.92%	
DR	€ 1.96 M	€ 0.90 M	€ 8.05 M	8.29 Year	8.48%	61.19%	
OR	€ 2.08 M	€ 1.59 M	€ 16.22 M	6.94 Year	11.54%	72.88%	
All ancillary services together	€ 3.21 M	€ 1.82 M	€ 19.08 M	6.45 Year	12.94%	78.48%	

Ancillary services	GI	NI	NPV	BET	IRR	Profitability	Low-scenario
None	€ 1.90 M	€ 0.92 M	€ 8.34 M	7.66 Year	9.09%	66.97%	
VAR	€ 2.08 M	€ 1.12 M	€ 10.55 M	7.02 Year	10.48%	69.59%	
DR	€ 1.96 M	€ 1.06 M	€ 9.00 M	7.46 Year	9.48%	68.40%	
OR	€ 2.08 M	€ 1.64 M	€ 16.72 M	6.25 Year	11.90%	75.13%	
All ancillary services together	€ 3.21 M	€ 1.96 M	€ 20.54 M	5.81 Year	13.93%	84.47%	

Ancillary services	GI	NI	NPV	BET	IRR	Profitability	High-scenario
None	€ 1.90 M	€ 0.70 M	€ 6.36 M	9.36 Year	6.93%	51.09%	
VAR	€ 2.08 M	€ 0.90 M	€ 8.53 M	8.58 Year	8.48%	56.25%	
DR	€ 1.96 M	€ 0.79 M	€ 7.10 M	9.12 Year	7.48%	53.98%	
OR	€ 2.08 M	€ 1.54 M	€ 15.72 M	7.63 Year	11.18%	70.63%	
All ancillary services together	€ 3.21 M	€ 1.68 M	€ 17.62 M	7.10 Year	11.95%	72.48%	

Table 12. The effect of different energy price scenarios (Low: 50%; Mid: 100%; high: 150%) on the economic results for the distributed supply chain system.

Ancillary services	GI	NI	NPV	BET	IRR	Profitability	Mid-scenario
None	€ 1.96 M	€ 0.96 M	€ 9.52 M	7.55 Year	10.06%	67.15%	

VAR	€ 2.06 M	€ 1.06 M	€ 10.73 M	7.19 Year	10.92%	70.48%
DR	€ 2.01 M	€ 1.01 M	€ 10.17 M	7.35 Year	10.33%	68.96%
OR	€ 2.91 M	€ 1.60 M	€ 16.83 M	6.62 Year	12.43%	76.49%
All ancillary services together	€ 3.09 M	€ 1.87 M	€ 18.85 M	6.27 Year	13.49%	80.78%

Ancillary services	**GI**	**NI**	**NPV**	**BET**	**IRR**	**Profitability**	**Low-scenario**
None	€ 1.96 M	€ 1.06 M	€ 10.51 M	6.80 Year	11.11%	74.14%	
VAR	€ 2.06 M	€ 1.16 M	€ 11.74 M	6.47 Year	1.95%	77.13%	
DR	€ 2.01 M	€ 1.11 M	€ 11.18 M	6.62 Year	11.35%	75.79%	
OR	€ 2.91 M	€ 1.73 M	€ 18.21 M	5.96 Year	13.44%	82.76%	
All ancillary services together	€ 3.09 M	€ 1.99 M	€ 20.08 M	5.64 Year	14.37%	86.05%	

Ancillary services	**GI**	**NI**	**NPV**	**BET**	**IRR**	**Profitability**	**High-scenario**
None	€ 1.96 M	€ 0.86 M	€ 8.53 M	8.31 Year	9.01%	60.16%	
VAR	€ 2.06 M	€ 0.96 M	€ 9.72 M	7.91 Year	9.89%	63.83%	
DR	€ 2.01 M	€ 0.91 M	€ 9.16 M	8.09 Year	9.31%	62.13%	
OR	€ 2.91 M	€ 1.47 M	€ 15.45 M	7.28 Year	11.41%	70.23%	
All ancillary services together	€ 3.09 M	€ 1.75 M	€ 17.62 M	6.90 Year	12.61%	75.51%	

Furthermore, varying the capacity of the ancillary services has a direct effect on the revenue. This is because, as the ancillary services are issued, the system has more capacity left to support the grid. From this, it can be observed that the output of the systems is highly dependent on the input data. Because of this, the comparison between the scenarios, as well as the different operating conditions is trustworthy, however, the specific profitability numbers are more uncertain. This is due to the uncertainty in the future.

Moreover, changing the value of the aggregated penalty factors has no significant effect on the results. This is because most of the ancillary services signals are abided, and therefore, the aggregated value of penalty factors is relatively low. However, this would change when there is insufficient capacity or when more market players are introduced in the market. Following that, varying the ancillary services market price has a direct effect. This relation is logic, as the prices increases, it is more beneficial to support the grid by providing ancillary services. Controversially, as the prices decreases, the revenue of the ancillary service provisioning must be higher than the cost of supplying it, as well as the revenue from the mobility demand at that moment. Eventually, it is observed that the system obtained a lower revenue from the ancillary service contributions when the price decreases. However, this had no significant effect on the profitability.

Lastly, the changes of costs of the components due to the potential technological developments influences the viability of hydrogen generation and storage systems in a positive manner. As the capital cost and operating cost decreases, the profitability increases, or lower end-use prices can be offered, which could support the development of future hydrogen systems. The results of the last four sensitivity analyses are described in the appendix.

7. Discussion

In this chapter, the results of both supply chain systems under various operating conditions are compared. As a result, the optimal design for hydrogen fuelling supply chains can be described. From this, a recommendation will be given for investors or operators of the electricity grid. Subsequently, the limitations of the research will be delineated, whereafter possible future research possibilities are substantiated.

7.1. Comparison of results

In this thesis, two configurations of hydrogen generation and supply chains under various operating conditions are compared. From this, it can be observed that both supply chains, the decentralized and centralized hydrogen supply chain, indicate technical viability. This means that both configurations including its technologies, such as gaseous storage and electrolyzer technologies, can be technically utilized for hydrogen fuel supply to the transportation sector and various ancillary services to the grid.

Furthermore, similar profitability trends are shown in each scenario. More specifically, a positive enhancement of the financial parameters is observed due to the joint application of the hydrogen generation and storage supply chains. However, the distributed supply chain system dominates the centralized supply chain system by means of the economic parameters under the operating conditions of this optimization.

As both systems are able to provide joint applications, it can be seen as a means for providing flexibility in the energy sectors. The systems can channel VRE and store the electricity in times of oversupply, it can transfer renewable energy from the power sector into sectors which are difficult to decarbonize, such as the mobility sector, and it offers a re-electrification pathway to support the electricity grid in times of a supply and demand mismatch or to increase the quality of electricity. However, comparing both scenarios, it is observed that the centralized supply chain presents better technical characteristics, where it enables more flexibility to the operation of power grids than the distributed supply chains. This can be observed by the changes in power demand patterns shown in Figure 30, as well as figure 35. As depicted in figure 30, the power demand is severely restricted by the lower capacity of the distributed supply chain and injectors of the power distribution systems. Since the centralized supply chain is connected to the bulk transmission system, such concerns are avoided. This can also be highlighted by the system's power losses incurred by the grids as a result of operating the hydrogen generation and storage supply chains.

Moreover, the results show that the distributed supply chain system entails higher power losses than the centralized system. As the electrolyzers are distributed throughout the system, it causes strains in the system, resulting in increased losses. This increase is relatively small for the centralized supply chain. This is due, once again, to the larger capacity of the transmission infrastructure, which allows for a stronger corridor for electricity supply. The participation of the ancillary services, on the other hand, does not significantly increase the system losses. Both scenarios indicate that no significant increase can be observed.

Additionally, the functioning of the centralized supply chain in the transmission grid can lead to greater values for the investor. This is due to the higher output potential of the centralized supply chain and the greater capacity of the power line corridor, which generally allows larger contributions to the ancillary services market.

From this, including techno-economic optimization of two different supply chain configurations under various operating conditions, the main research question can be answered. The main research question aimed to answer in this thesis was:

What are potential designs of hydrogen fuelling supply chains powered by solar and wind energy that can effectively serve the mobility sector demand of a region, as well as providing balancing services to the power grid?.

To answer this research question, different configurations of hydrogen generation and storage supply chains were considered in this thesis. From this, it is indicated that both the distributed and centralized supply chain systems are technically and effectively viable to serve the mobility sector demand of a region, as well as providing balancing services to the power grid. Whereas both designs were able to channel and use the provided renewable electricity in an effective manner, the systems were also able to deal with the fluctuating supply and demand patterns, such as the demand from the mobility sector, and the volatile supply of electricity from renewable energy sources. The results have also shown that the profitability patterns of the distributed and centralized supply chain systems are comparable under various conditions. While the distributed supply chain system presents better profitability patterns than the centralized supply chain systems under the performed conditions, the centralized hydrogen supply chain has greater technological benefits than the distributed supply chain. Yet, both designs can offer more flexibility in the energy sectors and can be seen as a means for balancing and supporting the electricity grid.

7.2. Scientific contribution

To combat climate change, ambitious decarbonization targets are implemented. Energy sector coupling is considered to be critical in achieving these targets. In literature, studies have shown the ability of sectors to incorporate renewable electricity from the power sector. Along with these changes, the energy system requires even more flexibility options. Furthermore, research has examined sector coupling of the power sector with easy-to-decarbonize sectors, such as the heating sector. However, literature on sector coupling of the transportation sector can be enhanced. Therefore, this thesis contributes to the academic knowledge by proposing a modelling approach to determine optimal designs for hydrogen fuelling supply chains to fulfil joint applications and provide flexibility in the energy sectors. This thesis enhances the understanding of the effect of different technical and economic configurations when implementing such supply chain designs. The model allows to make quantified decisions in a systematic manner for complex systems where the operation includes multiple components on various levels.

Furthermore, the thesis provided deployment and scheduling of hydrogen generation and storage supply chains to utilize the full system benefit. This included understanding of using such systems for the mobility sector, as well as enhancing the economics of seasonal storage and flexibility to the electricity sector and to maximize the profitability of such systems.

The findings of the study have shown that sector coupling between the energy and transportation sector with hydrogen as a nodal connector can significantly improve the performance of the energy system, allowing the sectors to utilize resources more efficiently, and increase the profit of the system. However, trade-offs between profit and flexibility should be made according to the size of the hydrogen demand and the ancillary services, and the needs of the sector coupling. Second, hydrogen can be a nodal connector between sectors, whereas it utilizes the full system benefit, as well as providing flexibility options. However, in this work hydrogen is utilized in the most efficient way, but it is dependent on different developments in the energy sector, for example, the development of batteries or the inclusion of other flexibility options.

Furthermore, different supply chain configurations, which resembles possible future scenarios, are implemented in the model. This resulted in a better understanding of the effects of future electricity on the outcomes of such systems, as well as cost reductions of technologies and components. It appeared that the electricity prices are critical for the determination of the hydrogen prices, which eventually has a major effect on the outcome or the selling price to the mobility demand. Furthermore, the change in electricity price also affected the allocation of power in the system. Lower electricity prices resulted in more supply to the mobility demand while higher electricity prices resulted in an enhancement of the profitability due to balancing the electricity grid.

7.3. Investment and policy recommendations

This section discusses the investment and policy recommendations based on the results retrieved from the optimization approach. First, the investment recommendations will be described. After that, the policy recommendation will be discussed.

7.3.1. Investment recommendations

This thesis is partly meant for assessing the economic viability of different configurations of hydrogen supply chains to assist private investors in decision-making regarding which investment is more profitable and to provide insights into the benefits of coupling the transportation and energy sectors. However, the determination of optimal design is a complex task due to various reasons. First, the operation and interconnection of the hydrogen systems with different sectors result in large-scale operation with components on various levels, such as multiple small compliances to the integration of renewable energy plants, where multiple configurations are possible (Seifi, 2011). Additionally, energy infrastructures are extremely capital demanding, requiring hundreds of millions of euros investments costs (Melese, 2014). Long lifetimes must also be acknowledged, which leads to decision-making in the face of uncertainty (Melese, 2014). Lastly, the socio-technical features of the energy system cause that the institutional and economic aspects must be considered next to the technical components (Farrokhifar, 2020). The modelling results contributed to these investment dilemmas by giving a quantitative tool for discovering the optimal investment designs in a systematic manner. From the results, it can be observed that the profitability patterns of the distributed and centralized supply chain systems are comparable under the operating conditions. However, while the distributed supply chain system presents better profitability patterns than the centralized supply chain systems under the performed conditions, the centralized hydrogen supply chain has greater technological benefits than the distributed supply chain. Whether the centralized or the distributed supply chain is the better investment option depends on the size of the hydrogen demand and the ancillary services, and the needs of the sector coupling. Whereas the decentralized supply chain is more beneficial for smaller demands, the operation of the centralized supply chain can bring higher values to investors that have to deal with larger demands and more interconnected systems. Since most of these systems will be operated by larger system operators, and the supply chain including the fuelling stations will be more connected to the energy sectors instead of operated alone, the centralized option is considered to be the most beneficial investment.

7.3.2. Policy recommendations

Aside from the technical and economic aspects of the system, the social aspects, such as institutions, policies, and regulations must be considered for the effectiveness of the systems. There are several recommendations that could enable sector coupling (GIE, 2018). The first is the implementation of fair grid charges. Grid charges or tariffs has a significant influence on the total cost and profitability of power to gas facilities. By utilizing the power conversion services, as well as the underlying gas infrastructure, unnecessary investments in the power grid can be avoided. Such operational value offered by the gas network towards the prospective power system must be represented in the regulatory framework. As a result, the method of cost reflectivity in calculating grid charges should be expanded to consider the role of energy generating and storage systems in avoiding electrical grid restrictions and grid expansion costs, and the curtailment of intermittent renewable power production (GIE, 2018).

There must also be some clarification on who will operate the hydrogen generation and storage facilities. At this moment, transmission system operators (TSOs) and storage system operators (SSOs) are involved in energy conversion activities. However, the power conversion will be critical in balancing the VRE production. In order to comply with existing European regulations, all market participants should be entitled to own, develop, operate, and manage the conversion and storage facilities. This is to deliver the most efficient operation of these services in a non-discriminatory manner (GIE, 2018).

Furthermore, increased coordination between power and other generation and storage infrastructure would be beneficial. This means introducing better institutionalizing and communications schemes between power and facility operators to balance the supply and demand of energy in a more efficient way. This might be accomplished by increasing network planning efforts and improving the energy sector independence (GIE, 2018).

Another measure would be introducing incentives for the use of advanced fuels, such as hydrogen, in transportation or industrial sectors. For this, it is important to better represent the corresponding CO_2 emission reduction objectives for vehicle and truck companies. For example, if hydrogen is completely produced by renewable power, it should be permitted to count as emission reduction (GIE, 2018).

Moreover, even though this thesis supports that hydrogen generation and supply chains are important in the transition of the energy system and the transportation sector, a future perspective is used. However, scaling up the infrastructure and developing the technologies also require experience in how to integrate these facilities into the existing energy system. Therefore, support for pilot projects at European level needs to be established (GIE, 2018).

All in all, there are four core principles of regulatory and market framework measures for efficient sector coupling: the recognition of values provided to the energy system by various energy sources and infrastructures, the creation of a fair playing field for various energy sources and facilities to include these various services, promotion of competition and innovation among energy sources and facilities to increase the level of supply by many services required by the energy system, and the establishing of a comprehensive approach for such generation and storage systems by governance mechanisms and planning tools (GIE, 2018).

7.4. Limitations

In this research, a modelling approach is used to determine the optimal design for hydrogen generation and storage supply chains. By using iterative optimization algorithms, a techno-economic analysis is performed. However, a model is a simplification of the real world used to visualize, explain, and make predictions on the outcomes (Nikolic, 2019). Because of this, details can be missed since not all the details of complex natural phenomena can be incorporated (Melese, 2014). During this process, assumptions are made to resemble the real world. For example, assumptions are made about who will own, operate, and invest in the hydrogen generation and supply chain, as well as the establishment of the system boundaries, interactions, and relationships within the model. However, also other viewpoints could be proposed, for example, with more connections or integrated with other sectors. For instance, within this system, collaborations with third parties are required, however, in this thesis only the overall profitability is examined to determine the optimal design for the joint application. More specifically, if third parties are included, the cost and profit allocations are becoming more complex.

Additionally, assumptions are made about which technologies should be included in this model. These assumptions are substantiated through reviewing literature; however, alongside the changing electricity market, many developments will be implemented. This could, in turn, result in the implementation of new entrants or other technologies that could exist or develop, which may be a better fit in the future system. One important development will be the hydrogen backbone, which could, in turn, drastically change the setup. This is, however, not considered in the model. Moreover, one could argue that if technologies and components are cheaper, which is a realistic prospective, more profit for the system can be obtained. Nonetheless, this would have no significant effect on the outcome because the main focus was comparing different configurations of hydrogen generation and storage supply chains. By including other technologies, the comparison would still be fair. Also, one scenario in this model included the use of pipelines, this could therefore easily be connected to the hydrogen backbone.

Above all, we are currently living in a turbulent electricity system and hydrogen period. The whole electricity system is changing rapidly, including the hydrogen market. Since this thesis includes a model that reflects various future scenarios, it could result in some values used in this thesis already been obsolete, such as the hydrogen selling price. Furthermore, it also decreases the credibility of the model since the future is uncertain. For instance, there is uncertainty in the generation capacity and mix of renewable energy sources, the electricity prices, the demand and prices of the ancillary services signals, as well as the ancillary services penalty factors, mobility demand, as well as other future market changes.

Regarding the energy mix and electricity price, it is expected that when more renewable generation capacity exists, the lower the electricity prices will become. Also, other factors can influence the electricity price, such as war or insufficient capacity of a generating source, such as the natural gas supply. Besides this, the location of the systems, and thus, the wind speed and solar irradiance, is crucial in reducing the cost of the hydrogen production. This indicates that the profitability is strongly associated with the capacity factor of the electrolyzer. The above-mentioned points bring uncertainties in the outcome of the model. Furthermore, in this thesis, electricity market data from 2018 is used instead of more actual data. This was because the war in Ukraine and the influence of Covid impacted the electricity price profiles. Additionally, in this thesis it is assumed that there is always sufficient generating capacity to satisfy the mobility demand. This could, however, also not be the case. However, the usage of the 2018 data and the generation capacity has no or little effect on the outcome of the thesis. This is because the main goal was to compare the scenarios and not necessarily gain the exact profit numbers.

Moreover, uncertainties exist in the demand and prices of the ancillary services signals, as well as the ancillary services penalty factors in the model. In this thesis, slack variables are used to resemble the ancillary service signals retrieved from the market systems operators. This is adapted from the average moments the ancillary services occur in a year from the IESO. However, the future demand of ancillary services maintains uncertain. The capacities and times of occurrence of the ancillary services are depending on the balancing of supply and demand. Since, the supply of electricity will become more volatile due to the introduction of more renewable energy sources, and the demand is changing as well, and hence, the ancillary services cannot be exactly estimated.

Furthermore, the ancillary services are optimized per 15 minutes, however, a smaller time horizon would be better for balancing the grid and supporting the power quality. For this, signals per minute could be implemented. This could influence the results since ancillary service contribution per minute causes that the storage must react faster. However, the size of the services would not differ since the sum of all signals per minute would be similar to the total amount per 15 minutes. To gain more information, a better scheduling scheme and coordination with the system operators need to be considered, or pilots must be implemented. This is also related to the requirements of the changing electricity market whereby new measures must be considered for these systems to be successful, such as a pricing mechanism or the opening up of the market for new entrants.

As mentioned before, this thesis includes a model that reflects various future scenarios. As a result, predictions are made to replicate the hydrogen mobility demand in the model. For this, data from the NREL is adapted to create a realistic image based on the demand of gasoline cars of today, which enabled the comparison between outcomes and benefits of the various supply chain designs. This could, however, differ from the actual demand in the future. For example, there might be better future sustainable mobility options, such as EVs or other new entrants, or only a part will be driving on hydrogen. The electricity price has a major effect on this, since a higher electricity price increases the hydrogen price, which makes driving FCEVs less attractive. Nonetheless, the thesis provides useful outcomes in terms of enhancing the knowledge regarding sector coupling and its advantages. As mentioned before, the transportation demand could also be substituted with another sector, such as the heating sector or industry.

Lastly, other future market changes could have influence on the model credibility. For example, the changing electricity market causes different pricing structures or policy measures. Also new market entrants could be introduced. If more competitors will arrive in the ancillary service market, the profitability, and hence, the attractiveness to perform the joint services will decrease. Besides this, the cost and profit allocation are also more difficult. So, the situation could be completely different when more competition is introduced.

All these uncertainties have influence on the credibility of the economic analysis. The economic analysis may be limited because of this; however, the main focus of this thesis was to compare different designs of hydrogen generation and storage supply chains. Because of this, the comparison, even with completely other future values, stays trustworthy. Trustworthy in the sense that the design comparison stays fair, and thus the results will remain the same under the operating conditions. Important contribution are: while the distributed supply chain system is better for lower hydrogen demand, the centralized supply chain system is the better option for larger demands. Moreover, the centralized supply chain system could provide more flexibility.

Furthermore, the credibility of the model is increased by using data from larger more reliable sources. Also, the sensitivity analyses have shown the influence of varying the parameters. However, for the simplicity of this thesis, three scenarios of electricity prices are considered to estimate future electricity price scenarios. Moreover, the input variables are taken from reliable sources, such as the NREL. However, these sources could also be verified by experts or comparing them to other reliable sources. For some data for example, the average over a longer time period could be taken to enhance the credibility instead of using one year.

Besides the uncertainties in estimating future values, the sample size of the model might also be a limitation of the thesis. For the performed operating conditions, the distributed supply chain system obtained better economic values. However, as mentioned before, the decentralized is better for smaller demands, yet the centralized can obtain better values for the investor since it has more capacity for ancillary service provisioning. The centralized system has hereby more potential, which can be observed from the power consumption figure, but also by optimizing a larger sample size system or region.

Lastly, other validations processes could be implemented. This is not fully accomplished since there was limited time for full validation. However, a pilot could be introduced. Otherwise, more literature could be investigated, for example with other sectors, and investigate whether the size and method used in this thesis of the results are trustworthy.

7.5. Future work

After the definition of the limitations of this thesis, future research opportunities are identified. The first opportunity for future research should be the focus on alternative or additional configurations of the hydrogen generation and storage supply chain. One possibility is exploring different modes of transportation. For instance, in the future energy system, it is expected that a hydrogen backbone will be implemented in the Netherlands. This would provide an opportunity to invest in the situation in which hydrogen is supplied to the fuelling stations via the pipelines from the backbone.

Furthermore, while wind and solar resources are projected to be the primary energy sources in the Netherlands, other different energy sources, such as biomass or hydropower, could be included in studies as well. This is in line with that the energy system will be more connected, so more secure, and reliable energy options are required, which also requires testing and research. Also, it would be interesting to vary the generation capacity of the energy sources instead of only varying the electricity prices. This would give insights on the effect of the energy sources, including the wind speed and solar irradiance on the outcomes. From this, the optimal design for different locations can be observed.

Besides that, this thesis only considers the sector integration of the energy and transportation sector. However, there is still more to be researched by incorporating other sectors, such as the heating or industrial sector. This has the potential to significantly reduce carbon emissions from various areas, making it an appealing study topic. The inclusion of batteries, such as neighbourhood batteries would also be an interesting opportunity.

As explained before, lower electricity prices would increase the willing to buy more electricity and produce more hydrogen and provide more ancillary services. However, if more investors or operators would do this, the whole market or idea of balancing the grid would change. Therefore, it is interesting to investigate the possible development paths of the hydrogen and ancillary service market. The understanding both markets diffusion will provide different scenarios of electricity supply and hydrogen production, which will then guide possible solutions for hydrogen generation and storage systems and its applications, especially for balancing the grid. If a scaled-up market is expected, and if the demand of hydrogen can be integrated with other applications, such as demand for fuel-cell-driven trains, the role of the refuelling station will change, and consequently its cost will alter. The market mechanism will adapt accordingly to the new developments. For this, new market mechanisms should be developed. Therefore, it would be interesting to study or identify possible dynamic ancillary service pricing if it will not be operated by own single system operator. Also, future research could consider dynamic hydrogen pricing and demand uncertainty. Another interesting opportunity is to engage in various distribution modalities with global demand points, in which the connection with other nations could be investigated. For this, a pricing framework needs to be considered.

Lastly, while this thesis focused mostly on the techno-economic side of the systems, cost and profit allocations will be increasingly important in the future. This is vital to study since additional connections, including more stakeholders will exist, resulting in a more complicated system. The issue of accountability will also be important.

8. Conclusion

This thesis proposed a modelling technique for maximizing the net return of hydrogen generation and storage supply chain systems by fulfilling a hydrogen mobility demand while also offering numerous ancillary services to the power grid. The proposed method is utilized to conduct a techno-economic analysis of two hydrogen supply chain configurations: distributed onsite hydrogen generation and centralized offsite generation. Both scenarios are analysed throughout different operating conditions, such as providing or not providing ancillary services to the grid, using real-world power market data. The results display that both distributed and centralized hydrogen generation and storage supply chains can be used to offer hydrogen fuel to the transportation sector as well as provide different ancillary services to the grid. Furthermore, the numerical findings show that when both supply chains are planned and run concurrently for various ancillary services, the highest improvement in terms of financial parameters can be observed. The results also indicate that the profitability of the distributed and centralized supply chain is comparable under various operating conditions. However, while the distributed supply chain system presents better economic performances than the centralized supply chain system under the performed conditions, the centralized hydrogen supply chain has greater technological benefits than the distributed supply chain in terms of flexibility. Whereas the decentralized supply chain is more beneficial for smaller demands and a more isolated operation, the centralized supply chain can provide higher values to investors who must deal with larger demands and more interconnected systems. Because the majority of these systems will be operated by larger system operators, and the supply chain, including fuelling stations, will be increasingly connected to the energy sectors rather than operating independently, the centralized alternative is likely to be the most beneficial investment. The analyses reported in this study are useful to interconnected investors or system operators for assessing the technical and economic viability of the widespread deployment of distributed and centralized hydrogen generation and storage supply chains integrated with the power grid. Future research might investigate other system configurations, such as including the hydrogen backbone into the operation or integrating the hydrogen supply chain with diverse industries, such as the heating sector. Different renewable energy sources, such as biomass or hydropower, might also be included. Other research might involve dynamic hydrogen pricing or the engagement of various distribution modalities with global demand points. Finally, for the supply chain systems to be successful, the social aspect must be considered, in which numerous market regulatory and governance impediments must be identified and exploited.

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Appendix:

33 bus:

Branch data info

```
% |Branch number|FromBus|ToBus|Impedance|LineCharging|TAP|
d=[1    1     2     0.0922  0.047   5.234 1
2       2     3     0.493   0.2511  0 1
3       3     4     0.366   0.1864  0 1
4       4     5     0.3811  0.1941  0 1
5       5     6     0.819   0.707   0 1
6       6     7     0.1872  0.6188  0 1
7       7     8     1.7114  1.2351  0 1
8       8     9     1.03    0.74    0 1
9       9     10    1.04    0.74    0 1
10      10    11    0.1966  0.065   0 1
11      11    12    0.3744  0.1238  0 1
12      12    13    1.468   1.155   0 1
13      13    14    0.5416  0.7129  0 1
14      14    15    0.591   0.526   0 1
15      15    16    0.7463  0.545   0 1
16      16    17    1.289   1.721   0 1
17      17    18    0.732   0.574   0 1
18      2     19    0.164   0.1565  0 1
19      19    20    1.5042  1.3554  0 1
20      20    21    0.4095  0.4784  0 1
21      21    22    0.7089  0.9373  0 1
22      3     23    0.4512  0.3083  0 1
23      23    24    0.898   0.7091  0 1
24      24    25    0.896   0.7011  0 1
25      6     26    0.203   0.1034  0 1
26      26    27    0.2842  0.1447  0 1
27      27    28    1.059   0.9337  0 1
28      28    29    0.8042  0.7006  0 1
```

29	29	30	0.5075	0.2585	0 1	
30	30	31	0.9744	0.963	0 1	
31	31	32	0.3105	0.3619	0 1	
32	32	33	0.341	0.5302	0 1];	

Bus data info:
Slack=1;
PV=2;
PQ=3;
% |Bus | Type | Vsp |del| PGi | QGi | PLi | QLi |

d=[1	Slack	1	0	0	0	0	0
2	PQ	1	0	0	0	100	60
3	PQ	1	0	0	0	90	40
4	PQ	1	0	0	0	120	80
5	PQ	1	0	0	0	60	30
6	PQ	1	0	0	0	60	20
7	PQ	1	0	0	0	200	100
8	PQ	1	0	0	0	200	100
9	PQ	1	0	0	0	60	20
10	PQ	1	0	0	0	60	20
11	PQ	1	0	0	0	45	30
12	PQ	1	0	0	0	60	35
13	PQ	1	0	0	0	60	35
14	PQ	1	0	0	0	120	80
15	PQ	1	0	0	0	60	10
16	PQ	1	0	0	0	60	20
17	PQ	1	0	0	0	60	20
18	PQ	1	0	0	0	90	40
19	PQ	1	0	0	0	90	40
20	PQ	1	0	0	0	90	40
21	PQ	1	0	0	0	90	40
22	PQ	1	0	0	0	90	40
23	PQ	1	0	0	0	90	50
24	PQ	1	0	0	0	420	200
25	PQ	1	0	0	0	420	200
26	PQ	1	0	0	0	60	25
27	PQ	1	0	0	0	60	20
28	PQ	1	0	0	0	60	20
29	PQ	1	0	0	0	120	70
30	PQ	1	0	0	0	200	600
31	PQ	1	0	0	0	150	70
32	PQ	1	0	0	0	210	100
33	PQ	1	0	0	0	60	40];

30 bus:
% |Branch number|FromBus|ToBus|Impedance|LineCharging|TAP|

d=[1	1	2	0.0922	0.047	5.234 1

2	2	3	0.493	0.2511	0 1
3	3	4	0.366	0.1864	0 1
4	4	5	0.3811	0.1941	0 1
5	5	6	0.819	0.707	0 1
6	6	7	0.1872	0.6188	0 1
7	7	8	1.7114	1.2351	0 1
8	8	9	1.03	0.74	0 1
9	9	10	1.04	0.74	0 1
10	10	11	0.1966	0.065	0 1
11	11	12	0.3744	0.1238	0 1
12	12	13	1.468	1.155	0 1
13	13	14	0.5416	0.7129	0 1
14	14	15	0.591	0.526	0 1
15	15	16	0.7463	0.545	0 1
16	16	17	1.289	1.721	0 1
17	17	18	0.732	0.574	0 1
18	2	19	0.164	0.1565	0 1
19	19	20	1.5042	1.3554	0 1
20	20	21	0.4095	0.4784	0 1
21	21	22	0.7089	0.9373	0 1
22	3	23	0.4512	0.3083	0 1
23	23	24	0.898	0.7091	0 1
24	24	25	0.896	0.7011	0 1
25	6	26	0.203	0.1034	0 1
26	26	27	0.2842	0.1447	0 1
27	27	28	1.059	0.9337	0 1
28	28	29	0.8042	0.7006	0 1
29	29	30	0.5075	0.2585	0 1];

Bus data info:
Slack=1;
PV=2;
PQ=3;
% |Bus | Type | Vsp |del| PGi | QGi | PLi | QLi |

d=[1	Slack	1	0	0	0	0	0
2	PQ	1	0	0	0	100	60
3	PQ	1	0	0	0	90	40
4	PQ	1	0	0	0	120	80
5	PQ	1	0	0	0	60	30
6	PQ	1	0	0	0	60	20
7	PQ	1	0	0	0	200	100
8	PQ	1	0	0	0	200	100
9	PQ	1	0	0	0	60	20
10	PQ	1	0	0	0	60	20
11	PQ	1	0	0	0	45	30
12	PQ	1	0	0	0	60	35
13	PQ	1	0	0	0	60	35
14	PQ	1	0	0	0	120	80

15	PQ	1	0	0	0	60	10
16	PQ	1	0	0	0	60	20
17	PQ	1	0	0	0	60	20
18	PQ	1	0	0	0	90	40
19	PQ	1	0	0	0	90	40
20	PQ	1	0	0	0	90	40
21	PQ	1	0	0	0	90	40
22	PQ	1	0	0	0	90	40
23	PQ	1	0	0	0	90	50
24	PQ	1	0	0	0	420	200
25	PQ	1	0	0	0	420	200
26	PQ	1	0	0	0	60	25
27	PQ	1	0	0	0	60	20
28	PQ	1	0	0	0	60	20
29	PQ	1	0	0	0	120	70
30	PQ	1	0	0	0	200	600];

Parameters	Value
Optimization time interval (h)	0.25
Hydrogen demand in transportation system ($\frac{m^3}{h}$)	155
Hydrogen sale prices in transport system ($\frac{€}{m^3}$)	0.3525
Electricity market price ($\frac{€}{MWh}$)	Dynamic price profile from Entsoe transparency platform
SoC reserve margin for VAR support to grid (m^3)	Reserve margin = SoC – supply to road mobility
SoC reserve margin for DR support to grid (m^3)	Reserve margin = SoC – supply to road mobility
SoC reserve margin for OR support to grid (m^3)	Reserve margin = SoC – supply to road mobility
Binary parameter representing VAR contribution mode	0 or 1
Binary parameter representing DR contribution mode	0 or1
Binary parameter representing OR contribution mode	0 or 1
Aggregated value of penalty factors (€)	
Ancillary service VAR signal (MVAr)	
Ancillary service DR signal (MW)	
Ancillary service OR signal (MW)	

Input variables	Output variables
Slack variable for DR management (MW)	Generated revenue (€)
Slack variable for management of electrolyzer VAR (MVAr)	Hydrogen consumption of fuel cell unit ($\frac{m^3}{h}$)
Slack variable for management of electrolyzer DR signal (MW)	Power generation of fuel cell unit (MW)
Slack variable for DR management (MW)	VAR of electrolyzer (MVAr)
Slack variable for management of electrolyzer OR signal (MW)	Adjusted power consumption of electrolyzer (MW)
Hydrogen storage SoC (m^3)	Power consumption of electrolyzer (MW)
Voltage angle at power system buses (Rad)	Power consumption of hydrogen transport (MW)
Voltage of power system buses (pu)	Hydrogen generation of electroyzer (m^3)
Active power injected to power system buses (MW)	
VAR injected to power system buses (MVAr)	