STRATEGIC DESIGN OF A HYDROGEN INFRASTRUCTURE UNDER UNCERTAINTY

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SUMMARY

Due to an increasing demand for electric energy and a decreasing amount of fossil fuel sources, renewable and clean energy systems are positioned as alternative energy supply options. A transformation of the supply of energy from fossil to renewable sources of energy is accompanied by substantial challenges such as their intermittent behavior and integrating high shares in transportation sector, which require smart transition strategies.

In this thesis, special attention is given to the concept for integrating renewable energy into transportation sector through applying hydrogen-based system, given the high penetration rate of fuel cell electric vehicles into passenger transport. Mathematical modeling and optimization tools are used at the network level. A hydrogen production network defined as a supply chain is modeled and Germany is chosen as a case study due to its progressive policies towards increasing the use of renewable energy sources and lowering greenhouse gas emissions.

First, a Mixed Integer Linear Programming (MILP) model is developed to solve a hydrogen supply chain (HSC) network design problem forecasting up to 2050. It is based on the concept of determining the best hydrogen infrastructure pathways where the interaction between four echelons of the supply chain is considered. The main decisions are the procurement, production, inventory, and distribution. As a result, two configurations are proposed based on coal gasification and water electrolysis technologies. Moreover, renewable energy as a power source shows the potential to replace commonly used fossil fuels in the near future: renewable electricity production can satisfy a hydrogen based fuel demand.

Secondly, the proposed MILP model is extended by considering different objectives, i.e. cost, environmental impact and safety. By balancing three objectives, a set of solutions approximating the Pareto front is generated using the ε-constraint method. The proposed trade-off solution enhances the design decisions and proposes a safer and decentralized HSC where water electrolysis is the main technology. Moreover, the competitive hydrogen costs compared to the average fuel cost used in the modern internal combustion vehicle demonstrates feasibility of a hydrogen economy.

Finally, the sensitivity analysis is preformed to evaluate which model parameters have the strongest impact in the total daily network cost. The hydrogen demand is considered and analyzed as an uncertain parameter leading to a stochastic formulation. The outcomes of this stochastic optimization show that a small emissions fee for water electrolysis based hydrogen

production is observed while the price of production sites and raw material is three times higher as compared to the cost of conventionally produced hydrogen (e.g. steam methane reforming and coal gasification). Despite economic benefits, the use of fossil fuels and large CO_2 emissions will no longer be attractive and lead to network configurations that incorporate water electrolysis.

Overall it can be concluded that implementation of fuel cell electric vehicles powered by renewable hydrogen for the transport sector becomes feasible and actively contributes to the decarbonization of the energy system making the transport sector in Germany ready to shift to clean fuels.

ZUSAMMENFASSUNG

Aufgrund des steigenden Bedarfs an elektrischer Energie und der sinkenden Menge fossiler Brennstoffe sind erneuerbare und saubere Energiesysteme als alternative Energieversorgungsoptionen positioniert. Eine Umstellung der Energieversorgung von fossilen auf erneuerbare Energiequellen bringt erhebliche Herausforderungen, wie das intermetierende Verhalten der regenerativen Erzeuger, sowie die Integration hoher Anteile erneuerbarer Energien in den Verkehrssektor, mit sich. Diese Herausforderungen stellen Bedarf anintelligente Übergangsstrategien.

Angesichts der hohen Durchdringungsrate von Brennstoffzellen-Elektrofahrzeugen im Personenverkehr, wird mit der vorliegenden Arbeit besonderes Augenmerk auf das Konzept der Integration erneuerbarer Energien in den Verkehrssektor durch Anwendung eines auf Wasserstoff basierenden Systems gelegt. Mathematische Modellierungs- und Optimierungswerkzeuge werden, am Beispiel von Versorgungsnetzwerken von Wasserstoffproduktionsketten, auf Netzebene angewandt. Hierbei dient Deutschland aufgrund seiner fortschreitenden Politik zur verstärkten Nutzung erneuerbarer Energien und zur Verringerungen von Treibhausgasemissionen als Fallstudie. Zunächst wird ein Gemischt-ganzzahliges lineares Modell (MILP) entwickelt. Dieses wird dazu verwendet, um ein potentielles Design einer Wasserstoffversorgungskette (HSC) für 2050 zu berechnen. Das entwickelte Modell basiert auf der Ermittlung der besten Wasserstoffinfrastrukturpfade, bei denen die Interaktion zwischen vier Ebenen von der Lieferkette berücksichtigt werden. Die wichtigsten Entscheidungen sind Beschaffung, Produktion, Lagerhaltung und Verteilung. Die Optimierung resultiert in zwei potentiellen Konfigurationen, die auf Kohlevergasungs- und Wasserelektrolyse-Technologien basieren. Erneuerbare Energien als Energiequelle zeigen zudem das Potenzial, in naher Zukunft häufig verwendete fossile Brennstoffe zu ersetzen: Die Stromerzeugung aus erneuerbaren Energieträgern kann einen auf Wasserstoff basierenden Brennstoffbedarf decken.

Im zweiten Schritt wird das vorgeschlagene MILP-Modell durch Berücksichtigung verschiedener Kriterien, d. H. Kosten, Umweltauswirkungen und Sicherheit, erweitert. Durch die Berücksichtigung der multiplen Kriterien wird mit der ε-Constraint-Methode eine Reihe von Lösungen erzeugt, die sich der Pareto-Front annähern. Die vorgeschlagene Trade-Off-Lösung verbessert die Entscheidungsfindung in der Designphase und schlägt eine sicherere und dezentralisierte HSC vor, bei der die Wasserelektrolyse die Haupttechnologie darstellt. Darüber hinaus zeigen die wettbewerbsfähigen Wasserstoffkosten im Vergleich zu den

durchschnittlichen Kraftstoffkosten, die in einem modernen Verbrennungsfahrzeug verwendet werden, die Realisierbarkeit einer Wasserstoffwirtschaft.

Im letzten Schrittwird eine Sensitivitätsanalyse durchgeführt, um zu bewerten, welche Modellparameter die stärksten Auswirkungen auf die täglichen Gesamtnetzkosten haben. Die Unsicherheit des Wassertoffbedarfes wird in Form einer stochastischen Optimierung analysiert. Die Ergebnisse der stochastischen Optimierung zeigen, dass eine geringe Emissionsgebühr für die auf Wasserelektrolyse basierende Wasserstofferzeugung beobachtet wird, während der Preis von Produktionsstätten und Rohmaterial dreimal höher ist als der Preis von herkömmlich erzeugtem Wasserstoff (z. B. Dampfmethanreformierung und Kohlevergasung). Trotz der wirtschaftlichen Vorteile wird der Einsatz fossiler Brennstoffe und das Emittieren hoher CO_2 Werte nicht mehr attraktiv sein und zu Netzwerkkonfigurationen mit Wasserelektrolyse führen.

Insgesamt kann der Schluss gezogen werden, dass die Einführung von Brennstoffzellen-Elektrofahrzeugen, die mit regenerativem Wasserstoff betrieben werden, für den Verkehrssektor machbar wird und aktiv zur Dekarbonisierung des Energiesystems beiträgt, wodurch der Verkehrssektor in Deutschland bereit ist, auf saubere Kraftstoffe umzusteigen.

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1. INTRODUCTION

1.1.BACKGROUND

Energy plays a crucial role in the modern society starting from residential services to industrial application. An increasing population consumes more and more energy year after year. Based on a report by the International Energy Agency (IEA) and the U.S. EIA, the global energy demand will have grown with 30% in 2040 [1] [2]. Up until now, fossil fuels, which include natural gas, oil, and coal, are the primary energy sources for transportation, electricity, and residential services. Increasing energy demand means a progressively growing fuel consumption in the near future. Moreover, due to increasing fuel consumption, a cause of concern is the fast rise of CO_2 levels, now already exceeding 400 ppm and when, left unmitigated, possibly increases in the coming 100 years up to 800 ppm [3]. Additionally, fossil fuel is a nonrenewable energy source. The depletion time for fossil fuel is estimated to be around 100 years, where oil and gas will be exhausted earlier than coal [4].

Due to the increasing demand of electric energy and a decreasing amount of fossil fuel sources, the development of alternative ways for energy production is required [5]. On 28 September 2010 the German government presented a long-term political timetable for decarbonization of the energy supply by renewable energy production and decided to completely phase out nuclear energy by 2022 ("Energiewende"). It aims at an 80%-95% greenhouse gas (GHG) reduction from 1990 level by the year 2050. Renewable energy sources have to contribute with 35%, 50, 65, 80% to the total energy generation by 2020, 2030, 2040, 2050 respectively [6] [7]. Renewable energy generation reached already 40% of the total energy generation in 2018 (see Figure 1.1) [8].

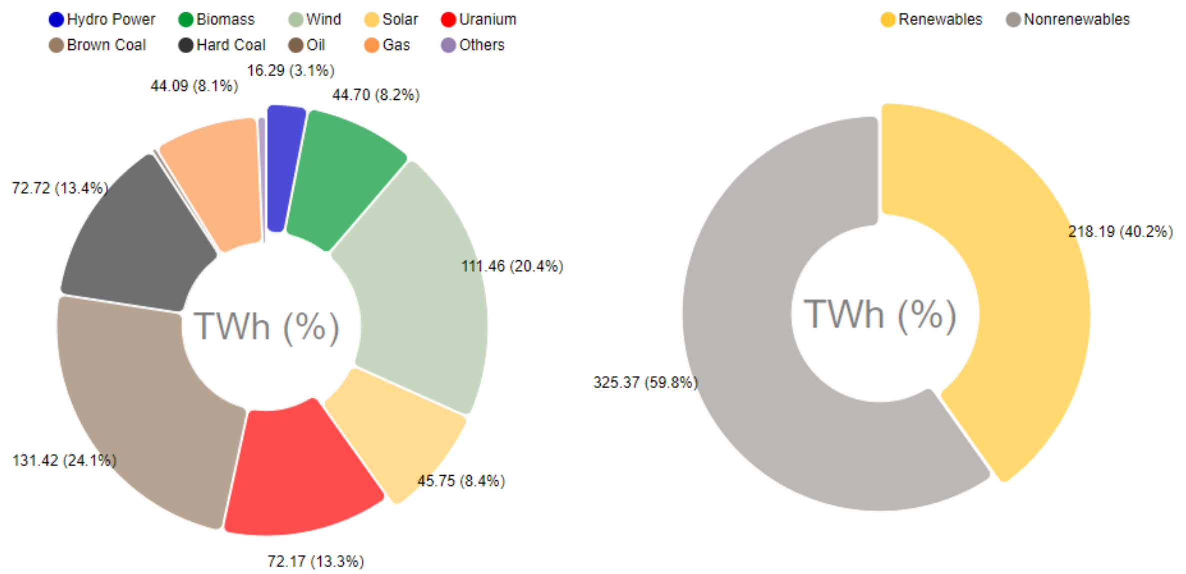

Figure 1.1 - Net public electricity generation in Germany in 2018 [8]

The largest part of renewable power will come from solar and wind as shown in Figure 1.2. Electric power from wind mills is expected to increase its contribution by 225 TWh in 2050, which is 39% of the overall produced energy; solar contributes 17%, at 100 TWh per year, while biomass reaches 60 TWh per year.

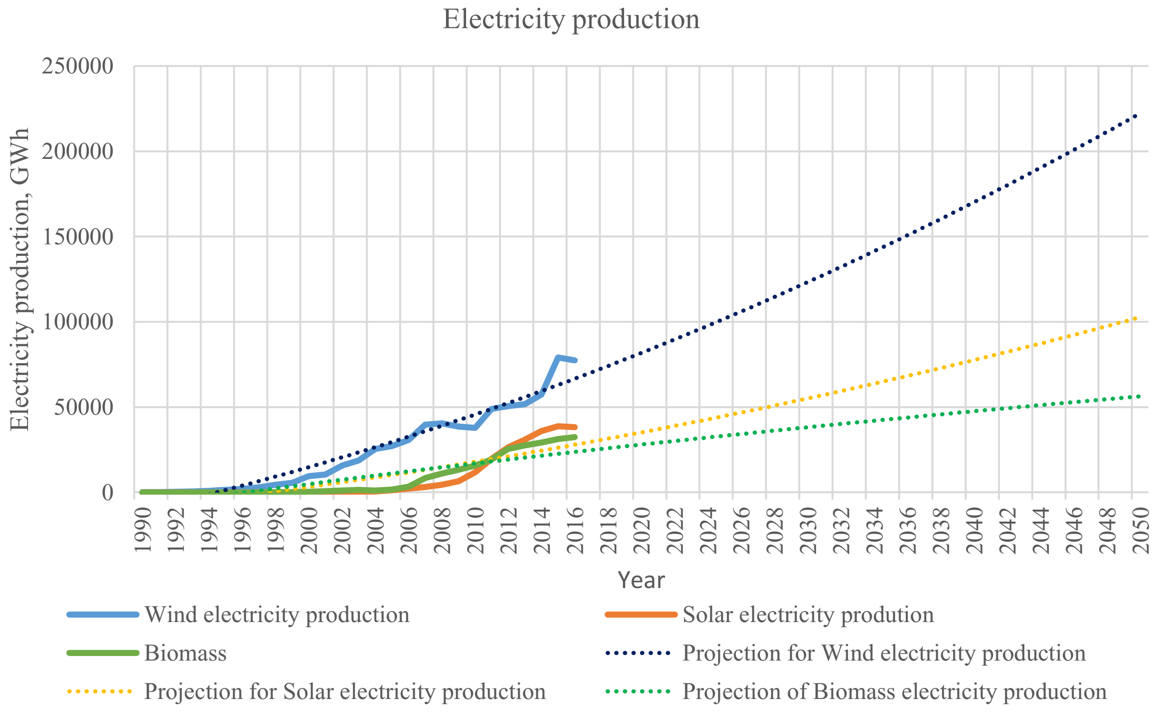

Figure 1.2 - Projection of energy generation

A transformation of the supply of energy from fossil to renewable sources is accompanied by substantial challenges. While biomass as a raw material might be stored for a long period of time, wind and solar are more difficult to handle. As battery systems do currently not have enough capacity and storage of electricity is very expensive, the developments in new long-term storage technology is one of the main challenges. Industrial key players like Siemens currently work on a new type of energy storage system based on hydrogen production [9]. The main idea is that excess energy from renewable energy sources can be converted into hydrogen from water by electrolysis, which is a non-toxic source of energy to consumers allowing a greater energy security and flexibility. As soon as there is energy shortage, hydrogen might be used in different applications such as power generation, domestic and industrial services, navigation and space [10].

Another challenge of the transformation is the concept for integrating high shares of renewables in the transport sector, which still faces environmental burdens. The transportation sector, which depends strongly on oil, is the second largest contributor of carbon dioxide (CO_2) emissions worldwide. The German's transportation sector faced an increase in energy requirements from 26.1% to 29.8%, where only 2% of GHG emissions have been reduced from

1990 to 2015 [11] - [13]. Integrating renewable energy into the transport sector is accompanied by the requirements to improve of fuel efficiency. The use of electricity in low carbon energy-efficient transport based on renewable energy sources is standing among promising alternatives for conventional fuel such as biodiesel, methanol. Currently, battery electrical vehicles (BEV) and fuel cell electrical vehicles (FCEV) are two promising options for a green transportation system. However, a shift to clean fuels will require new infrastructures and smart transition strategies. On the one hand, BEVs can already use the existing electricity generation and transportation and distribution (T&D) infrastructure. On the other hand, battery technology has still serious obstacles to be countered before it can be used safely in a consumer market. Issues with battery technology relate to for example the trade-off between energy capacity and weight, and recharging time. Unlike BEV-based mobility (with higher overall efficiency), FCEV powered by hydrogen could be considered as a flexible option in terms of a long range and shorter charging time. In addition, analysis of large-scale integration of these vehicles technologies showed a competitive advantage of FCEVs [14]. Moreover, hydrogen can be stored and transported at a lower cost than the cost of electrical energy. However, hydrogen is not a naturally occurring fuel of mineral origin; it can be produced from both renewable and non-renewable resources: from coal and biomass gasification, the reforming of natural gas, from water electrolysis, photo-electrolysis, water-splitting thermochemical cycle, photobiological production, and high temperature decomposition. Most of the conventional lower cost hydrogen production techniques lead to emission of significant amounts of CO_2 (about 500g CO2/kWhH_2), which diminishes the advantage of hydrogen [15]. Figure 1.3 shows the cost increase for hydrogen production versus the maturity level of the industry from the lowest cost hydrogen generation from natural gas up to expensive technologies using renewable sources, which are still not developed for market levels. Despite the expenses from using renewable technologies, CO2 emission levels are reduced as far as hydrogen production costs increase.

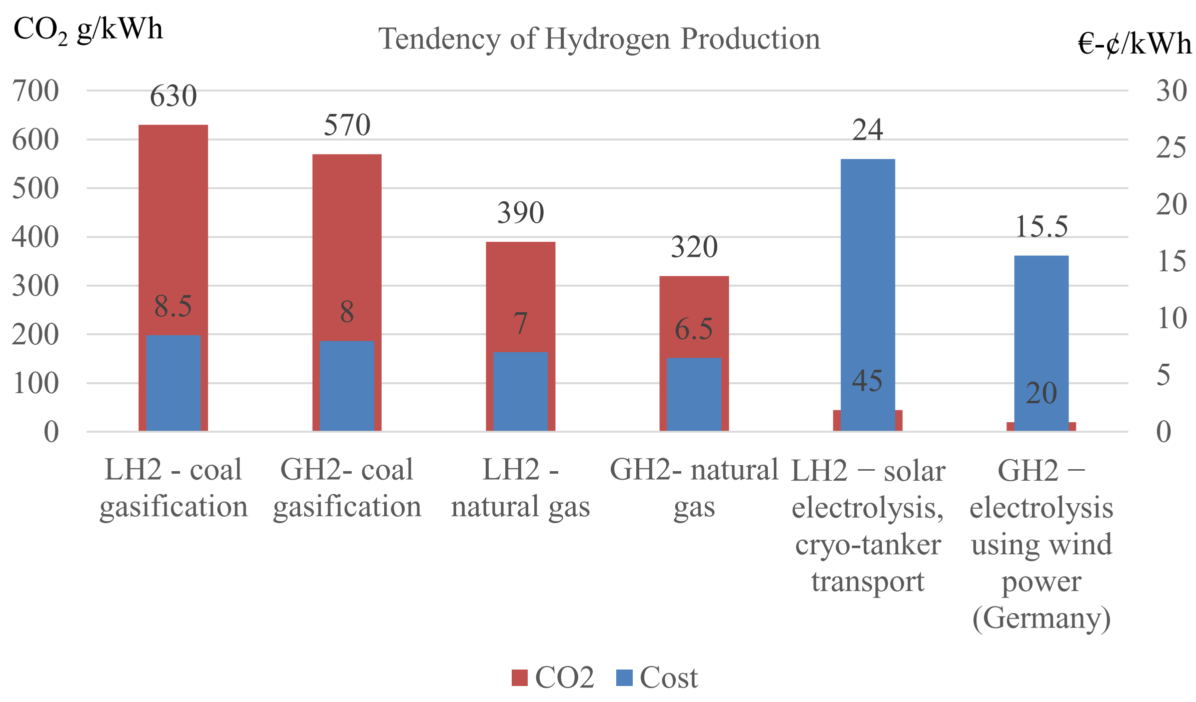

Figure 1.3 - Hydrogen costs (left) and CO2 emissions (right) per kWh H2 from selected hydrogen production from non-renewable (natural gas, coal) and renewable sources (solar, wind, nuclear) [15]

Moreover, hydrogen generation is only a part of the hydrogen production network, which can be defined as a supply chain consisting of several components (such as production, storage and distribution). For each of these stages a wide range of potential technological options exist. However, there are several factors, which should be considered when assessing the development of a hydrogen economy such as 1) energy efficiency, 2) environmental impact and 3) cost effective delivering pathways. Following those interests, alternative strategies to meet the most efficient, sustainable and cost-effective supply chains can be designed.

This thesis investigates the feasibility of hydrogen as transportation fuel from a supply chain point of view.

1.2. MAIN STATUS OF HYDROGEN FUELING AND ELECTRIC CHARGING

Transportation is one of the most promising sectors where the energy transition goals in Germany can be achieved. The Federal Government has supported the development of BEVs and FCEVs to make the transport sector more energy efficient, reduce its environmental impact and make it more sustainable. The government aims to install 5,000 fast charging and 10,000 standard charging stations between 2017 and 2020, and 400 hydrogen filling stations by 2023. Based on the total number of hydrogen fueling stations worldwide, Germany is currently taking 3d place with 13% after Japan (44 %) and USA (17 %). Currently Germany’s hydrogen fueling station network consists of 62 (108 in Europe) stations by mid-March 2019 while an additional 32 (49 in Europe) stations were under construction or being planned [16]. In addition, the number of charging points in Germany in December 2017 is estimated around 12,500, including more than 850 fast charging points [17]. The increase in the number of vehicles powered by alternative fuel leads to a rise in electricity demand and a moderate increase in demand for electricity from renewable sources.

1.3. HYDROGEN AND CHARGING INFRASTRUCTURE ANALYSIS

Shifting to hydrogen fuel requires building up a completely new hydrogen generation network considering an investment in large-scale FCEV production and high FCEV demand uncertainty. It stands behind the development of a hydrogen supply chain (HSC). HSC based on renewable electricity will increase total demand for electricity. Thus, it will raise integration rate of renewable electricity into energy supply chain. Due to HSC is able to use local renewables as primary energy carriers, reducing of overall dependence on imported energy will increase geopolitical fuel supply security. Additionally, the hydrogen infrastructure can be used to supply all vehicles types and has the potential to supply other transportation modes such as ships, trains or plains (see Figure 1.4). Moreover, hydrogen refueling is similar to a conventional fueling process perceived from a customer’s view (it is clear that a hydrogen infrastructure is very different than the current gasoline/gas network infrastructure).

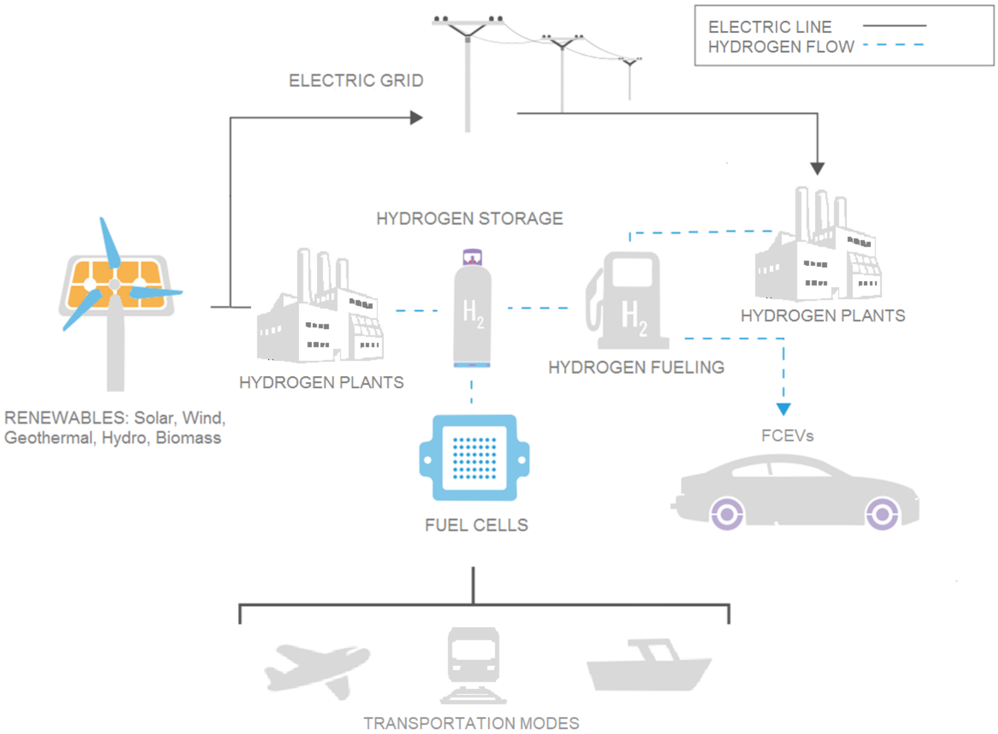

Figure 1.4 - Diagram of hydrogen transportation application

Moreover, it can be easily adapted to different demand situations such as “hydrogen as fuel” demand or “hydrogen as feedstock” demand (synergies with other Power-to-X technologies). Noted, hydrogen itself is regarded as suitable option for long-term storage of excess renewable energy. However, the development of a HSC requires a fundamental change in the existing fuel infrastructure. A depreciation of the installed fossil infrastructure will lead to lock-in a developing hydrogen infrastructure.

On the other hand, there is a well developed electric grid, which can guarantee the stability of BEVs charging. In addition, charging infrastructure can easily be extended. Moreover, BEVs can use electricity directly from the grid making them more efficient than FCEVs. In addition, BEVs can be home-charged in the private parking spaces. The charging infrastructure can also be used to supply only light duty vehicles and passenger cars. In addition, BEV charging time is higher than FCEV fueling. As batteries of BEV are designed for daily use, there are no options for seasonal storage capacities that hydrogen can offer. Results of infrastructure analysis for both configurations are presented in Table 1.1.

Table 1.1 - Infrastructure analysis

	Hydrogen infrastructure	Charging infrastructure
+	• Suitable for all vehicle types • inbuilt large-scale energy storage • Synergies with other PtX technologies • No change in the fueling process	• Existing infrastructure • Efficiency of the electricity supply chain • Home charging
-	• No developed infrastructure • Efficiency of the hydrogen supply chain • Lock-in effects	• Limited applications • No inherent seasonal energy storage • Charging time

1.4. CHALLENGES IN OPTIMAL DESIGN AND PLANNING

The work presented in this thesis shows how mathematical modeling and optimization tools can be used to describe, analyze and optimize a HSC network addressing the aforementioned challenges of the supply transformation to renewable sources of energy such as integrating high shares of renewables in the transportation sector. A thorough literature review on the use of mathematical programming to study supply chain design reveals that this is a powerful approach [18]–[21] . Development and evaluation of an optimization model that can be used to solve a HSC network design problem are required. This model can assist in determining the optimal configuration of the network considering supply and demand requirements. The Advanced Integrated Multidimensional Modeling System (AIMMS) is used as optimization platform for the implementation of the network model.

1.5. SCOPE AND OBJECTIVES

Hydrogen offers a multitude of advantages over existing fuels, especially in transportation applications: the energy density of hydrogen is much higher than other fuels such as methanol, diesel, kerosene or petrol. The FCEV fuelled by hydrogen can enhance the decarbonization of the transport sector. The use of hydrogen can also improve the security of primary energy supplies increasing the role of renewable energy. However, one of major challenge is the high final cost to of hydrogen infrastructures as compared to the current fuels. In addition, there are still many safety concerns for hydrogen which can be hazardous, and risk management is essential to ensure the save use of hydrogen. However, it is no more dangerous than other flammable fuels such as natural gas and gasoline.

In this thesis, a hydrogen production infrastructure for the transport sector is mapped that is sustainable and functions under varying conditions. Germany is chosen as a case study due to its progressive policies towards increasing the use of renewable energy sources and lowering greenhouse gas emissions.

The aim of this thesis is to prove that the transport sector in Germany is ready to shift from fossil fuels to hydrogen and to develop a strategy for evaluating the feasibility of a hydrogen economy.

In this thesis an optimization model is developed and evaluated that can be applied to solve a HSC network design problem forecasting up to 2050 considering the different objectives, i.e. cost, environmental impact, safety.

The developed model of HSC is designed to answer the following questions:

- Is the hydrogen fuel cost competitive with the current fuel cost?
- Does a hydrogen infrastructure offer a sustainable solution to the decarbonization problem?
- Which is the safest configuration for the HSC?
- What is the best option for production, storage and distribution of hydrogen?
- What are the most cost effective configuration of a HSC in case we include demand uncertainty?

1.6.THESIS OUTLINE

In **Chapter 2**, a snapshot mathematical model of HSC network is developed. The model is used to identify the best hydrogen infrastructure pathways making decisions regarding the primary energy source, production, storage and distribution networks. In this chapter, the HSC infrastructure is setup for passenger transport in Germany in 2030 and 2050. Two scenarios are evaluated, including a full range of conventional- and only renewable resources to produce hydrogen. **Chapter 3** extends the HSC model considering environmental impact and safety issues. This chapter gives an analysis of mono- and multi-objective approaches, where the trade-off results are obtained by using the epsilon constraint method. **Chapter 4** addresses the demand uncertainty issues through stochastic optimization. A stochastic model is setup and compared with its deterministic equivalent. Finally, the overall conclusion and recommendations are presented in **Chapter 5**. In this chapter, alternative strategies for hydrogen application are discussed to ensure economic feasibility.

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2. DESIGN OF HYDROGEN SUPPLY CHAINS

This chapter presents a comprehensive investigation of the feasibility of hydrogen as transportation fuel from a supply chain point of view. It introduces an approach for the identification of the best hydrogen infrastructure pathways making decisions regarding primary energy source, production, storage and distribution networks in Germany. The objective is to minimize of the total hydrogen supply chain (HSC) network cost for Germany in 2030 and 2050 years. Two scenarios are evaluated, including a full range of conventional- and "green" technologies using only renewable resources. The resulting model is a mixed integer linear program (MILP) that is solved with the Advanced Integrated Multidimensional Modeling System (AIMMS). It is noted that, renewable energy as a power source has a potential to replace commonly used fossil fuels in the near future: renewable electricity production can satisfy personal needs such as household's energy demand and hydrogen based fuel demand. Due to the high energy consumption a water electrolysis technology becomes very competitive – if electricity prices decrease significantly. Implementation of fuel cell electric vehicles (FCEVs) powered by renewable hydrogen for the transport sector becomes feasible and actively contributes to the decarbonization of the energy system.

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2.1. INTRODUCTION

Due to increasing demand for energy, the development of sustainable and environmental friendly concepts such as the HSC is needed to replace non-sustainable alternatives to meet the global need for energy [1]. Many studies in the area of HSC design focus on network evaluation. The work of Hugo et al. takes all possible hydrogen alternatives for the design of an optimal hydrogen infrastructure in Germany in to consideration [2]. However, their model does not include the distribution of the energy sources and the ability of centralized hydrogen storage to satisfy the local demand. A study of Almansoori and Betancourt-Torcat investigated a number of strategic decisions for hydrogen fuel production and hydrogen delivery networks in Germany at large-scale considering emission targets and carbon tax as a part of the model formulation for 2030 [3]. The main objective in that study was to satisfy the hydrogen demand, which was determined by a fuel cell electric vehicles (FCEVs) penetration of 10% of the overall passenger transport. The results showed that liquefied hydrogen production by coal gasification facilities at large-scale and delivery via railway tank cars results in the best HSC network structure. Large-size facilities showed benefit compared to a small-scale facility because large facilities have a higher energy efficiency. Renewable energy such as wind- and solar energy were not included in that study due to technical- and economic hurdles such as the electricity price for water electrolysis technology and size-independent electrolyzer efficiency. The rate of renewable energy consumption to generate a unit of hydrogen for both sizes of electrolysis facility is identical as the electrolyzer efficiency is independent of the facility size. A similar model was developed for the United Kingdom [4]. The objective was the minimization of the cost of the network considering capital- and operating costs. The results showed the dominance of steam methane reforming technology. Large-scale electrolysis facilities were not considered due to a size-independent electrolyzer efficiency that was mentioned before.

This chapter introduces an approach to develop and evaluate an optimization model that can be used to solve a HSC network design problem forecasting for 2030 and 2050 while considering a full range of local factors such as i) energy sources distribution for hydrogen production, ii) local hydrogen demand and iii) distribution between the place of hydrogen production and hydrogen demand. The model is used to define the procurement of energy sources from the supplier, the type, the number and the location of a production facility, the hydrogen production form and the delivery of hydrogen to consumers. The logistics of renewable sources is also included into the model by accounting for personal needs such as household energy and hydrogen based fuel consumption. Moreover, all techno-economic parameters were collected for 2015. The German landscape provides an important case study as Germany has an immense potential to develop a sustainable hydrogen infrastructure [5].

2.2. NETWORK DESCRIPTION AND PROBLEM STATEMENT

2.2.1. PROBLEM STATEMENT

Given are the location and capacity of energy source suppliers, capital and operating costs for a large-scale hydrogen production, transportation and storage facilities of the network, under the conditions that:

1. location of storage facilities is fixed;
2. all natural gas is imported (despite a national 12% production of natural gas);
3. weighted average cost of capital for production, transportation and storage is 8%;
4. electricity is the main energy source to power rail freight transport [6];
5. the way of handling of residual waste is not considered;
6. secondary energy carriers have no economic value in this network model;
7. electricity price based on industrial electricity price for Germany.

The HSC consists of energy sources from different origins, large-scale hydrogen production technologies, hydrogen product form and the hydrogen distribution and storage (see Figure 2.1). Five types of energy sources are considered: wind- and solar energy, biomass, natural gas and coal. In addition, four hydrogen production technologies are included into the model: steam methane reforming, coal gasification, biomass gasification and water electrolysis. As hydrogen might be generated by different production technologies, it may be transported into two forms (i.e. liquid or gaseous), which determines the transportation mode that will be used. The liquid form (LH) could be stored in super-insulated spherical tanks and be distributed via two types of transportation modes: by railway tank car or via tanker truck. Gaseous hydrogen (CH) could be stored into pressurized cylindrical vessels and distributed via railway tube car or tube trailer. Each facility of the HSC includes: a technological option, a capacity, a location. The problem is concerned with finding the number and locations of the production facilities for a given demand, while minimizing the total operating HSC network cost.

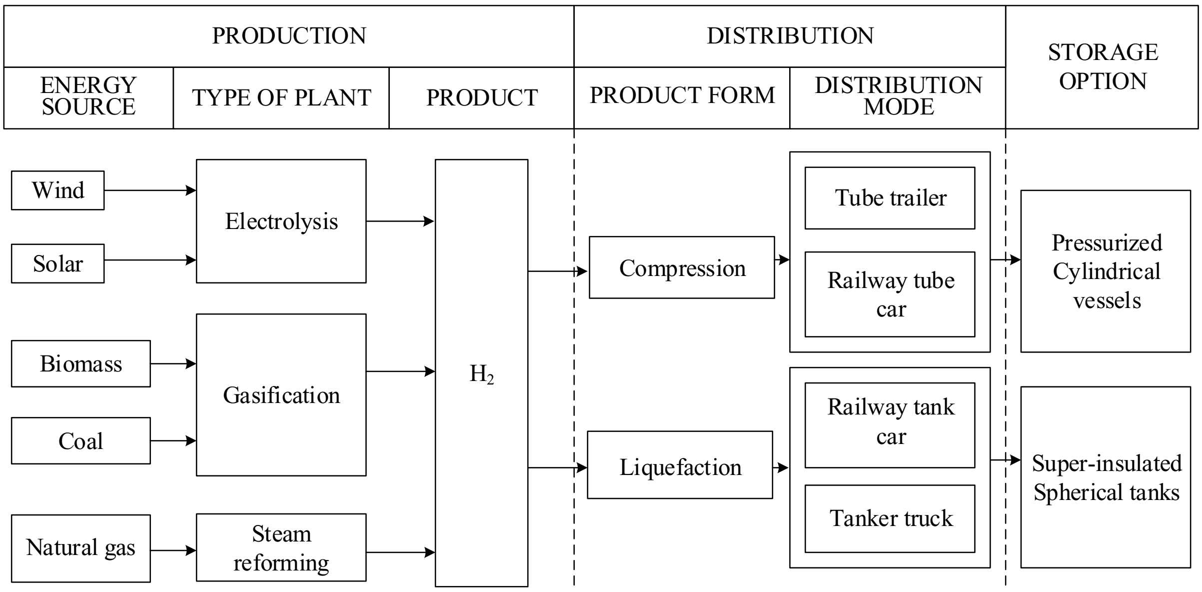

Figure 2.1 - Structure of the hydrogen supply and delivery chain

2.2.2. MODEL DESCRIPTION

In Figure 2.2 the superstructure of HSC model is shown [2]. The superstructure includes all possible connections between the model components. Ultimately, an optimization algorithm is used to search for the best strategy to minimize the costs of the HSC network. The superstructure consists a set of grid points (*g*, each grid point represents a German state), energy sources (*e*), different transportation (*t*) modes, different hydrogen production- (*p*) and storage (*s*) facilities. The transportation modes are used to distribute different types of hydrogen (*f*) from production facility to storage facility. In the following subsections, each component of the HSC model will be described in more detail.

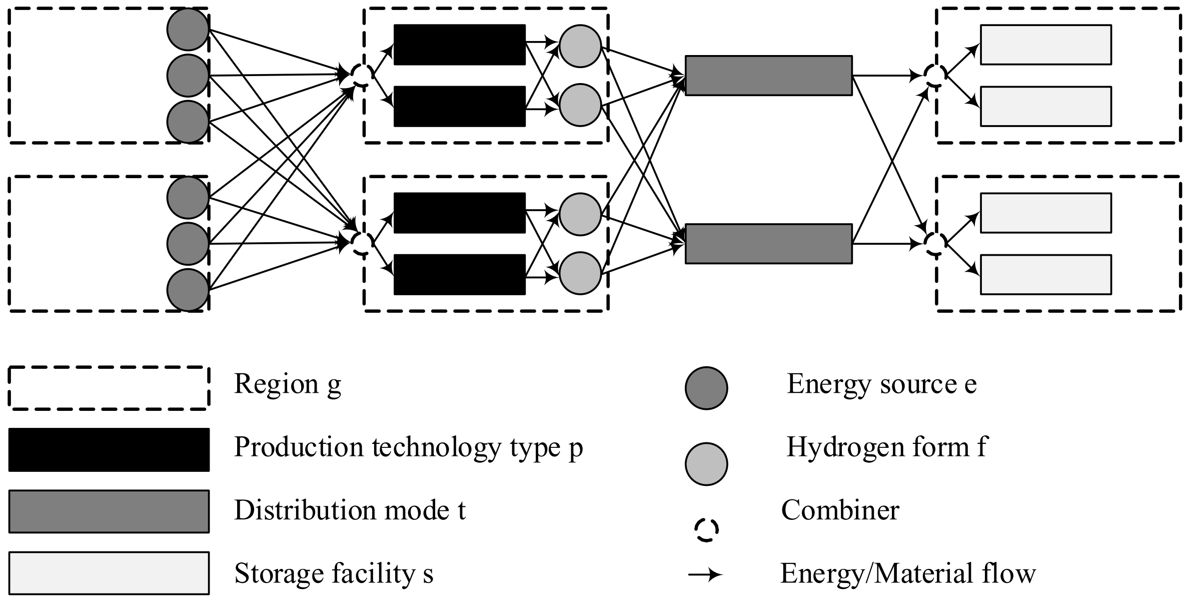

Figure 2.2 - Model superstructure

2.2.2.1.Grid

The territory of Germany is divided into 16 grid points, each of these grid points represents a German region. Moreover, the region's largest city is taken as the potential center for a hydrogen production facility and for a storage facility to satisfy the local demand and further product distribution to another region [3]. The total hydrogen demand was estimated based on FCEVs integration rate into the total number of passenger transports (public buses, light motor vehicle) available by 2030, and 2050, the average distance travelled and transport fuel economy (see Table 2.2) [7]. 2015 was used as the reference year for the calculations. All relevant parameters are listed in Table 2.1 [8]. Based on the projections of energy consumption from 1960 to 2050 (as shown in Figure 2.3), the household energy demand was forecasted.

Table 2.1 - Parameters used for total hydrogen demand calculation in Germany

Parameter	Passenger transport system in Germany in y year
Average distance travelled, AvD (km y^{-1} capita^{-1})	$44.3 \cdot y - 77407$
Fuel economy, FE (kg H2 km^{-1})	0.01
FCEV penetration rate, γ (%)	$0.83 \cdot y - 1674.93$

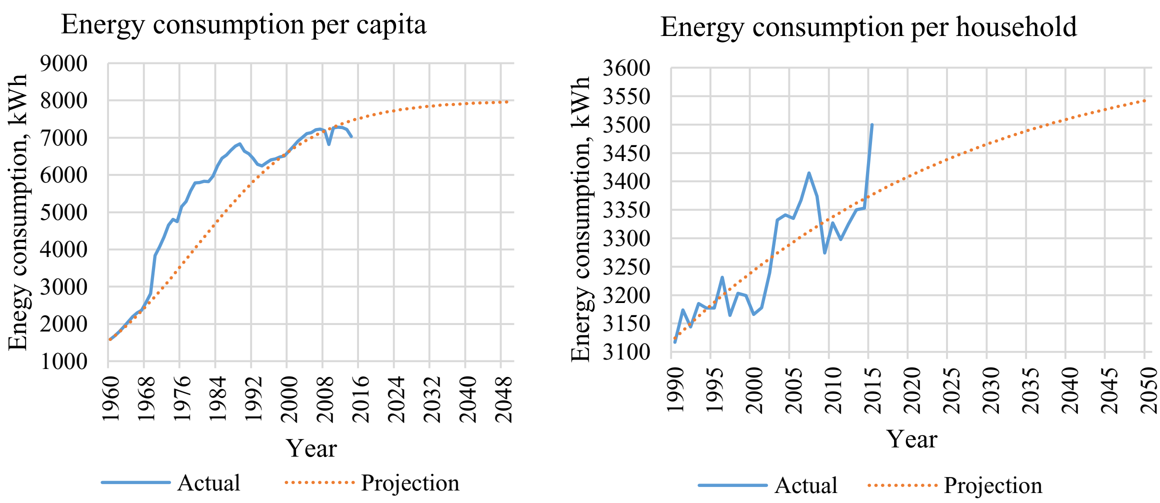

Figure 2.3 - Projection of energy consumption

Table 2.2 - Local energy and hydrogen demand for the 2030 and 2050

Grid points, g	German region	Population (MM)		Household energy Consumption (GWh d^{-1})		Hydrogen demand (ton d^{-1})	
		2030	2050	2030	2050	2030	2050
1.	Baden-Wurttemberg	10.80	10.10	34.20	32.74	372.51	995.20
2.	Bavaria	12.90	12.10	40.85	39.23	444.21	1181.43
3.	Berlin	3.70	3.60	11.72	11.67	127.00	354.89
4.	Brandenburg	2.30	1.90	7.28	6.16	80.55	191.13
5.	Bremen	0.60	0.60	1.90	1.95	22.24	59.12
6.	Hamburg	1.80	1.80	5.70	5.84	63.20	176.81
7.	Hesse	6.00	5.60	19.00	18.16	208.38	550.35
8.	Mecklenburg-Vorpommern	1.40	1.20	4.43	3.89	259.96	661.37
9.	Lower Saxony	7.50	6.70	23.75	21.72	50.12	118.55
10.	North Rhine-Westphalia	16.90	15.30	53.52	49.60	586.78	1515.14
11.	Rhineland-Palatinate	3.80	3.40	12.03	11.02	132.46	335.54
12.	Saarland	0.90	0.80	2.85	2.59	30.91	74.41
13.	Saxony	3.80	3.30	12.03	10.70	130.73	325.80
14.	Saxony-Anhalt	1.90	1.60	6.02	5.19	66.47	153.56
15.	Schleswig-Holstein	2.80	2.40	8.87	7.78	95.57	240.81
16.	Thuringia	1.90	1.60	6.02	5.19	66.35	157.81

2.2.2.2.Primary energy sources

Hydrogen can be produced from different sources such as water, natural gas, biomass and coal. This resource availability at each grid point plays an important role in defining the type and location of production technologies. In addition, the main problem of a domestic production facility is concerned with finding an appropriate energy source supplier. There are three opportunities related with the energy source consumption from i) a domestic grid point or ii) supply from neighboring grid points or iii) import from abroad.

2.2.2.3.Hydrogen production

Considering that hydrogen is not a naturally occurring fuel of mineral origin, different production technologies, including steam methane reforming, coal gasification, biomass gasification and water electrolysis, are generally used to generate it. Each alternative has fixed capital and operational costs (see Table A.1). The main decisions are to determine the type, location and number of production facilities. Each facility carries out large-scale hydrogen production (960 t H_2 d^{-1}) (see Table 2.3).

Table 2.3 - Capital and unit production costs of hydrogen production technologies [9].

Parameters	Facility type: Steam reforming		Coal gasification		Electrolysis		Biomass gasification	
Capacity (kg d^{-1})	960 000		960 000		960 000		960 000	
Product form	LH	CH	LH	CH	LH	CH	LH	CH
Facility capital cost (Mio $)	1082	775	1667	1123	1819	1572	1824	1454
Unit production cost ($ kg^{-1})	2.45	1.29	2.53	1.23	5.80	4.68	3.03	1.84

2.2.2.4.Hydrogen physical form

Hydrogen can be carried in two physical forms: liquid and gaseous. Each form is distributed by different transportation modes and might be stored in special storage facilities. The hydrogen form plays an important role in defining which transportation mode and storage facilities should be used. These decisions affect the final costs of the HSC network.

2.2.2.5.Transportation mode

The transportation mode is related to the hydrogen form (gas or liquid). The main decisions are to define the type transportation mode and its number of vehicles used to deliver the final product from production point to storage point. Each transportation mode has a specific capacity, capital cost, operating cost and delivery distance (see Table 2.4). It is noted that the operating cost is associated with the delivery distance.

Table 2.4 - Parameters used to estimate the capital and operating costs of transportation modes [10].

Transpiration mode	Tanker truck	Tube trailer	Railway tank car	Railway tube car
Capacity (kg $trip^{-1}$)	4082	181	9072	454
Total cost ($)	500000	250000	500000	300000
Fuel economy (km $unit^{-1*}$)	2.85		1.133	
Fuel price ($ $unit^{-1*}$)	1.22		0.07	

*unit for truck and trailer in l, for railway car in kWh

2.2.2.6.Storage facility

The storage facility, just like the transportation mode, is linked to the hydrogen form. Each type has a specific capacity, capital and operating cost (see Table 2.5). Storage facilities are installed at each grid point to satisfy the local hydrogen demand. Storage facilities could be located next to production plant or away from it.

Table 2.5 - Capital and unit storage costs of hydrogen storage facilities [4]

Storage type	Super-insulated spherical tanks	Pressurized cylindrical vessel
Product form	LH	CH
Capacity (kg)	540 000	540 000
Storage capital cost (M $)	122	1894
Unit storage cost ($ kg^{-1} d^{-1})	0,005	0,076

2.3. MODEL FORMULATION

This section represents the model constraints, the components and objective function, resulting in a MILP.

2.3.1. HOUSEHOLD ENERGY DEMAND

As mentioned earlier, the household's energy demand by grid point was estimated via projections of the German population [11] and energy consumption till 2050. The household's energy demand can be calculated as follows:

$$HHED_g = PN_g AvCon, \quad \forall g \tag{2.1}$$

where $HHED_g$ is the total energy demand at grid point g, PN_g represents the population at grid point g, $AvCon$ denotes average of household energy consumption. The demand must be covered by local energy sources generation and/or imports from neighboring grid points as follows:

$$HHED_g \le \sum_e \left(EESAv_{g,e} + \sum_{g''} EESN_{g'',g,e} \right), \quad \forall g \tag{2.2}$$

where $EESAv_{g,e}$ is amount of available energy source e in grid point g, which is used to satisfy the energy demand in grid point g, and $EESN_{g'',g,e}$ is the flowrate of the supplied energy source e from neighboring grid point g'' to grid point g. Preferably, the renewable energy source e will be used to satisfy the household energy demand.

2.3.2. DEMAND FOR A CERTAIN ENERGY SOURCE

The demand for a certain energy source must be satisfied to ensure production. The demand for a certain energy source is calculated as follows:

$$ESD_{g,p,e} = \sum_f HP_{g,p,f} \alpha_{e,p}, \quad \forall e,p,g \tag{2.3}$$

where $HP_{p,g,f}$ denotes the amount of produced hydrogen in the production facility p in the form f at grid point g and $\alpha_{e,p}$ denotes the ratio between *the* energy sources e consumption to produce 1 kg of hydrogen in production facility p. The demand must be covered by local power generation and/or imports from neighboring grid points as follows:

$$ESD_{g,p,e} \leq \sum_{g''} PESAv_{g'',g,p,e} + PES\mathrm{Im}_{g,p,e}, \quad \forall e,g \tag{2.4}$$

where $PESAv_{g'',g,p,e}$ is energy source flowrate to meet demand for a certain energy source e from the grid point g'' to the grid point g for production plants type p, and $PESIm_{g,e}$ is the flowrate importing energy source e to grid point g for production plants type p.

The price for the energy source consumed in year y is calculated as follows:

$$\begin{aligned} ESC = & \sum_{g'',g,p,e} \left(PESAv_{g'',g,p,e} (ESDis_e \, Dis_{g'',g} + ESCost_e) \right) + \\ & + \sum_{g,p,e} PES\mathrm{Im}_{g,p,e} \, ESICost_e \end{aligned} \tag{2.5}$$

where $ESICost_e$ represents the energy source e import price, $ESCost_e$ denotes the energy source e price, generated locally, $ESDis_e$ is the delivery price for energy source e, and $Dis_{g'',g}$ is the distance between grid points.

2.3.3. HYDROGEN DEMAND

The hydrogen demand HD_g by grid point p can be calculated as follows:

$$HD_g = \gamma PN_g AvD \cdot FE, \quad \forall g \tag{2.6}$$

where γ represents the FCEVs penetration rate, AvD is the average distance travelled by a person, and FE denotes the fuel economy. The demand must be satisfied by local production and/or import from neighboring grid points as follows:

$$HD_g \leq \sum_{f,t,g'} HF_{g',g,t,f}, \quad \forall g \tag{2.7}$$

where $HF_{g',g,t,f}$ is hydrogen flowrate in the form f from a neighboring grid point g' to g via transportation mode t.

2.3.4. HYDROGEN GENERATION.

The hydrogen production is described as follows:

$$HP_{g,f} = \sum_p HP_{g,p,f}, \quad \forall g,f \tag{2.8}$$

where $HP_{g,f}$ represents the hydrogen generation in the form f at grid point g, and $HP_{p,g,f,}$ denotes the amount of produced hydrogen in the production facility p in the form f at grid point g. The hydrogen production rate is constrained by a maximum and minimum capacities as follows:

$$MinPCap_p NPF_{g,p,f} \leq HP_{g,p,f} \leq MaxPCap_p NPF_{g,p,f}, \quad \forall g,p,f \tag{2.9}$$

where $MaxPCap_p$, $MinPCap_p$ is the max/min production capacity for hydrogen production facility p, $NPF_{g,p,f}$ represents number of installed production technologies p at grid point g. Each production plant has an associated capital- and operating cost, the total daily production cost is given by:

$$PC = \sum_{g,p,f} \left(\left(PCC_{p,f} NPF_{g,p,f} AF_p \right) / OP + HP_{g,p,f} POC_{p,f} \right) \quad (2.10)$$

where $PCC_{p,f}$ represents the capital cost of facility p, producing hydrogen in form f, AF_p is an annuity factor for facility p, OP represents the operating period, and $POC_{p,f}$ denotes the hydrogen production cost in form f at facility p.

2.3.5. HYDROGEN DISTRIBUTION

The hydrogen flow in form f from grid point g to grid point g' will exist if the transportation mode t has been settled:

$$MinHF_{t,f}\, X_{g,g',t,f} \le HF_{g,g',t,f} \le MaxHF_{t,f}\, X_{g,g',t,f}, \quad \forall g,g',t,f \quad (2.11)$$

where $MinHF_{t,f}$, $MaxHF_{t,f}$ are min/max product flow rate, $X_{g,g',t,f}$ is binary variable, which equals 1 if product transportation in form f from grid point g to grid point g' by transportation mode t is established. It is noted that products can be imported to a particular grid point from neighboring grid points or be exported to other grid points in one direction:

$$Q_{g,f} \ge X_{g,g',t,f}, \quad \forall g,g',t,f: g <> g' \quad (2.12)$$

$$W_{g,f} \ge X_{g',g,t,f}, \quad \forall g,g',t,f: g <> g' \quad (2.13)$$

$$W_{g,f} + Q_{g,f} \le 1, \ \forall g,f \quad (2.14)$$

where $Q_{g,f}$, $W_{g,f}$ are binary variables, which equal 1 if product in form f is exported/imported respectively. The product flowrate by transportation mode t from g to g' is given as follows:

$$HP_{g,f} \ge \sum_{t,g'} HF_{g,g',t,f}, \quad \forall g,f \quad (2.15)$$

It is noted that the product can only move in one direction between grid points. The total distribution cost, calculated as the sum of the operating and capital costs, is represented as:

$$TC = \sum_{f,t,g,g'} \left(\left(TCC_{t,f} NTU_{g,g',t,f} AF_t \right) / OP \right) + FC + LC + MC \quad (2.16)$$

where $TCC_{t,f}$ denotes the capital cost of transport mode t for the distribution of hydrogen in form f, $NTU_{g,g',t,f}$ is the number of transport unit t used for the hydrogen distribution in the form f from g to g', AF_t is an annuity factor for transport mode t, FC is fuel cost, LC is labour cost, MC is maintenance cost.

The number of vehicles t required in grid point g to serve local and regional demand of hydrogen produced in the form f is given as follows:

$$NTU_{g,g',t,f} \ge HF_{g,g',t,f} \left(\frac{2Dis_{g,g',t}}{AvS_t} + LUT_t \right) \Big/ \left(MA_t \cdot TCap_{t,f} \right) + ExT_{g,g',t,f}, \quad (2.17)$$

$$\forall sc,ts,g,g',t,f$$

where $Dis_{g,g',t}$ is average distance travelled by transportation mode t to serve local and regional demand, AvS_t is average speed of transportation mode t, LUT_t is load/unload time for transportation mode t, MA_t is transportation mode t availability, $TCap_{t,f}$ is capacity of transportation mode t to distribute produced hydrogen in form f, $ExT_{g,g',t,f}$ is continuous variable in scenario sc with value between 0 and 1, which is used to take an integer value for $NTU_{g,g',t,f}$ (modification was suggested by De-León Almaraz et al [12]).

The daily fuel cost is calculated as follows:

$$FC = \sum_{g,g',t,f} \frac{FP_t}{FET_t} 2Dis_{g,g',t} HF_{g,g',t,f} \Big/ TCap_{t,f} \tag{2.18}$$

where FP_t represents fuel price for transportation mode t, FET_t denotes the fuel economy for transportation mode t.

The labor cost is calculated as follows:

$$LC = \sum_{g,g',t,f} DW_t \, HF_{g,g',t,f} \left(\frac{2Dis_{g,g',t}}{AvS_t} + LUT_t \right) \Big/ TCap_{t,f} \tag{2.19}$$

where DW_t represents driver wage, who drives transportation mode t.

The maintenance cost is calculated as follows:

$$MC = \sum_{g,g',t,f} ME_t \, 2Dis_{g,g',t} HF_{g,g',t,f} \, / TCap_{t,f} \tag{2.20}$$

where ME_t denotes maintenance cost for transportation mode t.

2.3.6. HYDROGEN STORAGE

The required hydrogen storage is constrained by maximum and minimum capacities as follows:

$$MinSCap_{s,f} NSF_{g,s,f} \leq HSInv_{g,s,f} \cdot \tau \leq MaxSCap_{s,f} NSF_{g,s,f}, \quad \forall g,s,f \tag{2.21}$$

where $NSF_{g,s,f}$ denotes the number of storage facilities s holding hydrogen in form f at grid point g, and $MaxSCap_{s,f}$, $MinSCap_{s,f}$ represent the maximum and minimum capacities of storage facility s for holding hydrogen in the from f, $HSInv_{g,s,f}$ is inventory of product f in the storage facility s at grid point g, τ is total product storage period.

The hydrogen inventory level at the storage facility is described as follows:

$$\sum_{s,f} HSInv_{g,s,f} = HD_g, \quad \forall g \tag{2.22}$$

The total hydrogen storage cost is calculated as follows:

$$SC = \sum_{g,s,f} \left(\left(SCC_{s,f} NSF_{g,s,f} AF_s \right) / OP + SOC_{s,f} HSInv_{g,s,f} \right) \tag{2.23}$$

where $SCC_{p,f}$ denotes the capital cost for storage facility s holding hydrogen in the form f, AF_s is annuity factor for the s storage facility, $SOC_{p,f}$ is the operating cost to store 1 kg of hydrogen in the form f at storage facility s.

2.3.7. OBJECTIVE FUNCTION

The total cost of HSC network is given as follows:

$$TotalCost = PC + SC + TC + ESC \qquad (2.24)$$

The right-hand side of Eq. (2.24) contains four parts: the costs of hydrogen production (*PC*), transport (*TC*), storage (*SC*), and energy sources (*ESC*). The objective is to minimize the total cost finding the combination of network components to satisfy the local hydrogen demand under the given constraints. The model is coded in AIMMS and is solved with CPLEX 12.8. The model consists 21253 constraints and 16852 continuous variables, and 4353 integer variables.

2.4. CASE STUDY

Almansoori and Betancourt-Torcat [3] concluded that the development of a HSC in Germany is economically feasible for the following reasons: the government is reaching the decarbonization target for private transport and reduction of greenhouse gases of at least 85% by 2050.

To validate the model, a future HSC scenario analysis for Germany was performed. The data was collected from the Federal Statistical Office of Germany [11], the Fraunhofer Institute [13] for Solar Energy Systems ISE, and Almansoori and Betancourt-Torcat [3].

This chapter considers two case studies. Each case represents a design of an HSC network for Germany for 2030 and 2050. The first case study considers a scenario to satisfy local hydrogen demand on the HSC by using the whole range of available technologies. The second case considers a "green" scenario, which represents the ability to satisfy local personal needs (local household's energy demand first and hydrogen based fuel demand after using rest of energy sources) by using only renewable sources (see Table A.5).

2.5. RESULTS AND DISCUSSION:

2.5.1. BASE CASE SCENARIO

The optimization results show that 3 and 8 large coal gasification hydrogen facilities are selected as most economic option to satisfy hydrogen demand in 2030 and 2050 respectively for the first scenario (see Table A.2). Capital and operating costs for a coal gasification facility are very low: in energy use the coal gasification facility only costs 0.03 \$ kg^{-1} which is around 5 times less then natural gas (0.14 \$ kg^{-1}) and 1.7 times less than biomass or wind and solar energy (0.05 \$ kg^{-1}) (see Table A.1). Facilities and their interconnections are shown in Figure 2.4. The result is comparable with the outcomes of the work by Almansoori [3] for 2030. In both studies, coal gasification technology is selected as the most economic option. One of the production facilities is installed in Potsdam, another in Cologne, and the last one in Munich for both studies. The locations of the production facilities promote the product distribution to regional storage facilities. Additionally, each production facility includes nearby storage facilities to satisfy the local hydrogen demand.

Figure 2.4 - Hydrogen supply chain network for 2030 (Base scenario)

Furthermore, hydrogen is generated in liquid form. Germany has a well-developed railway infrastructure, i.e. the railway tank car is selected as preferred transportation mode in both studies. It is noted that a large part of the German rail freight transport is electrified, which means that the rail transport is a clean type of distribution. As hydrogen is generated in liquid form, super-insulated spherical tanks are used to minimize heat loss. The total cost of the HSC is approximately 10.9 and 27.9 Mio \$ d^{-1} for 2030 and 2050 respectively, which means 3.98 and 3.93 \$ kg^{-1} of H_2 (the hydrogen price is 1.3% less in 2050 than in 2030). In case the hydrogen price is decreasing in 2050, it might motivate a replacement of gasoline cars by

FCEVs. However, the hydrogen price (3.98 \$ kg^{-1}) is higher than as the one in Almansoori's work (3.03 \$ kg^{-1}) as electricity price at that Almansoori is using equals 0.12 \$ kWh^{-1} when Almansoori assumed 0.05 \$ kWh^{-1}, and it is close to the average unit cost expected in Europe in 2030 (around 3.2 \$ kg^{-1}). In 2050, plants are installed in Stuttgart, Berlin, Frankfurt, Hamburg, Rostock and Manz (see Figure 2.5).

Figure 2.5 - Hydrogen supply chain network for 2050 (Base scenario)

2.5.2. THE "GREEN" SCENARIO

Despite the costs for water electrolysis technology, the "green" scenario considers the opportunity to satisfy the local hydrogen demand and the household energy demand by wind- and solar energy (see Table A.3). It was found out that, after meeting the household's energy demand, 3 and 8 large electrolysis-based facilities are required in 2030 and 2050 respectively. The "green" scenario shows that hydrogen facilities need to be built in Munich, Potsdam and Hannover by 2030 (see Figure 2.6), and in 2050 they need to be installed in Hannover, Potsdam, Munich, Stuttgart, Rostock, Halle, Cologne and Mainz (see Figure 2.7). The total costs of the HSC are approximately 28.7 and 74.0 Mio \$ d^{-1} for 2030 and 2050 respectively, which means 10.49 and 10.43 \$ kg^{-1} of H_2. The hydrogen price decreased by 0.5% from 2030 to 2050. However, this is not a reasonable price for industry. In addition, expenses related with the household's energy consumption account for 25.3 and 23.4 Mio \$ d^{-1} for 2030 and 2050 respectively, which shows electricity price reduction for this sector.

Figure 2.6 - Hydrogen supply chain network for 2030 ("green" scenario)

Figure 2.7 - Hydrogen supply chain network for 2050 ("green" scenario)

2.5.3. CASE COMPARISON

As shown in Table 2.6, the cost analysis has been done for the two cases in 2030. For the hydrogen pathways, water electrolysis consumes more electricity than other technologies (see Table A.1). This energy consumption is about 47.3 kWh kg^{-1} H_2, with a specific power cost to supply the electrolysers of 0.07 \$ kWh^{-1} and additional 11 kWh kg^{-1} H_2 with the price 0.12 \$ kWh^{-1} for hydrogen liquefaction/compression. The capital- and operating costs for a hydrogen production facility are only related to the required power to achieve the targeted hydrogen production rate. The specific energy consumption hydrogen production facility's is the sum of the specific power demand for hydrogen production and the general power demand for any electrical facility. Due to the high energy consumption an electricity price reduction can make water electrolysis technology feasible (see Table A.4).

Table 2.6 - HSC cost for two case studies in 2030

Network Expenses	Base Scenario	“Green” scenario
Raw material Cost M$ d^{-1}	0.44	9.17
Production Capital Cost M$ d^{-1}	1.40	1.52
Production Operating Cost M$ d^{-1}	6.94	15.89
Storage Capital Cost M$ d^{-1}	1.97	1.97
Storage Operating Cost M$ d^{-1}	0.01	0.01
Transportation Capital Cost M$ d^{-1}	0.02	0.03
Transportation Operating Cost M$ d^{-1}	0.09	0.13
Total Cost M$ d^{-1}	10.88	28.73
Hydrogen cost $ kg^{-1}	**3.98**	**10.49**

The electricity price might be decreased by several strategies such as integration of more renewable electricity generation facilities such as wind mills, solar panels, wave pumps, or using off-peak electricity. However, the installation of new energy facilities is only realistic in places with suitable geographical conditions (location with high availability of renewable energy sources) providing continuous energy generation. Moreover, the modification of existing conventional methods or development of innovative methods is necessary for reduction of conversion losses and capital costs investment. There are a number of problems related with conventional electrolysers such as safety risks due to leaks, stack degradation, membrane deterioration, difficulties with starting the system after shutdown, and freezing of membranes, especially during cold weather. All these problems require technological improvements. In addition, analysis of the impact of intermittency of renewable energy sources on the electrolysis system performance and reliability is required to map the uncertainty.

2.6. CONCLUSION

In this chapter, a general optimization model for a HSC network is proposed. The results show that renewable energy has the potential to replace fossil fuels as a power source, especially in transportation sector: renewable electricity production can satisfy personal needs such as household’s energy demand and hydrogen based fuel demand by the currently installed wind- and solar power plants. The model was applied to design strategies of developing the future structure of a HSC network for Germany, considering a full range of local factors and geographical conditions. Due to the high energy consumption an low electricity price, water electrolysis technology becomes very competitive. Hydrogen production in liquid form is preferable, distributed via railway tank car and stored into super-insulated spherical tanks. Moreover, the case analysis shows that the hydrogen price decreases significantly up till 2050, which motivates a replacement of gasoline cars by FCEVs. This transition also enables a full decarbonization of power sector.

2.7.NOMENCLATURE

INDICES

e	type of energy source
f	type of hydrogen physical form
g	grid points, each grid point represents German state
p	type of hydrogen production facility
s	type of storage facility
t	type of transportation mode

ABBREVIATIONS

AIMMS	Advanced Integrated Multidimensional Modeling System
CH	compressed-gaseous hydrogen
FCEV	fuel cell electric vehicle
HSC	hydrogen supply chain
LH	liquid hydrogen
MILP	mixed integer linear program

CONTINUOUS VARIABLES

$EESAv_{g,e}$	amount of available energy source *e* in the grid point *g*, which is used to satisfy energy demand in grid point *g* [kWh d^{-1}]
$EESN_{g",g,e}$	the flowrate of the supplied energy source *e* from neighboring grid point *g”* to grid point *g,* , which is used to satisfy energy demand in grid point *g* [kWh d^{-1}]
ESC	total cost for the energy source consumed for hydrogen production [$ d^{-1}]
$ESD_{g,p,e}$	daily energy source demand [kWh d^{-1}]
$ExT_{g,g',t,f}$	continuous variable in scenario sc with value between 0 and 1, which is used to take an integer value for $NTU_{g,g',t,f}$
FC	fuel cost [$ d^{-1}]
$HF_{g,g',t,f}$	hydrogen flowrate in the form *f* from grid point *g* to *g’* via transportation mode *t* [kg d^{-1}]

$HP_{g,f}$	hydrogen generation in the form *f* at grid point *g* [kg d^{-1}]
$HP_{g,p,f}$	amount of produced hydrogen in the production facility *p* in the form *f* at grid point *g* [kg d^{-1}]
$HSInv_{g,s,f}$	inventory of product *f* in the storage facility s at grid point *g* [kg]
LC	labour cost [$ d^{-1}]
MC	maintenance cost [$ d^{-1}]
PC	daily production costs[$ d^{-1}]
$PESAv_{g'',g,p,e}$	energy source flowrate to meet demand for a certain energy source *e* from the grid point *g''* to the grid point *g,* which is used to satisfy energy source demand for hydrogen production [unit e d^{-1}]
$PESIm_{g,p,e}$	flowrate importing energy source *e* to grid point *g*, which is used to satisfy energy source demand for hydrogen production [unit e d^{-1}]
SC	daily storage costs[$ d^{-1}]
TC	daily distribution cost [$ d^{-1}]
TotalCost	total daily cost of HSC network [$ d^{-1}]

INTEGER VARIABLES

$NPF_{g,p,f}$	number of production facility *p* generating hydrogen in from *f* at grid point *g*
$NSF_{g,s,f}$	number of storage facility *s* holding hydrogen in the form *f* at grid point *g*
$NTU_{g,g',t,f}$	the number of transport mode *t* used for hydrogen distribution in the form *f* from *g* to *g'*

BINARY VARIABLES

Xg,g',t,f	1 if product transportation in form *f* from grid point *g* to grid point *g'* by transportation mode t is established, otherwise 0
$Q_{g,f}/W_{g,f}$	1 if product in form *f* is exported/imported, otherwise 0

PARAMETERS

AvCon	average of household energy consumption [kWh d^{-1}]
AvD	the average distance travelled by personal car [km y^{-1}]
AvS_t	average speed of transportation mode *t* [km h^{-1}]
AF_p	annual factor for the facility *p* [%]
AF_s	annual factor for the *s* storage facility *s* [%]

AF_t	annual factor for the transport mode t [%]
$Dis_{g'',g}$	distance between grid points [km]
$Dis_{g,g',t}$	distance between grid points depending of type of transport [km]
DW_t	driver wage [$ h^{-1}]
$ESCost_e$	energy source e price in year y, generated locally [$ $unit^{-1}$ e]
$ESDis_e$	delivery price for energy source e [$ $unit^{-1}$ km^{-1}]
$ESICost_e$	energy source e import price [$ $unit^{-1}$]
FE	the fuel economy [kg H_2 km^{-1}]
FET_t	the fuel economy for transportation mode t [unit km^{-1}]
FP_t	fuel price for transport mode t [$ l^{-1}]
HD_g	hydrogen demand by grid point [kg d^{-1}]
$HHED_g$	total energy demand in the grid point g [kWh d^{-1}]
LUT_t	load/unload time for transportation mode t [h]
MA_t	transportation mode t availability [h]
$MinHF_{t,f}$/ $MaxHF_{t,f}$	min/max product flow rate [kg d^{-1}]
$MaxPCap_p$/ $MinPCap_p$	max/min production capacity for hydrogen production facility p [kg d^{-1}]
$MaxSCap_{s,f}$/ $MinSCap_{s,f}$	max/min capacity of storage facility s for holding hydrogen in the from f [kg]
ME_t	maintenance cost for transportation mode t [$]
OP	operating period [d y^{-1}]
$PCC_{p,f}$	capital cost of facility p, producing hydrogen in form f [$]
PN_g	population at the grid point g
$POC_{p,f}$	hydrogen production operating cost in form f at facility p [$ kg^{-1}]
$SCC_{s,f}$	capital cost for storage facility s holding hydrogen in the form f [$]
$SOC_{s,f}$	operating cost to store 1 kg of hydrogen in the from f inside of storage facility s [$ kg^{-1} d^{-1}]
$TCap_{t,f}$	capacity of transportation mode t to distribute produced hydrogen in form f [kg]
$TCC_{t,f}$	capital cost of transport mode t for distribution hydrogen in the form f [$]

GREEK LETTERS

$\alpha_{e,p}$	the ratio between energy sources *e* consumption to produce 1 kg [unit e kg^{-1} H_2]
γ	FCEVs penetration rate [%]
τ	total product storage period [d]

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APPENDIX A

Table A.1 - Capital and unit production costs of hydrogen production technologies [8]

Production technology	Steam reforming	Coal gasification	Water electrolysis	Biomass gasification
Product form	LH	LH	LH	LH
Design production capacity ton d^{-1}	960.00	960.00	960.00	960.00
Plant availability d	329	329	329	329
Annual production 10^3 ton	315.84	315.84	315.84	315.84
Fuel required per H_2 generated unit kg^{-1} H_2	3.16	5.33	47.60	11.26
Fuel consumed unit d^{-1}	3033.60	5116.80	45696.00	10809.60
Fuel price \$ $unit^{-1}$	0.14	0.03	0.05	0.05
CO_2 produced kg kg^{-1} H_2	17.40	30.30	0.00	32.10
SMR/Gasifier/Electrolyzer \$ $unit^{-1}$	317.25	239.85	1023.40	506.70
CO2 cost \$ kg^{-1}	0.06	0.06	0.06	0.06
Energy cost \$ kW^{-1}			516.00	
CO shift, cool and cleanup \$ kg^{-1} d^{-1} CO_2		20.00		15.00
Air separation unit \$ kg^{-1} d^{-1} O_2		28.00		27.00
O_2 consumed per H_2 generated		1.08		1.41
Dispenser rate kg h^{-1}	4000.00	4000.00	4000.00	4000.00
Number of Dispenser	10.00	10.00	10.00	10.00
H_2 Dispenser unit cost k\$	100.00	100.00	100.00	100.00
Power consumption kWh kg^{-1} H_2	11.00	11.00	11.00	11.00
Electricity cost \$ kWh^{-1}	0.12	0.12	0.12	0.12
Unit cost \$ kg^{-1} d^{-1} H2	318.22	877.74	1023.45	1027.94
Size factor Process	0.75	0.75	0.75	0.80
Unit liq/gas cost \$ kg^{-1} d^{-1} H_2	700.00	700.00	700.00	700.00
Size factor liq/gas	0.75	0.75	0.75	0.75
Unit storage cost \$ kg^{-1} H_2	19.00	19.00	19.00	19.00
Size factor of storage	0.70	0.70	0.70	0.70
Total process unit cost (UC) M\$	**746.89**	**1149.74**	**1254.65**	**1307.23**
General facilities cost 20% of UC M\$	149.38	229.95	250.93	261.44
Engineering Permitting 10% of UC M\$	74.69	114.97	125.46	130.72
Contingencies 10% of UC M\$	74.69	114.97	125.46	130.72
Working Capital, Land 5% of UC M\$	37.34	57.49	62.73	65.36
Total Capital Cost (CC) M\$	**1082.99**	**1667.13**	**1819.24**	**1895.48**
O&M 3% of CC M\$ y^{-1}	32.48	50.01	54.57	56.86
Fuel price M\$ y^{-1}	139.73	50.50	1052.38	177.82
Electricity cost M\$ y^{-1}	416.91	416.91	416.91	416.91
Fixed Operating Cost 5% M\$ y^{-1}	54.15	83.36	90.96	94.78
Capital Charges 12% of capital M\$ y^{-1}	129.96	200.06	218.31	227.46
Total Operating Cost M\$ y^{-1}	**773.24**	**800.84**	**1833.13**	**973.82**
Unit Production cost \$ kg^{-1}	**2.45**	**2.54**	**5.80**	**3.08**

Table A.2 - Results of the hydrogen supply by grid point (Base scenario)

Grid point, g	Year 2030			Year 2050		
	H2 produced (ton d^{-1})	H2 imported (ton d^{-1})	Local use (ton d^{-1})	H2 produced (ton d^{-1})	H2 imported (ton d^{-1})	Local use (ton d^{-1})
1		372.51		960.00	35.20	960.00
2	826.14		444.21	960.00	221.43	960.00
3		127.00			354.89	
4	952.77		80.55	960.00		191.13
5		22.24			59.12	
6		63.20		670.56		176.81
7		208.38		960.00		550.35
8		259.96		661.37		661.37
9		50.12			118.55	
10	958.54		586.78	960.00	555.14	960.00
11		132.46		960.00		335.54
12		30.91			74.41	
13		130.73			325.80	
14		66.47			153.56	
15		95.57			240.81	
16		66.35			157.81	
Total	**2737.44**	**1625.90**	**1111.54**	**7091.93**	**2296.72**	**4795.2**

Table A.3 - Results of the hydrogen supply by grid point ("Green" scenario)

Grid point, g	Year 2030			Year 2050		
	H2 produced (ton d^{-1})	H2 imported (ton d^{-1})	Local use (ton d^{-1})	H2 produced (ton d^{-1})	H2 imported (ton d^{-1})	Local use (ton d^{-1})
1		372.51		960.00	35.20	960.00
2	825.79		444.21	960.00	221.43	960.00
3		127.00			354.89	
4	951.65		80.55	546.02		191.13
5		22.24			59.12	
6		63.20			176.81	
7		208.38			550.35	
8		259.96		902.17		661.37
9	960.00		50.12	946.79		118.55
10		586.78		958.35	556.79	958.35
11		132.46		959.99		335.54
12		30.91			74.41	
13		130.73			325.80	
14		66.47		858.61		153.56
15		95.57			240.81	
16		66.35			157.81	
Total	**2737.44**	**2162.57**	**574.88**	**7091.93**	**2753.42**	**4338.5**

Table A.4 - HSC network cost depending of the energy price

Network Expenses "Green" scenario	Electricity price reduction		
	10%	50%	90%
Raw material Cost M$ d^{-1}	8.26	4.61	0.96
Production Capital Cost M$ d^{-1}	1.52	1.52	1.52
Production Operating Cost M$ d^{-1}	14.98	11.33	7.68
Storage Capital Cost M$ d^{-1}	1.97	1.97	1.97
Storage Operating Cost M$ d^{-1}	0.01	0.01	0.01
Transportation Capital Cost M$ d^{-1}	0.03	0.03	0.03
Transportation Operating Cost M$ d^{-1}	0.13	0.13	0.13
Total Cost M$ d^{-1}	26.90	19.61	12.31
Hydrogen cost $ kg^{-1}	9.83	7.16	4.50

Table A.5 - Initial availability of energy sources

Grid point, g	Primary energy source, e						
	Biomass (ton d^{-1})	Coal (ton d^{-1})	Natural gas (ton d^{-1})	Renewable energy source (GWh d^{-1})			
				Base scenario		"Green" scenario	
				2030	2050	2030	2050
1	1.99	0.00	0.00	25.85	43.57	0.00	10.83
2	4.62	0.00	0.00	61.50	104.09	20.64	64.87
3	0.00	0.00	0.00	0.34	0.57	0.00	0.00
4	1.92	95890.41	0.00	55.73	98.52	37.07	81.26
5	0.00	0.00	0.00	1.70	3.04	0.00	1.09
6	0.00	0.00	0.00	0.59	1.04	0.00	0.00
7	1.13	0.00	0.00	16.43	28.60	0.00	10.45
8	4.39	0.00	0.00	32.51	57.78	28.08	53.89
9	5.34	0.00	0.00	112.46	200.64	88.51	178.92
10	2.19	293041.10	0.00	46.47	81.43	0.00	31.83
11	0.63	0.00	0.00	29.67	52.37	0.00	41.34
12	0.06	0.00	0.00	3.81	6.63	0.63	4.04
13	2.46	95890.41	0.00	15.58	27.09	3.55	16.39
14	3.07	26027.40	0.00	42.32	75.07	36.31	69.88
15	2.91	0.00	0.00	47.50	84.74	33.52	72.16
16	2.26	0.00	0.00	14.38	25.22	8.36	20.04
Total	**32.97**	**510849.32**	**0.00**	**506.85**	**890.41**	**256.67**	**656.99**

3. MULTI-OBJECTIVE OPTIMIZATION DESIGN OF HYDROGEN SUPPLY CHAINS

This chapter presents a strategy for the design of a hydrogen supply chain network in Germany for minimum daily supply costs, minimum mitigation costs of CO2 and maximum network safety. The aim is to identify the best hydrogen infrastructure pathways while taking into account local factors such as the location of the hydrogen supply and demand, and distribution between the hydrogen production location and hydrogen demand points. In this chapter, extended model is solved as a multi-criterion decision making problem, where three objectives (costs, safety and environmental impact) are balanced. A three dimensional Pareto front is created using the epsilon constraint method. Utopia point analysis is used to make trade-off decisions in the Pareto front. Compared to the current internal combustion vehicle fuel with an average cost of 0.0645 $ per km, the hydrogen cost, of 0.0762 $ per km, proofs the potential for a hydrogen economy.

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3.1. INTRODUCTION

The transport sector, which depends strongly on oil, is the second largest contributor to carbon dioxide (CO_2) emissions worldwide. Significant improvements of fuel efficiency is required to reduce the carbon dioxide emissions. Among promising alternatives for conventional fuel such as biodiesel, methanol, the use of electricity in low carbon energy-efficient transport based on renewable energy sources such as fuel cell electrical vehicles (FCEV) powered by hydrogen. However, a shift to clean fuels will require new infrastructures and smart transition strategies. The main challenge is to build up a completely new hydrogen generation network considering an investment in large-scale FCEV production and high FCEV demand uncertainty [1]. It stands behind the development of a hydrogen supply chain (HSC) considering safety, economic and environmental impact issues.

A study of Jiyong Kim and Il Moon considers a bi-creterion assessment of a HSC network. The model they proposed determines cost-safety objectives, where the safety objective is based on the so called risk index method. However, the environmental impact is not considered [2]. The study of De-León Almaraz et al. focuses on the design of a HSC considering three objectives: cost, environmental impact and risk. It is solved by ε-constraint method. It is noted that this model does not include the energy source distribution [3]. The work of Almansoori investigated a number of strategic decisions to design HSC networks in Germany at large-scale considering emission targets and carbon taxes as a part of the model formulation for 2030 [4]. The study focuses on meeting the hydrogen demand, which was determined by a 10% implementation of FCEVs into the passenger transport system. Renewables were not included in that work due to technical- and economical hurdles related with size-independent electrolyzer efficiency and expenses for water electrolysis technology. The study of Lahnaoui focused on the identification of a cost-effective hydrogen infrastructure based on excess electricity from wind energy by 2050. It shows potential of FCEVs implementation into transport sector [5], however, also in this study the environmental impact was not considered.

In this chapter, the model that was developed in Chapter 2 is extended and used to identify the best hydrogen infrastructure pathways in Germany while balancing between multiple, conflicting objectives: the minimum daily supply costs, the minimum mitigation costs of CO2 and the maximum network safety. The extended model of the HSC network is focused on the passenger transport in Germany. It is solved as a multi-criterion decision making problem: costs, safety and environmental impact are balanced via the epsilon constraint method to generate the Pareto front. Often multi-objective optimization only considers two dimensions, the current work evaluates three target simultaneously through a Pareto trade-off. Four types of technologies to produce hydrogen are evaluated, namely coal gasification, steam methane reforming, biomass gasification and water electrolysis.

3.2. NETWORK DESCRIPTION AND PROBLEM STATEMENT

The problem statement introduced in Chapter 2 will be extended in this chapter with three important additions. Firstly, it is assumed that the relative risk of production plants, storage facilities and transportation modes are expected not to change under the various demand scenarios. Secondly, each production technology is coupled with an index *h* to consider different sizes, referred to as small (up to 10 t H_2 d^{-1}), medium (up to 150 t H_2 d^{-1}), and large (up to 480 t H_2 d^{-1}). Finally, the problem is concerned with finding the number and locations of the production facilities for a given demand, considering the minimum total operating cost, the minimum safety risk and the minimum environmental impact of HSC network.

3.3. INDEX-BASED RISK ASSESSMENT METHOD

Hydrogen is a flammable fuel just as gasoline and natural gas. Hydrogen can behave dangerously under specific conditions and wrong use may result in fatal accidents due to its burning or explosion. Thus, safety considerations must be satisfied for a sustainable hydrogen economy. The risk method described by Kim and Moon is applied in this study using the relative risk level for each type of hydrogen activity (production, storage, transportation) and relative impact levels of regions that may be a cause of harmful consequences [2]. The relative risk levels of the hydrogen activities are determined based on the results of Norsk Hydro ASA and the DNV report[6], where five risk levels from V to I according harmful consequences to people, the environment and facilities are described. The acceptance criterion of levels are as follows:

- ***Level V***

  People: Minor injury,

  Environment: Minor environment damage,

  Facilities: Minor;

- ***Level IV***

  People: Medical treatment and lost time injury,

  Environment: damage of short duration (<1 month),

  Facilities: Minor structural damage, minor influence on operations;

- ***Level III***

  People: Permanent disability,

  Environment: Time for restitution of ecological resource <2 year,

  Facilities: Considerable structural damage, operation interrupted for weeks;

- ***Level II***

  People: One fatality,

  Environment: Time for restitution of ecological resource 2-5 years,

  Facilities: Loss of main part of station, production interrupted for months;

- ***Level I***

  People: Several fatalities,

  Environment: Time for restitution of ecological resource >5 years,

  Facilities: Total loss of station, major structural damages outside station area.

Based on this report, all hydrogen activities considered in the current model are marked as Levels IV and III. Water electrolysis technology, transportation modes distributing gaseous hydrogen and gaseous storage can be classified as risk level IV. It was assumed that biomass and coal gasification technologies have risk level III as well as steam methane reforming (SMR). The relative impact level of regions is determined based on regional characteristics such as population density. When the population of a particular region is over 16.3 million, the region is considered to be Level I. Regions with Level II have a population between 16.3 million and 12.23 million, Level III regions have population levels between 12.23 million and 8.15 million, for Level IV – the population is between 8.15 million and 4.08 million. Finally, regions have Level V if their population is less than 4.08 million.

Three indicators were taken as rating parameters for the safety risk assessment such as the weight factor of each activity, the population weight factor and weight factor of transport line. Based on relative risk level, each type of hydrogen activity has a score 3 or 5 classifying its weight factor (see Table 3.1). The weight factor of the transportation line is sum of weight factors of the population at grid points which transportation unit t is transiting through or passing close according the geographic location (see Table B.1). Based on the population level, each grid point has a score (1, 3, 5, 7, 9) classifying its population weight factor (see Table 3.2). It is noted that the each risk factor of a transportation line is calculated as an effect of the transportation path through grid points using GIS (Geographic Information System) of Germany.

Table 3.1 - Relative risk level of hydrogen activities and weight factor for production and storage sites and transportation mode

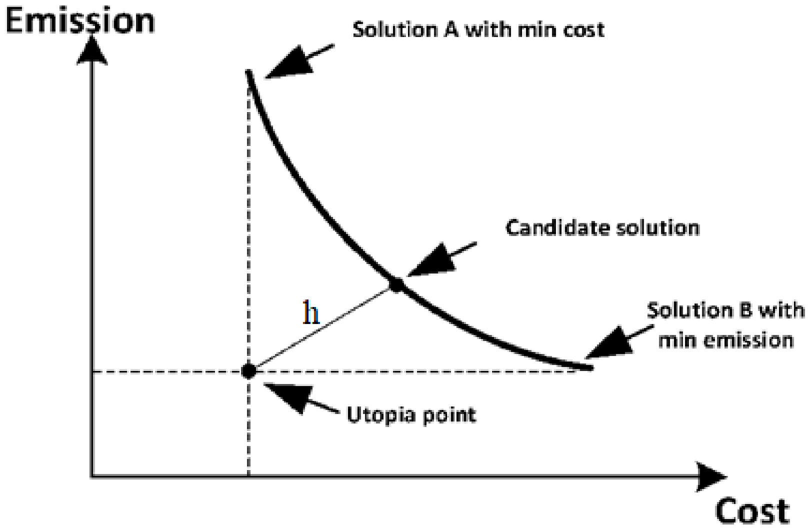
	Relative risk level	Weight factor
Production type		
Coal gasification	III	5
Water electrolysis	IV	3
Steam reforming	III	5
Biomass gasification	III	5
Storage type		
Cryogenic spherical tank	III	5
Pressurized cylindrical vessel	IV	3
Transportation type		
Tanker truck	III	5
Tube trailer	IV	3
Tank railcar	III	5
Tube railcar	IV	3

Table 3.2 - Weight factor for the effect of transportation of hydrogen into the region

Grid	Population level	Weight factor of transiting through a grid point (<1 km)	Weight factor of passing close to a grid point (1-10 km)
Baden-Wurttemberg	III	5	3
Bavaria	II	7	5
Berlin	V	1	1
Brandenburg	V	1	1
Bremen	V	1	1
Hamburg	V	1	1
Hesse	IV	3	1
Mecklenburg-Vorpommern	IV	3	1
Lower Saxony	V	1	1
North Rhine-Westphalia	I	9	7
Rhineland-Palatinate	V	1	1
Saarland	V	1	1
Saxony	V	1	1
Saxony-Anhalt	V	1	1
Schleswig-Holstein	V	1	1
Thuringia	V	1	1

3.4. THE ε-CONSTRAINT METHOD

The ε-constraint method is used to consider three objectives. The optimum solution with respect to each objective is obtained first from a single objective optimization, to evaluate the lower bounds (utopia points) of each objective in the feasible space and upper bounds (nadir points) on the Pareto surface. Then, multiple solutions between these lower and upper bounds are obtained by constraining two objectives and minimizing the last one [7]. In this chapter, the minimization of the total daily cost can be regarded as the objective function while the GHG and total risk are considered as inequality constraints. In addition, 56 points are considered to obtain a good representation of the Pareto front: 4 epsilon points between the lower and upper bounds of the risk objective and 14 points for GHG emissions. The proposed trade-off solution of the multi-objective optimization was obtained by calculation of the shortest distance between the utopia point and all points on the Pareto front (see Figure 3.1).



$$h = \sqrt{(x_s - x_u)^2 + (y_s - y_u)^2 + (z_s - z_u)^2}$$

Figure 3.1 - Solution strategy

3.5.MATHEMATICAL FORMULATION

The proposed model is applied to design HSC is addressed to minimize three targets separately and simultaneously through a Pareto trade-off:

1. Total cost of the network
2. Environmental impact in terms of CO_2 emissions
3. Total relative risk of the network.

The following subsections discuss the model constraints and objectives functions in more detail.

3.5.1. CONSTRAINTS

3.5.1.1.Demand constraints for a certain energy source

The demand for a certain energy source must be satisfied to ensure production. The demand for a certain energy source is calculated as follows:

$$ESD_{g,p,e} = \sum_{f,h} HP_{g,p,h,f} \alpha_{e,p,h} , \qquad \forall e,p,g \tag{3.1}$$

The demand must be covered by local power generation and/or imports from neighboring grid points as follows:

$$ESD_{g,p,e} \leq \sum_{g''} PESAv_{g'',g,p,e} + PES\,\mathrm{Im}_{g,p,e}\;, \qquad \forall e,g \tag{3.2}$$

3.5.1.2.Hydrogen demand constraints

The hydrogen demand by grid point can be calculated as follows:

$$HD_g = \gamma PN_g AvD \cdot FE\,, \qquad \forall g \tag{3.3}$$

The demand must be satisfied by local production and/or import from neighboring grid points as follows:

$$HD_g \leq \sum_{f,t,g'} HF_{g',g,t,f}\,, \qquad \forall g \tag{3.4}$$

3.5.1.3.Hydrogen generation constraints.

The hydrogen production is described as follows:

$$HP_{g,f} = \sum_{p,h} HP_{g,p,h,f}\,, \qquad \forall g,f \tag{3.5}$$

The hydrogen production rate is constrained by a maximum and minimum capacities as follows:

$$MinPCap_{p,h} NPF_{g,p,h,f} \leq HP_{g,p,h,f} \leq MaxPCap_{p,h} NPF_{g,p,h,f}\,, \qquad \forall g,p,h,f \tag{3.6}$$

It is noted that coal and biomass gasification plants cannot be developed at small-scale, and electrolysis-based plant cannot be developed at large-scale due to technical and economic limitations of those technologies such environmental hazard and size-independent efficiency.

3.5.1.4.Hydrogen distribution constraints

In Chapter 2 was outlined that the product can only move in one direction between grid points. The product flowrate by transportation mode *t* from *g* to *g'* is given as follows:

$$HP_{g,f} \geq \sum_{t,g'} HF_{g,g',t,f}\,, \qquad \forall g,f \tag{3.7}$$

3.5.1.5.Hydrogen storage constraints

The required hydrogen storage is constrained by maximum and minimum capacities as follows:

$$MinSCap_{s,f} NSF_{g,s,f} \leq HSInv_{g,s,f} \cdot \tau \leq MaxSCap_{s,f} NSF_{g,s,f}\,, \qquad \forall g,s,f \tag{3.8}$$

The hydrogen inventory level at the storage facility is described as follows:

$$\sum_{s,f} HSInv_{g,s,f} = HD_g\;, \qquad \forall g \tag{3.9}$$

3.5.2. OBJECTIVE FUNCTION

3.5.2.1. Total daily cost

The first objective function describes the total annualized cost (*TotalCost*) of the HSC network. Based on work by Almansoori and Betancourt-Torcat. [4], it consists of the production, storage and transportation capital- and operating costs and expenses of energy sources. The right-hand side of Eq. (3.10) contains four parts: the costs of hydrogen production (*PC*), transport (*TC*), storage (*SC*), and energy sources (*ESC*).

$$TotalCost = PC + SC + TC + ESC \tag{3.10}$$

$$PC = \sum_{g,p,h,f}\left(\left(PCC_{p,h,f}NPF_{g,p,h,f}AF_{p}\right)\Big/OP + HP_{g,p,h,f}POC_{p,h,f}\right) \tag{3.11}$$

$$SC = \sum_{g,s,f}\left(\left(SCC_{s,f}NSF_{g,s,f}AF_{s}\right)\Big/OP + SOC_{s,f}HSInv_{g,s,f}\right) \tag{3.12}$$

$$TC = \sum_{f,t,g,g'}\left(\left(TCC_{t,f}NTU_{g,g',t,f}AF_{t}\right)\Big/OP\right) + FC + LC + MC \tag{3.13}$$

$$\begin{aligned} ESC = &\sum_{g'',g,p,e}\left(PESAv_{g'',g,p,e}(ESDis_{e}\,Dis_{g'',g} + ESCost_{e})\right) + \\ &+ \sum_{g,p,e} PESIm_{g,p,e}\,ESICost_{e} \end{aligned} \tag{3.14}$$

3.5.2.2. Total environmental impact

Based on the work of De-León Almaraz [3], the total daily greenhouse gas (GHG) emission that is associated with GHG in production, storage sites and transportation of HSC network can be given by:

$$TotalCO_2 = PCO_2 + SCO_2 + TCO_2 \tag{3.15}$$

where $TotalCO_2$ is the total daily amount of realized GHG emissions in the HSC network, PCO_2 is the daily GHG emission from the production sites, SCO_2 is the daily GHG emission from the storage sites, TCO_2 is the daily GHG emission during hydrogen delivery.

The total daily GHG emissions in production sites are associated with the produced hydrogen of the form *f* by the each production facility *p* at grid point *g* and the total daily GHG emissions in production facility *p* producing hydrogen of form *f*:

$$PCO_2 = \sum_{g,p,h,f} HP_{g,p,h,f}GEP_{p,f} \tag{3.16}$$

where $GEP_{p,f}$ is the amount of GHG emitted per kg H_2 produced in the form *f* in production facility *p*.

The total daily storage of emitted GHG is calculated as follows:

$$SCO_2 = \sum_{g,s,f} HSInv_{g,s,f} GES_f \tag{3.17}$$

where GES_f is the amount of GHG meitted per kg H_2 in the form f in storage side s.

The total daily transport GHG emissions are determined as follows:

$$TCO_2 = \sum_{g,g',t,f} 2Dis_{g,g',t,f} NTU_{g,g',t,f} GET_t \tag{3.18}$$

where GET_t is the amount of GHG emitted per km traveled distance of transportation mode t.

3.5.2.3. Total relative risk

The total relative risk is given by:

$$TotalRisk = TotalPRisk + TotalSRisk + TotalTRisk \tag{3.19}$$

where *TotalPRisk* is the total risk of the production facilities, *TotalSRisk* is the total risk of the storage facilities, *TotalTRisk* is total risk associated with hydrogen distribution between grid points.

The relative risk of production sites is linked with the number of installed production facilities p producing hydrogen in the form f at the grid point g multiplied with its relative risk level and a population weight factor, and it is calculated as follows:

$$TotalPRisk = \sum_{p,h,f,g} NPF_{p,h,f,g} PRisk_p PW_g \tag{3.20}$$

where $PRisk_p$ is the risk level of the production facility p, PW_g is the population weight factor at grid point g where the production or storage facilities are installed.

The relative risk of storage sites is given as follows:

$$TotalSRisk = \sum_{s,f,g} NSF_{s,f,g} SRisk_s PW_g \tag{3.21}$$

where $SRisk_s$ is the risk level of the storage facility s.

The transportation relative risk is calculated by:

$$TotalTRisk = \sum_{g,g',f,t} NTU_{g,g',f,t} DRisk_{g,g',t} TRisk_t \tag{3.22}$$

where $TRisk_t$ is the risk level of the transportation mode t, $DRisk_{g,g',t}$ is the road risk level between grid points for transportation mode t for hydrogen distribution in the form f.

3.5.2.4. Multi-objective problem

The tri-objective optimization problem is solved by implementing the epsilon constraint method. The HSC design problem in this work is given as follows:

$$\text{Minimize } \{TotalCost\} \tag{3.23}$$

Subject to:

$TotalRisk \leq \varepsilon_n$ (n=0,1,2,…,N)

$TotalCO_2 \leq \varepsilon_m$ (n=0,1,2,…,M)

AIMMS is used as optimization platform and CPLEX 12.6.8 is selected as the preferred solver. The model is formulated as a mixed integer linear programming model and it consists of 21862 constraints, 21718 variables.

3.6. CASE STUDY

The German government is aiming at reaching the decarbonization target for private transport and a reduction of 80-95% GHG emissions by 2050 as compared to the 1990 levels, the development of a HSC in Germany is economically feasible [8].

This chapter considers four case studies, which will be analysed and compared with each other. Three objectives were optimized separately to analyse how their optimal values are affected when executing a multi-objective optimization. Each case represents the design of a HSC network for Germany for 2030 and it consists of a minimization target. The data was collected from the Federal Statistical Office of Germany [9], the Fraunhofer Institute for Solar Energy Systems ISE [10], Almansoori and Betancourt-Torcat [4], Ruth [11]

3.7. RESULTS AND DISCUSSION

In this section, the results of each case and corresponding configurations are analysed and discussed. The results of each optimization cases can be seen in Table 3.3. The following subsections discuss each case in more detail.

Table 3.3 - Results of optimization among treated cases

	Total cost (M$ d^{-1})	Relative risk (units)	CO_2 gas emission (10^3 t CO_2 d^{-1})
Case 1 (Min Total Cost)	**10.8** (48.2%)	9315 (-8.3%)	97.7 (-58.8%)
Case 2 (Min Total Risk)	19.9 (4.4%)	**8328** (2.6%)	45.7 (-11.9%)
Case 3 (Min Total CO_2)	28.9 (-27.8%)	8438 (1.3%)	**17.2** (57.1%)
Case 4 (Multi-objective optimization)	**20.8**	**8546**	**40.2**

3.7.1. CASE 1: MINIMIZATION OF TOTAL DAILY COST

The optimization results for Case 1 show that 2 large-scale and 12 medium-scale production facilities with coal gasification are selected as most economic option to satisfy hydrogen demand in 2030 (see Table B.2). The total cost of the HSC is 10.81 Mio $ d^{-1} for 2030, which means 3.95 $ kg^{-1} of H_2 with a centralized HSC configuration. The results obtained for Case 1 are in agreement with the base case results of Chapter 2. However, in this model, each production technology is coupled with an index *h* to consider different sizes of production plant. This modification affected the locations of production plants and map of distribution. The production facilities locations promotes the product distribution to regional storage facilities involving 70 transportation units to cover the demand between grid points. Facilities and their interconnections are shown in Figure 3.2.

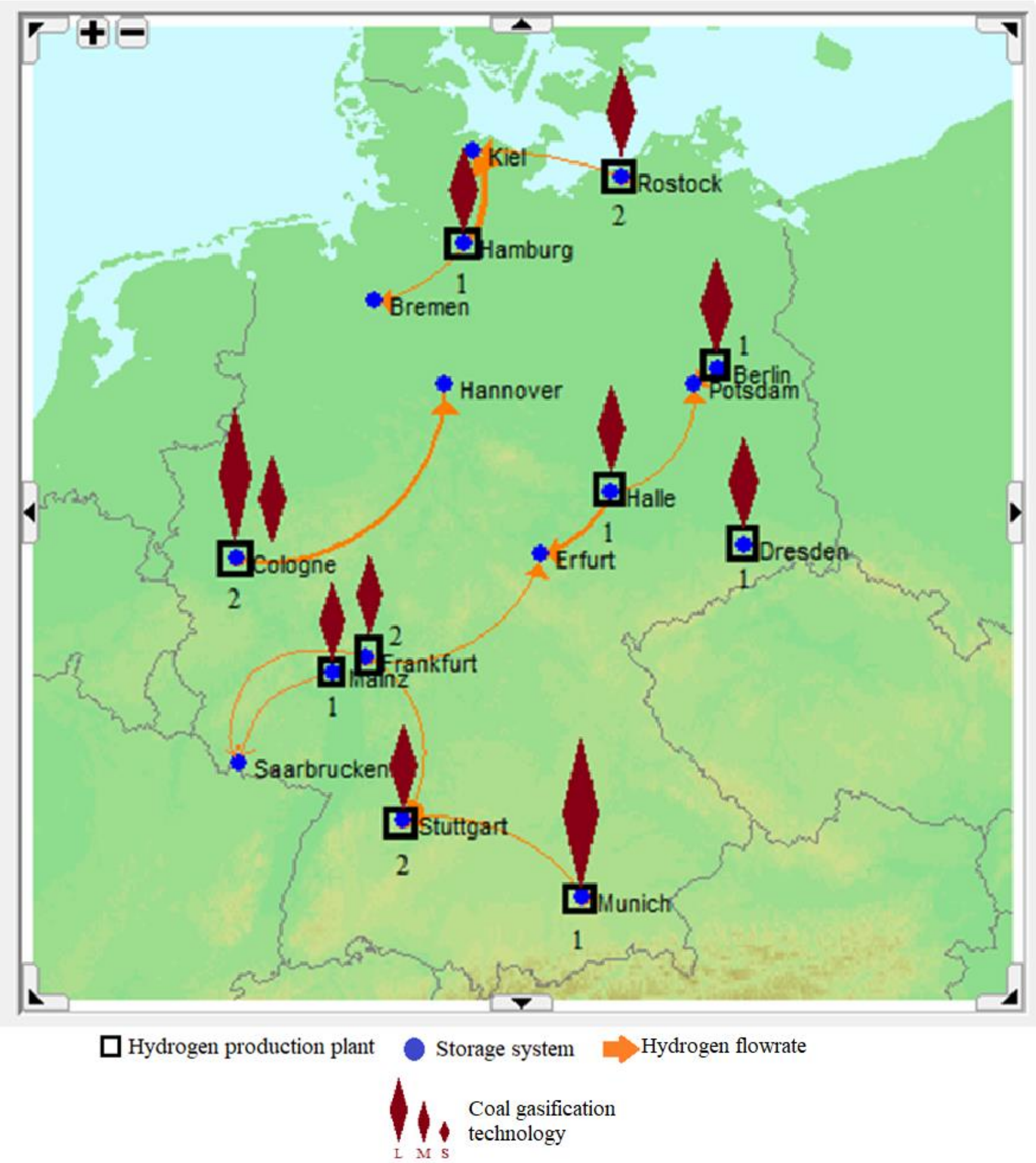


Figure 3.2 - Hydrogen supply chain network for Case 1: Minimization of total daily cost.

3.7.2. CASE 2: MINIMIZATION OF TOTAL RELATIVE RISK

Case 2 minimizes the total relative risk. In this case, the total cost of the HSC is 19.95 M$ involving 51 transportation vehicles to satisfy the local demand, the transportation relative risk was reduced to find the safest configuration. The network exhibits a decentralized configuration, where all grid points are autonomous in liquid hydrogen production (see Figure 3.3). Thus, the number of production facilities increased as compared to Case 1 (from 14 plants in Case 1 to 16 in this case) including water electrolysis and SMR technologies. That means a price of 7.28 \$ kg^{-1} of H_2. The total relative risk is mostly influenced by the storage risk since locations of storage facilities are fixed (see assumption 1 Chapter 2) to satisfy the local demand.

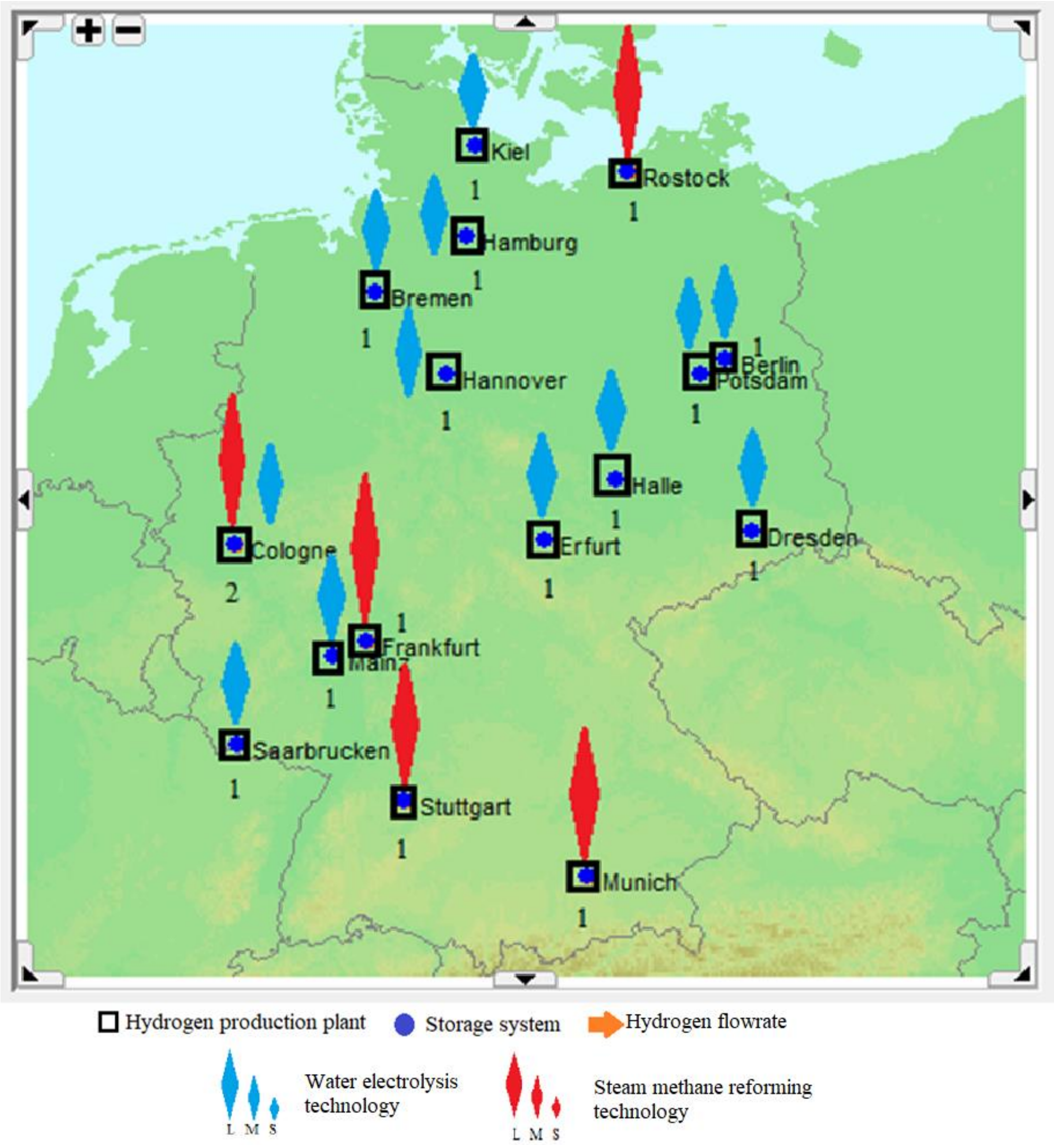


Figure 3.3 - Hydrogen supply chain network for Case 2: Minimization of total relative risk

3.7.3. CASE 3: MINIMIZATION OF TOTAL DAILY GHG EMISSION

This case minimizes the total daily GHG emission. The minimum GHG emission equals 17.25 x 10^3 t CO_2- eq. d^{-1}, which is much less than in previous two cases (97.73 x 10^3 t CO_2- eq. d^{-1} in Case 1 and 45.70 x 10^3 t CO_2- eq. d^{-1}in Case 2) However, in Case 3, there is a high risk of accidents as compared to Case 2 (8438 units for this case as compared to 8328 units for Case 2). However, the total cost of the HSC is 28.91 M\$ involving 51 transportation vehicles to satisfy the local demand, which results in a production price of 10.56 \$ kg^{-1} of H_2. The number of production plants increased considerably (from 14 plants in Case 1 to 30 in this case) and all of them are using water electrolysis technology leading to important decreases of the total CO_2 emissions of the HSC but it affects the total daily cost which is more than two times higher as compared to Case 1. The optimal configuration is similar to Case 2 in terms of degree of decentralization, with only 1 distribution links. Despite local production, Potsdam imports hydrogen from neighboring grid points due to their particularly high demand as shown in Figure 3.4.

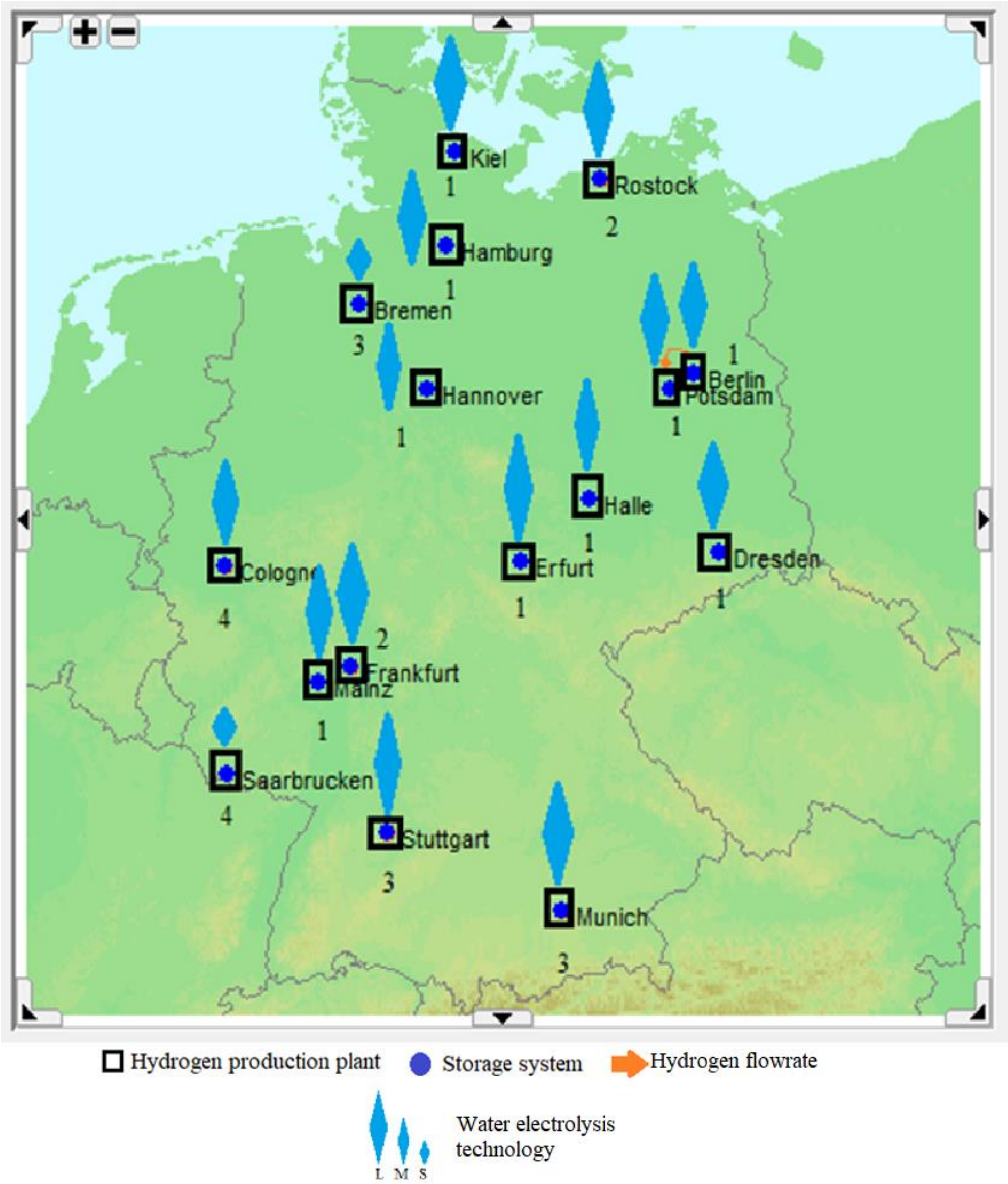


Figure 3.4 - Hydrogen supply chain network for Case 3: Minimization of total daily GHG emission

3.7.4. CASE 4: MULTI-OBJECTIVE MINIMIZATION

In this case study, the minimization of the total daily cost can be regarded as the objective function while the GHG and total risk are considered as inequality constraints. The best trade-off solution of the multi-objective optimization was obtained by calculation of the shortest distance between Utopia point and all combinations in the Pareto front (see Figure 3.5). The right figure has a pronounced bend at the place where the model changed network configuration from centralized to decentralized. Starting at the minimum total daily cost, the investment cost is less although CO_2 emissions are higher than other design strategies because the network exhibits a centralized configuration including coal gasification and SMR technologies. In contrast, the HSC can be designed environmental friendly in a decentralized fashion using water electrolysis technology (area at the minimum CO_2 emissions).

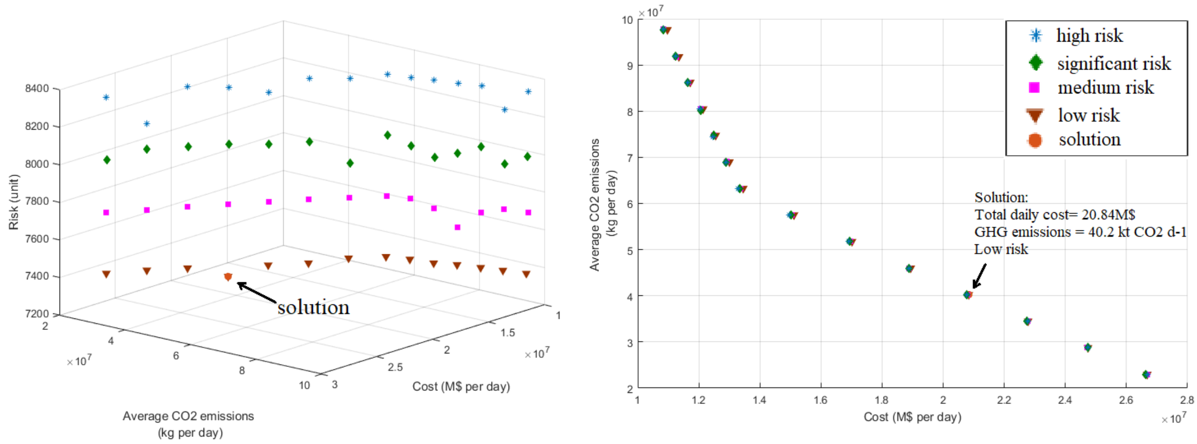


Figure 3.5 - Plot of Pareto front for multi-objective optimization (Cost vs Emissions, Risk)

The optimal configuration of the HSC for Case 4 involves 7 medium-scale and 40 small-scale production plants with water electrolysis technology and 3 large-scale and 1 medium-scale production plants with SMR (45% of hydrogen produced by water electrolysis technology and 55 % by steam methane reforming). The total HSC network costs are 20.86 M$ involving 53 transportation vehicles, CO_2 emissions are 40.20 x 10^3 t CO_2- eq. d^{-1} and the safety risk is very low. The network exhibits a decentralized configuration, where almost all grid points are autonomous in hydrogen production in liquid form, with only 6 distribution links. All grid points have domestic hydrogen production to satisfy local demand. Despite local production, Cologne, Frankfurt, Halle, Hamburg, Bremen and Potsdam import hydrogen from neighboring grid points due to their particularly high demand. Thus, the final cost for 1 kg of H_2 equals 7.62 \$ (0.0762 \$ km^{-1}). Compare to the modern internal combustion vehicle fuel with average cost 0.0645 \$ km^{-1}, the case clearly shows the potential for a hydrogen economy. Facilities and their interconnections are shown in Figure 3.6.

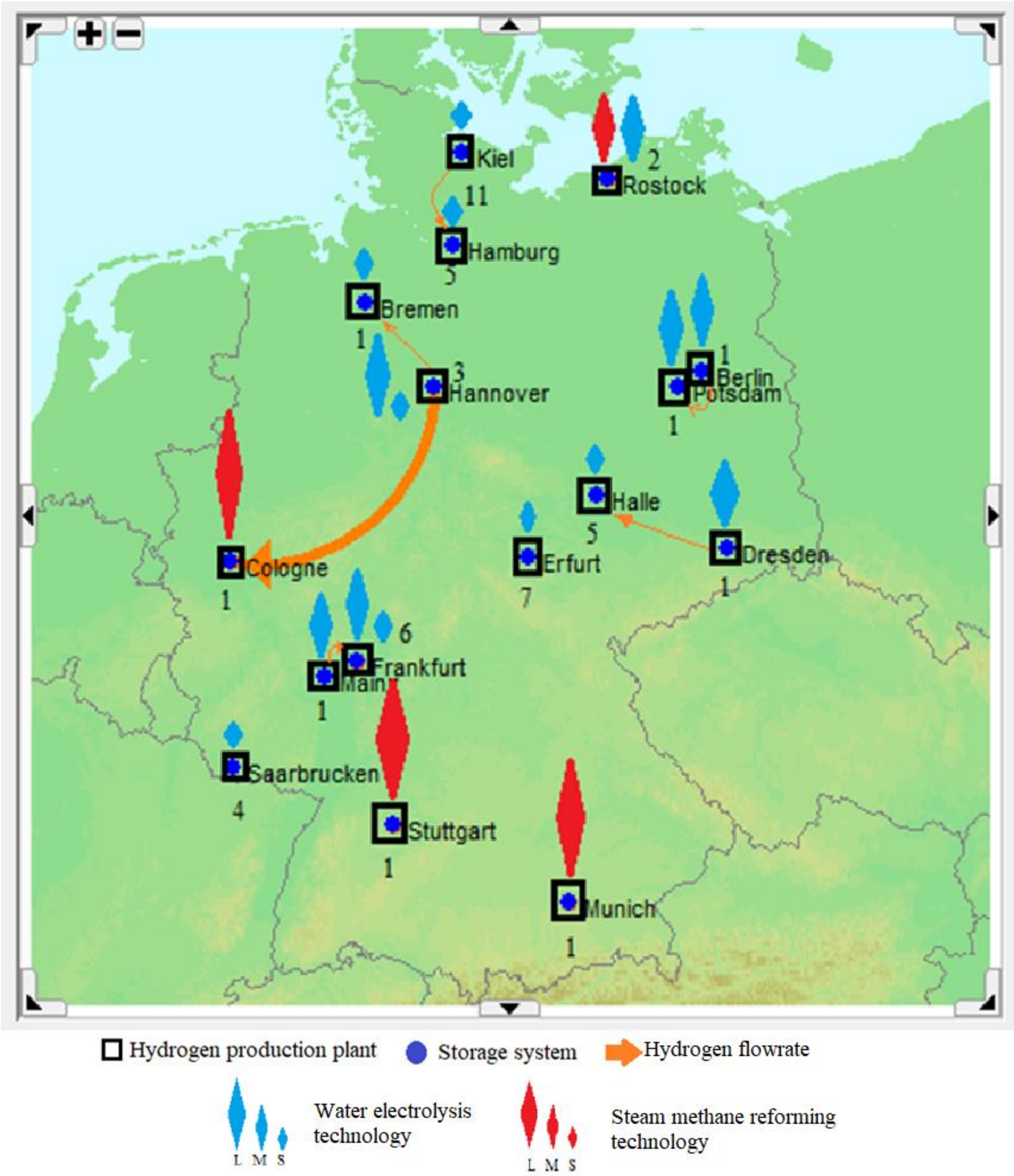


Figure 3.6 - Hydrogen supply chain network for Case 4: Multi-objective minimization

The results of this case are quite different from other cases. Table 3.3 shows that the trade-off solution obtained for the total costs in Case 4 is higher (by 48.2%) than Case 1. However, the CO_2 emissions decreased by 58.8%, and the safety improved by 8.3%. Compared to Case 2, the total cost increased with 4.4 % for Case 4 while the CO_2 emissions are lowered by 11.9%. However, the risk of hydrogen activities increased with 2.6%. In addition, the HSC network costs are lowered by 27.8%, CO_2 emissions and risk increased with 57.1% and 1.3% in Case 4 as compared with Case 3 respectively.

Finally, the hydrogen production costs vary between 3.95 and 10.56 $ per kg for all 4 cases. Centralized hydrogen production guarantees more financial benefits with less safe and environmental friendly construction unlike decentralized production [13].

3.8.CONCLUSIONS

In this chapter, a multi-criterion optimization approach was applied for the development of a sustainable HSC network in Germany. The three objectives considered were cost, safety, and environmental impact. Safety risk assessment allowed to specify hydrogen activity in every stage by its rating and to define safer HSC configurations. Four types of technologies to produce hydrogen were evaluated, namely coal gasification, steam methane reforming, biomass gasification, and water electrolysis. The ε-constraint method was applied to consider three objectives and to create a three-dimensional Pareto front, where the minimization of the total daily cost was regarded as the objective function while the environmental impact and safety were considered as inequality constraints. The best trade-off result of the multi-objective optimization was obtained by analysis of the shortest distance between the Utopia point and a trade-off point in the Pareto front. The proposed trade-off solution of multi-objective optimization shows the potential to build a safer HSC based on water electrolysis technology considering decentralized production configuration. Obtained results show that hydrogen costs vary between 3.95 and 10.56 \$ kg^{-1}. Compared to the modern internal combustion vehicle that uses fuel with average cost of 0.0645 \$ km^{-1}, the hydrogen cost, 0.0762 \$ km^{-1}, shows the feasibility of HSC network.

3.9. NOMENCLATURE

INDICES

e	type of energy source
f	type of hydrogen physical form
g	grid points, each grid point represents German state
p	type of hydrogen production facility
s	type of storage facility
t	type of transportation mode

ABBREVIATIONS

FCEV	fuel cell electric vehicle
GHG	greenhouse gas
HSC	hydrogen supply chain

CONTINUOUS VARIABLES

ESC	total cost for the energy source consumed for hydrogen production [\$ d^{-1}]
$ESD_{g,p,e}$	daily energy source demand [kWh d^{-1}]
FC	fuel cost [\$ d^{-1}]
$HF_{g,g',t,f}$	hydrogen flowrate in the form f from grid point g to g' via transportation mode t [kg d^{-1}]
$HP_{g,f}$	hydrogen generation in the form f at grid point g [kg d^{-1}]
$HP_{g,p,f}$	amount of produced hydrogen in the production facility p in the form f at grid point g [kg d^{-1}]
$HSInv_{g,s,f}$	inventory of product f in the storage facility s at grid point g [kg]
LC	labour cost [\$ d^{-1}]
MC	maintenance cost [\$ d^{-1}]
PC	daily production costs[\$ d^{-1}]
PCO_2	daily GHG emissions from production sites [kg d^{-1}]
$PESAv_{g'',g,p,e}$	energy source flowrate to meet demand for a certain energy source e from the grid point g'' to the grid point g, which is used to satisfy energy source demand for hydrogen production [unit e d^{-1}]
$PESIm_{g,p,e}$	flowrate importing energy source e to grid point g, which is used to satisfy energy source demand for hydrogen production [unit e d^{-1}]
SC	daily storage costs[\$ d^{-1}]
SCO_2	daily GHG emissions from storage sites [kg d^{-1}]
TC	daily distribution cost [\$ d^{-1}]
$TCO2$	daily GHG emissions during hydrogen delivery [kg d^{-1}]
$TotalCost$	total daily cost of HSC network [\$ d^{-1}]
$TotalCO_2$	total daily GHG emission of HSC network [kg d^{-1}]
$TotalRisk$	total daily relative risk of HSC network [unit d^{-1}]

INTEGER VARIABLES

$NPF_{g,p,f}$	number of production facility p generating hydrogen in from f at grid point g
$NSF_{g,s,f}$	number of storage facility s holding hydrogen in the form f at grid point g

$NTU_{g,g',t,f}$	the number of transport mode t used for hydrogen distribution in the form f from g to g'

PARAMETERS

AvD	the average distance travelled by personal car [km y^{-1}]
AvS_t	average speed of transportation mode t [km h^{-1}]
AF_p	annual factor for the facility p [%]
AF_s	annual factor for the s storage facility s [%]
AF_t	annual factor for the transport mode t [%]
$Dis_{g'',g}$	distance between grid points [km]
$Dis_{g,g',t}$	distance between grid points depending of type of transport [km]
$DRisk_{g,g',t,}$	risk level of hazard on the road passing by transportation mode t [unit]
$ESCost_e$	energy source e price in year y, generated locally [\$ $unit^{-1}$ e]
$ESDis_e$	delivery price for energy source e [\$ $unit^{-1}$ km^{-1}]
$ESICost_e$	energy source e import price [\$ $unit^{-1}$]
FE	the fuel economy [kg H_2 km^{-1}]
FP_t	fuel price for transport mode t [\$ l^{-1}]
$GEP_{p,f}$	GHG emitted in the production facility p to produce kg H2 in the form f [kg kg^{-1} H_2]
GES_f	GHG emitted in storage side to store kg H2 in the form f [kg kg^{-1} H_2]
GET_t	GHG emitted by transport mode t per 1 km [kg km^{-1}]
HD_g	hydrogen demand by grid point [kg d^{-1}]
$HHED_g$	total energy demand in the grid point g [kWh d^{-1}]
LUT_t	load/unload time for transportation mode t [h]
$MaxPCap_p$/ $MinPCap_p$	max/min production capacity for hydrogen production facility p [kg d^{-1}]
$MaxSCap_{s,f}$/ $MinSCap_{s,f}$	max/min capacity of storage facility s for holding hydrogen in the from f [kg]
OP	operating period [d y^{-1}]
$PCC_{p,f}$	capital cost of facility p, producing hydrogen in form f [\$]
PN_g	population at the grid point g
$POC_{p,f}$	hydrogen production operating cost in form f at facility p [\$ kg^{-1}]
$PRisk_p$	risk level of hazard of production facility p [unit]
PW_g	population weight factor in grid point g [unit]

$SCC_{s,f}$	capital cost for storage facility *s* holding hydrogen in the form *f* [$]
$SOC_{s,f}$	operating cost to store 1 kg of hydrogen in the from *f* inside of storage facility *s* [$ kg^{-1} d^{-1}]
$SRisk_s$	risk level of hazard of the storage facility *s* [unit]
$TCap_{t,f}$	capacity of transportation mode *t* to distribute produced hydrogen in form *f* [kg]
$TCC_{t,f}$	capital cost of transport mode *t* for distribution hydrogen in the form *f* [$]
$TRisk_t$	risk level of hazard of transportation mod t [unit]

GREEK LETTERS

$\alpha_{e,p}$	the ratio between energy sources *e* consumption to produce 1 kg [unit e kg^{-1} H_2]
γ	FCEVs intergradation rate [%]
τ	total product storage period [d]

3.10. REFERENCES

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APPENDIX B

Table B.1 - Relative risk matrix of the effect of transportation between various grid points

Road

Grid point	Stuttgart	Munich	Berlin	Potsdam	Bremen	Hamburg	Frankfurt	Rostock	Hannover	Cologne	Mainz	Saarbrucken	Dresden	Halle	Kiel	Erfurt
Stuttgart	5	12	13	13	18	18	9	20	17	18	6	7	14	14	18	13
Munich	12	7	12	12	12	12	15	15	12	25	11	14	9	10	13	8
Berlin	13	12	1	2	9	7	8	5	4	13	9	9	3	4	6	5
Potsdam	13	12	2	1	9	7	7	4	3	12	8	9	2	3	5	4
Bremen	18	12	9	9	1	3	15	7	2	11	15	13	4	3	4	4
Hamburg	18	12	7	7	3	1	6	5	2	11	6	8	8	3	2	4
Frankfurt	9	15	8	7	15	6	3	10	4	13	4	5	6	5	6	4
Rostock	20	15	5	4	7	5	10	3	6	15	11	16	6	6	4	7
Hannover	17	12	4	3	2	2	4	6	1	10	6	6	3	2	3	3
Cologne	18	25	13	12	11	11	13	15	10	9	13	11	16	15	13	14
Mainz	6	11	9	8	15	6	4	11	6	13	1	2	7	6	7	5
Saarbrucken	7	14	9	9	13	8	5	16	6	11	2	1	8	7	8	6
Dresden	14	9	3	2	4	8	6	6	3	16	7	8	1	2	7	3
Halle	14	10	4	3	3	3	5	6	2	15	6	7	2	1	4	2
Kiel	18	13	6	5	4	2	6	4	3	13	7	8	7	4	1	5
Erfurt	13	8	5	4	4	4	4	7	3	14	5	6	3	2	5	1

Railway

Grid point	Stuttgart	Munich	Berlin	Potsdam	Bremen	Hamburg	Frankfurt	Rostock	Hannover	Cologne	Mainz	Saarbrucken	Dresden	Halle	Kiel	Erfurt
Stuttgart	5	12	13	13	17	11	9	19	15	18	6	8	12	16	17	15
Munich	12	7	12	12	12	12	10	15	11	25	14	15	10	9	13	11
Berlin	13	12	1	2	10	8	12	5	4	13	8	14	3	4	8	5
Potsdam	13	12	2	1	10	8	12	5	4	13	8	14	4	2	8	5
Bremen	17	12	10	10	1	3	20	7	2	11	15	12	4	3	4	6
Hamburg	11	12	8	8	3	1	11	6	2	12	6	12	9	3	2	6
Frankfurt	9	10	12	12	20	11	3	13	9	13	4	10	12	5	11	9
Rostock	19	15	5	5	7	6	13	3	6	16	10	12	7	5	6	7
Hannover	15	11	4	4	2	2	9	6	1	10	5	16	3	2	3	5
Cologne	18	25	13	13	11	12	13	16	10	9	13	19	21	11	13	19
Mainz	6	14	8	8	15	6	4	10	5	13	1	7	12	11	12	10
Saarbrucken	8	15	14	14	12	12	10	12	16	19	7	1	18	17	18	16
Dresden	12	10	3	4	4	9	12	7	3	21	12	18	1	3	10	3
Halle	16	9	4	2	3	3	5	5	2	11	11	17	3	1	4	2
Kiel	17	13	8	8	4	2	11	6	3	13	12	18	10	4	1	7
Erfurt	15	11	5	5	6	6	9	7	5	19	10	16	3	2	7	1

Table B.2 - Results of Case 1: Minimization of Total daily cost

Production stage

Grid point	Type of technology	Size	Form	Number	Amount (t d^{-1})
Stuttgart	Coal gasification	Medium	Liquid	2	300.00
Munich	Coal gasification	Large	Liquid	1	479.68
Berlin	Coal gasification	Medium	Liquid	1	150.00
Hamburg	Coal gasification	Medium	Liquid	1	146.81
Frankfurt	Coal gasification	Medium	Liquid	2	288.97
Rostock	Coal gasification	Medium	Liquid	2	294.15
Cologne	Coal gasification	Medium	Liquid	1	147.83
Cologne	Coal gasification	Large	Liquid	1	480.00
Mainz	Coal gasification	Medium	Liquid	1	150.00
Dresden	Coal gasification	Medium	Liquid	1	150.00
Halle	Coal gasification	Medium	Liquid	1	150.00

Storage stage

Grid point	Type of technology	Form	Number	Amount (t d^{-1})
Stuttgart	Super-insulated spherical tanks	Liquid	7	372.51
Munich	Super-insulated spherical tanks	Liquid	9	444.21

Berlin	Super-insulated spherical tanks	Liquid	3	127.00
Potsdam	Super-insulated spherical tanks	Liquid	2	80.55
Bremen	Super-insulated spherical tanks	Liquid	1	22.24
Hamburg	Super-insulated spherical tanks	Liquid	2	63.20
Frankfurt	Super-insulated spherical tanks	Liquid	4	208.38
Rostock	Super-insulated spherical tanks	Liquid	5	259.96
Hannover	Super-insulated spherical tanks	Liquid	1	50.12
Cologne	Super-insulated spherical tanks	Liquid	11	586.78
Mainz	Super-insulated spherical tanks	Liquid	3	132.46
Saarbrucken	Super-insulated spherical tanks	Liquid	1	30.91
Dresden	Super-insulated spherical tanks	Liquid	3	130.73
Halle	Super-insulated spherical tanks	Liquid	2	66.47
Kiel	Super-insulated spherical tanks	Liquid	2	95.57
Erfurt	Super-insulated spherical tanks	Liquid	2	66.35

Transportation stage

From	To	Type	Form	Number	Amount (t d^{-1})
Stuttgart	Stuttgart	Railway tank car	Liquid	5	300.00
Munich	Stuttgart	Railway tank car	Liquid	2	35.47
Munich	Munich	Railway tank car	Liquid	7	444.21
Berlin	Berlin	Railway tank car	Liquid	2	127.00
Berlin	Potsdam	Railway tank car	Liquid	1	23.00
Hamburg	Bremen	Railway tank car	Liquid	1	22.24
Hamburg	Hamburg	Railway tank car	Liquid	1	63.20
Hamburg	Kiel	Railway tank car	Liquid	2	61.37
Frankfurt	Stuttgart	Railway tank car	Liquid	2	37.04
Frankfurt	Frankfurt	Railway tank car	Liquid	3	208.38
Frankfurt	Hannover	Railway tank car	Liquid	1	9.07
Frankfurt	Saarbrucken	Railway tank car	Liquid	1	13.37
Frankfurt	Erfurt	Railway tank car	Liquid	2	21.11
Rostock	Rostock	Railway tank car	Liquid	4	259.96
Rostock	Kiel	Railway tank car	Liquid	2	34.20
Cologne	Hannover	Railway tank car	Liquid	3	41.04
Cologne	Cologne	Railway tank car	Liquid	9	586.78
Mainz	Mainz	Railway tank car	Liquid	2	132.46
Mainz	Saarbrucken	Railway tank car	Liquid	1	17.54
Dresden	Potsdam	Railway tank car	Liquid	1	19.27
Dresden	Dresden	Railway tank car	Liquid	2	130.73
Halle	Potsdam	Railway tank car	Liquid	2	38.28
Halle	Halle	Railway tank car	Liquid	1	66.47
Halle	Erfurt	Railway tank car	Liquid	2	45.25

Summary

Energy Distribution and Purchase Cost M\$ d^{-1}	0.46
Production Capital Cost M\$ d^{-1}	1.34
Production Operating Cost M\$ d^{-1}	6.96
Storage Capital Cost M\$ d^{-1}	1.97

Storage Operating Cost M$ d^{-1}	0.01
Transportation Capital Cost M$ d^{-1}	0.01
Transportation Operating Cost M$ d^{-1}	0.04
Global warming potential 10ˆ3 t CO_2 d^{-1}	97.73
Risks	9315
Total Cost M$ d^{-1}	10.81
Hydrogen cost $ kg^{-1}	3.95

Table B.3 - Results of Case 2: Minimization of Total relative risk

Production stage

Grid point	Type of technology	Size	Form	Number	Amount (t d^{-1})
Stuttgart	Steam methane reforming	Large	Liquid	1	372.51
Munich	Steam methane reforming	Large	Liquid	1	444.21
Berlin	Water electrolysis	Medium	Liquid	1	127.00
Potsdam	Water electrolysis	Medium	Liquid	1	80.55
Bremen	Water electrolysis	Medium	Liquid	1	50.00
Hamburg	Water electrolysis	Medium	Liquid	1	63.20
Frankfurt	Steam methane reforming	Large	Liquid	1	208.38
Rostock	Steam methane reforming	Large	Liquid	1	259.96
Hannover	Water electrolysis	Medium	Liquid	1	50.12
Cologne	Water electrolysis	Medium	Liquid	1	150.00
Cologne	Steam methane reforming	Large	Liquid	1	436.78
Mainz	Water electrolysis	Medium	Liquid	1	132.46
Saarbrucken	Water electrolysis	Medium	Liquid	1	50.00
Dresden	Water electrolysis	Medium	Liquid	1	130.73
Halle	Water electrolysis	Medium	Liquid	1	66.47
Kiel	Water electrolysis	Medium	Liquid	1	95.57
Erfurt	Water electrolysis	Medium	Liquid	1	66.35

Storage stage

Grid point	Type of technology	Form	Number	Amount (t d^{-1})
Stuttgart	Super-insulated spherical tanks	Liquid	7	372.51
Munich	Super-insulated spherical tanks	Liquid	9	444.21
Berlin	Super-insulated spherical tanks	Liquid	3	127.00
Potsdam	Super-insulated spherical tanks	Liquid	2	80.55
Bremen	Super-insulated spherical tanks	Liquid	1	22.24
Hamburg	Super-insulated spherical tanks	Liquid	2	63.20
Frankfurt	Super-insulated spherical tanks	Liquid	4	208.38
Rostock	Super-insulated spherical tanks	Liquid	5	259.96
Hannover	Super-insulated spherical tanks	Liquid	1	50.12
Cologne	Super-insulated spherical tanks	Liquid	11	586.78
Mainz	Super-insulated spherical tanks	Liquid	3	132.46
Saarbrucken	Super-insulated spherical tanks	Liquid	1	30.91
Dresden	Super-insulated spherical tanks	Liquid	3	130.73
Halle	Super-insulated spherical tanks	Liquid	2	66.47

Kiel	Super-insulated spherical tanks	Liquid	2	95.57
Erfurt	Super-insulated spherical tanks	Liquid	2	66.35

Transportation stage

From	To	Type	Form	Number	Amount (t d^{-1})
Stuttgart	Stuttgart	Railway tank car	Liquid	6	372.51
Munich	Munich	Railway tank car	Liquid	7	444.21
Berlin	Berlin	Railway tank car	Liquid	2	127.00
Potsdam	Potsdam	Railway tank car	Liquid	2	80.55
Bremen	Bremen	Railway tank car	Liquid	1	23.37
Hamburg	Hamburg	Railway tank car	Liquid	1	63.20
Frankfurt	Frankfurt	Railway tank car	Liquid	3	208.38
Rostock	Rostock	Railway tank car	Liquid	4	259.96
Hannover	Hannover	Railway tank car	Liquid	1	50.12
Cologne	Cologne	Railway tank car	Liquid	9	586.78
Mainz	Mainz	Railway tank car	Liquid	2	132.46
Saarbrucken	Saarbrucken	Railway tank car	Liquid	1	30.91
Dresden	Dresden	Railway tank car	Liquid	2	130.73
Halle	Halle	Railway tank car	Liquid	1	66.47
Kiel	Kiel	Railway tank car	Liquid	2	95.57
Erfurt	Erfurt	Railway tank car	Liquid	1	66.35

Summary

Energy Distribution and Purchase Cost M$ d^{-1}	5.83
Production Capital Cost M$ d^{-1}	1.71
Production Operating Cost M$ d^{-1}	10.38
Storage Capital Cost M$ d^{-1}	1.97
Storage Operating Cost M$ d^{-1}	0.01
Transportation Capital Cost M$ d^{-1}	0.01
Transportation Operating Cost M$ d^{-1}	0.03
Global warming potential 10ˆ3 t CO_2 d^{-1}	45.70
Risks	8328
Total Cost M$ d^{-1}	19.95
Hydrogen cost $ kg^{-1}	7.28

Table B.4 - Results of Case 3: Minimization of Total GHG emissions

Production stage

Grid point	Type of technology	Size	Form	Number	Amount (t d^{-1})
Stuttgart	Water electrolysis	Medium	Liquid	3	372.51
Munich	Water electrolysis	Medium	Liquid	3	444.21
Berlin	Water electrolysis	Medium	Liquid	1	127.00
Potsdam	Water electrolysis	Medium	Liquid	1	80.55
Bremen	Water electrolysis	Small	Liquid	3	22.24

Hamburg	Water electrolysis	Medium	Liquid	1	63.20
Frankfurt	Water electrolysis	Medium	Liquid	2	208.38
Rostock	Water electrolysis	Medium	Liquid	2	259.96
Hannover	Water electrolysis	Medium	Liquid	1	50.12
Cologne	Water electrolysis	Medium	Liquid	4	586.95
Mainz	Water electrolysis	Medium	Liquid	1	132.46
Saarbrucken	Water electrolysis	Small	Liquid	4	30.91
Dresden	Water electrolysis	Medium	Liquid	1	130.73
Halle	Water electrolysis	Medium	Liquid	1	66.47
Kiel	Water electrolysis	Medium	Liquid	1	95.57
Erfurt	Water electrolysis	Medium	Liquid	1	66.35

Storage stage

Grid point	Type of technology	Form	Number	Amount (t d^{-1})
Stuttgart	Super-insulated spherical tanks	Liquid	7	372.51
Munich	Super-insulated spherical tanks	Liquid	9	444.21
Berlin	Super-insulated spherical tanks	Liquid	3	127.00
Potsdam	Super-insulated spherical tanks	Liquid	2	80.55
Bremen	Super-insulated spherical tanks	Liquid	1	22.24
Hamburg	Super-insulated spherical tanks	Liquid	2	63.20
Frankfurt	Super-insulated spherical tanks	Liquid	4	208.38
Rostock	Super-insulated spherical tanks	Liquid	5	259.96
Hannover	Super-insulated spherical tanks	Liquid	1	50.12
Cologne	Super-insulated spherical tanks	Liquid	11	586.78
Mainz	Super-insulated spherical tanks	Liquid	3	132.46
Saarbrucken	Super-insulated spherical tanks	Liquid	1	30.91
Dresden	Super-insulated spherical tanks	Liquid	3	130.73
Halle	Super-insulated spherical tanks	Liquid	2	66.47
Kiel	Super-insulated spherical tanks	Liquid	2	95.57
Erfurt	Super-insulated spherical tanks	Liquid	2	66.35

Transportation stage

From	To	Type	Form	Number	Amount (t d^{-1})
Stuttgart	Stuttgart	Railway tank car	Liquid	6	372.51
Munich	Munich	Railway tank car	Liquid	7	444.21
Berlin	Berlin	Railway tank car	Liquid	2	127.00
Berlin	Potsdam	Railway tank car	Liquid	1	10.21
Potsdam	Potsdam	Railway tank car	Liquid	1	70.34
Bremen	Bremen	Railway tank car	Liquid	1	22.24
Hamburg	Hamburg	Railway tank car	Liquid	1	63.20
Frankfurt	Frankfurt	Railway tank car	Liquid	3	208.38
Rostock	Rostock	Railway tank car	Liquid	4	259.96
Hannover	Hannover	Railway tank car	Liquid	1	50.12
Cologne	Cologne	Railway tank car	Liquid	9	586.78
Mainz	Mainz	Railway tank car	Liquid	2	132.46
Saarbrucken	Saarbrucken	Railway tank car	Liquid	1	30.91
Dresden	Dresden	Railway tank car	Liquid	2	130.73

Halle	Halle	Railway tank car	Liquid	1	66.47
Kiel	Kiel	Railway tank car	Liquid	2	95.57
Erfurt	Erfurt	Railway tank car	Liquid	1	66.35

Summary

Energy Distribution and Purchase Cost M$ d^{-1}	9.13
Production Capital Cost M$ d^{-1}	1.86
Production Operating Cost M$ d^{-1}	15.89
Storage Capital Cost M$ d^{-1}	1.97
Storage Operating Cost M$ d^{-1}	0.01
Transportation Capital Cost M$ d^{-1}	0.01
Transportation Operating Cost M$ d^{-1}	0.03
Global warming potential 10ˆ3 t CO_2 d^{-1}	17.25
Risks	8438
Total Cost M$ d^{-1}	28.91
Hydrogen cost $ kg^{-1}	10.56

Table B.5 - Results of Case 4: Multi-objective Minimization

Production stage

Grid point	Type of technology	Size	Form	Number	Amount (t d^{-1})
Stuttgart	Steam methane reforming	Large	Liquid	1	372.51
Munich	Steam methane reforming	Large	Liquid	1	444.21
Berlin	Water electrolysis	Medium	Liquid	1	140.11
Potsdam	Water electrolysis	Medium	Liquid	1	80.55
Bremen	Water electrolysis	Small	Liquid	1	10.00
Hamburg	Water electrolysis	Small	Liquid	5	49.73
Frankfurt	Water electrolysis	Small	Liquid	5	50.00
Frankfurt	Water electrolysis	Medium	Liquid	1	149.31
Rostock	Water electrolysis	Medium	Liquid	1	150.00
Rostock	Steam methane reforming	Medium	Liquid	1	96.85
Hannover	Water electrolysis	Small	Liquid	2	20.00
Hannover	Water electrolysis	Medium	Liquid	1	149.14
Cologne	Steam methane reforming	Large	Liquid	1	480.00
Mainz	Water electrolysis	Medium	Liquid	1	141.54
Saarbrucken	Water electrolysis	Small	Liquid	4	30.91
Dresden	Water electrolysis	Medium	Liquid	1	147.20
Halle	Water electrolysis	Small	Liquid	5	50.00
Kiel	Water electrolysis	Small	Liquid	11	109.03
Erfurt	Water electrolysis	Small	Liquid	7	66.35

Storage stage

Grid point	Type of technology	Form	Number	Amount (t d^{-1})
Stuttgart	Super-insulated spherical tanks	Liquid	7	372.51
Munich	Super-insulated spherical tanks	Liquid	9	444.21

Berlin	Super-insulated spherical tanks	Liquid	3	127.00
Potsdam	Super-insulated spherical tanks	Liquid	2	80.55
Bremen	Super-insulated spherical tanks	Liquid	1	22.24
Hamburg	Super-insulated spherical tanks	Liquid	2	63.20
Frankfurt	Super-insulated spherical tanks	Liquid	4	208.38
Rostock	Super-insulated spherical tanks	Liquid	5	259.96
Hannover	Super-insulated spherical tanks	Liquid	1	50.12
Cologne	Super-insulated spherical tanks	Liquid	11	586.78
Mainz	Super-insulated spherical tanks	Liquid	3	132.46
Saarbrucken	Super-insulated spherical tanks	Liquid	1	30.91
Dresden	Super-insulated spherical tanks	Liquid	3	130.73
Halle	Super-insulated spherical tanks	Liquid	2	66.47
Kiel	Super-insulated spherical tanks	Liquid	2	95.57
Erfurt	Super-insulated spherical tanks	Liquid	2	66.35

Transportation stage

From	To	Type	Form	Number	Amount (t d^{-1})
Stuttgart	Stuttgart	Railway tank car	Liquid	6	372.51
Munich	Munich	Railway tank car	Liquid	7	444.21
Berlin	Berlin	Railway tank car	Liquid	2	127.00
Berlin	Rostock	Railway tank car	Liquid	1	13.11
Potsdam	Potsdam	Railway tank car	Liquid	2	80.55
Bremen	Bremen	Railway tank car	Liquid	1	10.00
Hamburg	Hamburg	Railway tank car	Liquid	1	49.73
Frankfurt	Frankfurt	Railway tank car	Liquid	3	199.31
Rostock	Rostock	Railway tank car	Liquid	4	246.85
Hannover	Bremen	Railway tank car	Liquid	1	12.24
Hannover	Hannover	Railway tank car	Liquid	1	50.12
Hannover	Cologne	Railway tank car	Liquid	8	106.78
Cologne	Cologne	Railway tank car	Liquid	7	480.00
Mainz	Frankfurt	Railway tank car	Liquid	1	9.07
Mainz	Mainz	Railway tank car	Liquid	2	132.46
Saarbrucken	Saarbrucken	Railway tank car	Liquid	1	30.91
Dresden	Dresden	Railway tank car	Liquid	2	130.73
Dresden	Halle	Railway tank car	Liquid	1	16.47
Halle	Halle	Railway tank car	Liquid	1	50.00
Kiel	Hamburg	Railway tank car	Liquid	1	13.46
Kiel	Kiel	Railway tank car	Liquid	2	95.57
Erfurt	Erfurt	Railway tank car	Liquid	1	66.35

Summary

Energy Distribution and Purchase Cost M$ d^{-1}	6.34
Production Capital Cost M$ d^{-1}	1.27
Production Operating Cost M$ d^{-1}	11.21
Storage Capital Cost M$ d^{-1}	1.97
Storage Operating Cost M$ d^{-1}	0.01
Transportation Capital Cost M$ d^{-1}	0.01

Transportation Operating Cost M$ d^{-1}	0.04
Global warming potential 10ˆ3 t CO_2 d^{-1}	40.24
Risks	8546
Total Cost M$ d^{-1}	20.86
Hydrogen cost $ kg^{-1}	7.62

4. DESIGN OF HYDROGEN SUPPLY CHAINS UNDER DEMAND UNCERTAINTY

This chapter presents an approach for the design of a hydrogen supply chain network in Germany incorporating the uncertainty in the hydrogen demand. Uncertainty in hydrogen demand has a very strong impact on the overall system costs, i.e. it makes sense to generate a scenario tree for stochastic simulations incorporating the variation in hydrogen demand. The extended model considers two configurations, which are analyzed and compared to each other according to production types: water electrolysis vs steam methane reforming. Each configuration has a minimization target. The concept of value of stochastic solution (VSS) is used to evaluate the stochastic optimization results and compare them to their deterministic counterpart. The VSS of each configurations shows significant benefits of a stochastic approach for the extended model presented in this chapter, corresponding up to 26% of infrastructure investments savings.

This chapter was published in:

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4.1. INTRODUCTION

Many studies in the area of HSC design, mentioned in Chapter 2, focus on network evaluation using steady-state simulation. However, it was recognized that input data is uncertain in most real-world decision problems and it has a major effect on decisions in supply chain. Uncertainty can be identified as one of the major challenges in supply chain management [1]-[2]. The work of Kim et al. considers all possible hydrogen alternatives for an optimal hydrogen infrastructure taking into account demand uncertainty following a stochastic formulation based on two-stage programing approach. The model was applied to evaluate the HSC of South Korea [3]. The work of Almasoori takes into account uncertainty in hydrogen demand over long-term planning horizon using a scenario-based approach. A multi-stage stochastic mixed integer linear programming (MILP) model was proposed to determine possible configurations of HSC network in Great Britain [4].

This chapter builds on the model introduced in Chapter 3 to capture the hydrogen demand uncertainty, where the environmental impact is part of the network costs, and a penalty method is applied to analyze the economic value of supply security.

4.2.UNCERTAINTY

There are many problems in production planning and scheduling, location and transportation design requiring decisions to be made in the presence of uncertainty [5]. It is not easy to identify which parameters in the model are random. Moreover, optimization under uncertainty leads to solve a very large-scale optimization models. Thus, it is important to control the size of the model by only taking into account the uncertain parameters that have the largest impact. Uncertainty can be classified as presented in Table 4.1, where the first three classes are considered most often in supply chain management [6]:

Table 4.1 - Classification of uncertainty

UNCERTAINTY			
SUPPLY	PROCESS	DEMAND	EXTERNAL
Supplier failure Supplier insolvency	Delays Delivery constrains Production resources disturbances Production system input disturbances	Purchasing power Competitors	Outsourcing of production Behavioral Political and Social Disruptions

Supplier failure and Supplier insolvency are a source for uncertainties, which means the inability to handle demand fluctuations and quality problems at supplier plants.

Process uncertainties cover all risks associated with internal operations: delays caused by supply disruptions or problems in unloading and loading; the breakdown of machines (production resource disturbance); financial factors (production system input disturbance).

In literature attention is paid to modeling of system under demand uncertainty [4], [7], [8]. The demand quantity results in missed income, in case of under production, or high production and stocking costs (over production). Moreover, competitors can either produce a similar product or use a new approach for an existing product, which effect on product demand. In addition, the demand can decrease if the purchasing power decreases.

The last class of uncertainty sources includes outsourcing, behavioral, political and social, and disruptions sources. Outsourcing is associated with intellectual property risks (the risk of unlicensed production). Behavioral uncertainties arise from the lack of information sharing between different echelons in the supply chain such as retailers and suppliers. Political and social uncertainties cover laws and policies, social acceptance. Uncertainty of disruptions relates to the war, terrorism, natural disasters, and infrastructure risks.

4.3. SENSITIVITY ANALYSIS

It is important to identify which parameters in the model are uncertain. For this, a local sensitivity analysis is performed to evaluate which model parameters have the strongest impact on the objective function and the decision variables. From the aforementioned uncertainty sources, several parameters can be analyzed:

- the price of raw materials (supply uncertainty);
- operational problems in unloading and loading (process uncertainty);
- demand quantity (demand uncertainty);
- carbon tax (external uncertainty).

Each of the selected parameters is evaluated within a ±20% range from their base values and applied in the deterministic model. Figure 4.1 shows the sensitivities of all selected parameters on the objective function, while Figure 4.2 shows the sensitivities on the remaining decision variables of the model. Noted, hydrogen demand quantity has the greatest effect on the objective function compared to other evaluated parameters. Thus, it is considered as uncertain parameter in the stochastic formulation.

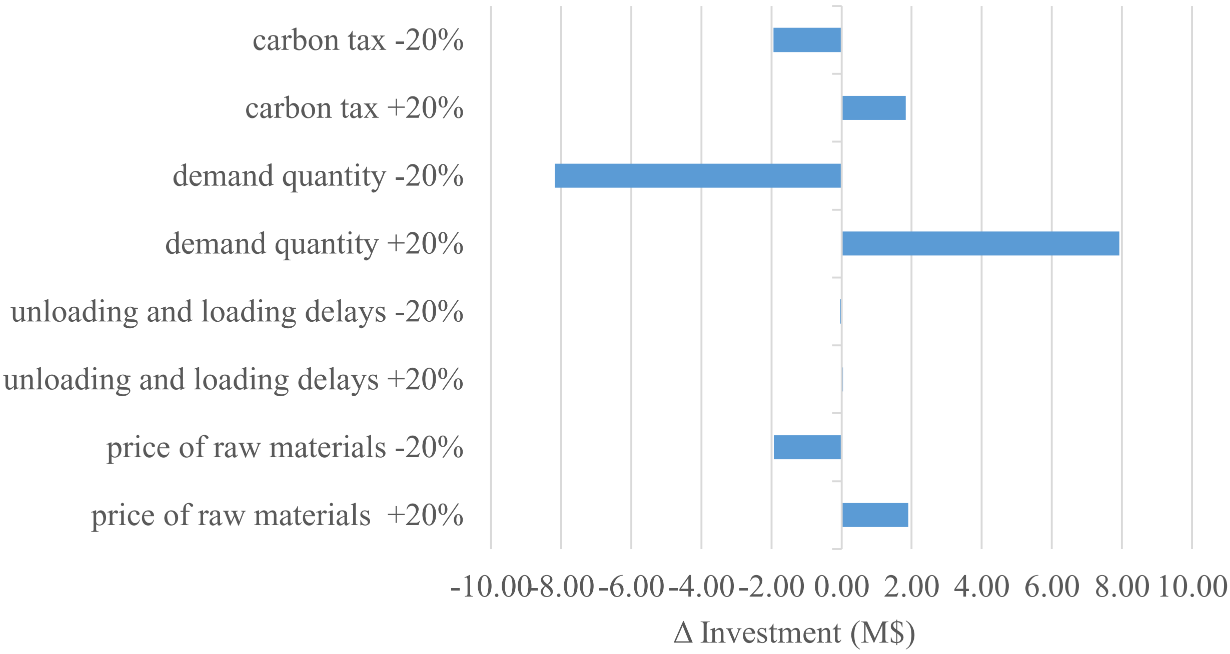

Figure 4.1 - Sensitivities of selected parameters on objective function (total daily cost)

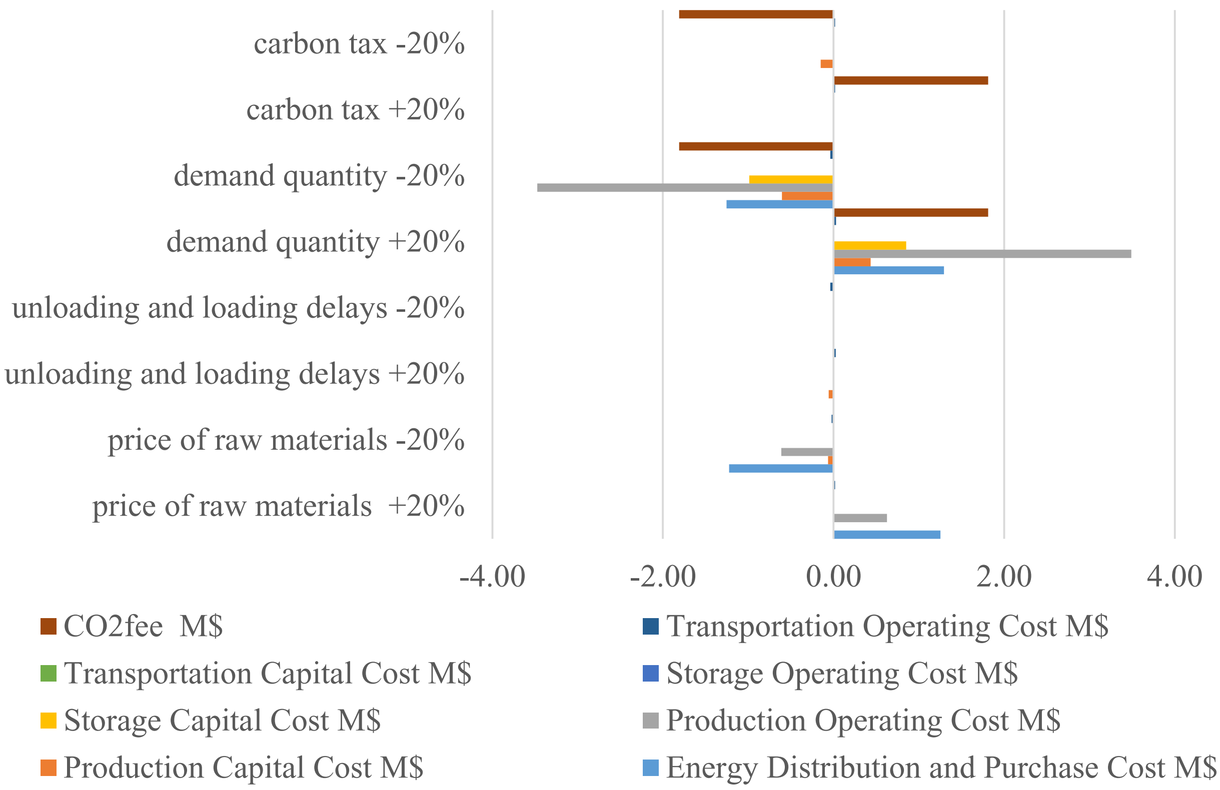

Figure 4.2 - Sensitivities of selected parameters on other decision variables in the model

4.4.NETWORK DESCRIPTION AND PROBLEM STATEMENT

The analysis performed in Chapter 3 shows that the combination of water electrolysis and steam methane reforming technologies can satisfy the hydrogen demand for trade-offs between costs, environmental impact and safety of the network. This chapter considers two configurations of a HSC, which are analyzed and compared to each other according to production types: water electrolysis vs steam methane reforming. Each configuration represents the design of a HSC network for Germany up to 2050 and it has a HSC cost minimization target. The two configurations are summarized as follows:

Configuration 1: Hydrogen can be produced in small-, medium-, and large-scale plants via steam methane reforming (SMR). Hydrogen distribution in two forms from production to storage sites via railway tank car and tanker truck (liquid hydrogen), and railway tube car and tube trailer (gaseous hydrogen), two types of storage technology (super-insulated spherical tank, pressurized cylindrical vessels). The stochastic behavior of the hydrogen demand is presented as multi-stage stochastic optimization problem with three demand scenarios, referred to as “high” (+20% expected demand), “medium” (expected demand), “low” (-20% expected demand) scenarios over five time periods of planning horizon and probability of their appearance equaled 0.3, 0.4, 0.3 respectively.

Configuration 2: Similar to the first configuration considering water electrolysis (WE) as a hydrogen production technology.

Each scenario includes a number of decisions that have to be taken. This chapter considers multi-stage stochastic MILP model representations including five time periods and eighty one scenarios. Each time period represents a 6-year interval starting from 2020 till 2050. Each scenario has a uniquely defined demand value as shown Figure 4.3. It is assumed that the demand is known at the first-stage, when at the next stages different corrective actions are taken according to unique demand values of all scenarios. The tree structure is formulated through using non-anticipativity constraints that do not allow the solution to anticipate on stochastic outcomes that lie beyond the stage. The problem is concerned with finding the size, capacity and locations of the production facilities for an uncertain demand, considering the minimum cost of the first-stage and the expected cost of the following stages. To analyze the economic value of supply security, a cost penalty for missing demand is applied. The main idea of penalty functions is to apply a penalty to feasible solutions when the constraint of the hydrogen demand requirements is violated [9]. To evaluate the stochastic optimization results and compare them to their deterministic counterpart the concepts of expected value of perfect information (EVPI) and value of stochastic solution (VSS) are used, where the EVPI measures the value of having accurate information for the future demand while the VSS assesses the value of cost when ignoring uncertainty in the demand [10].

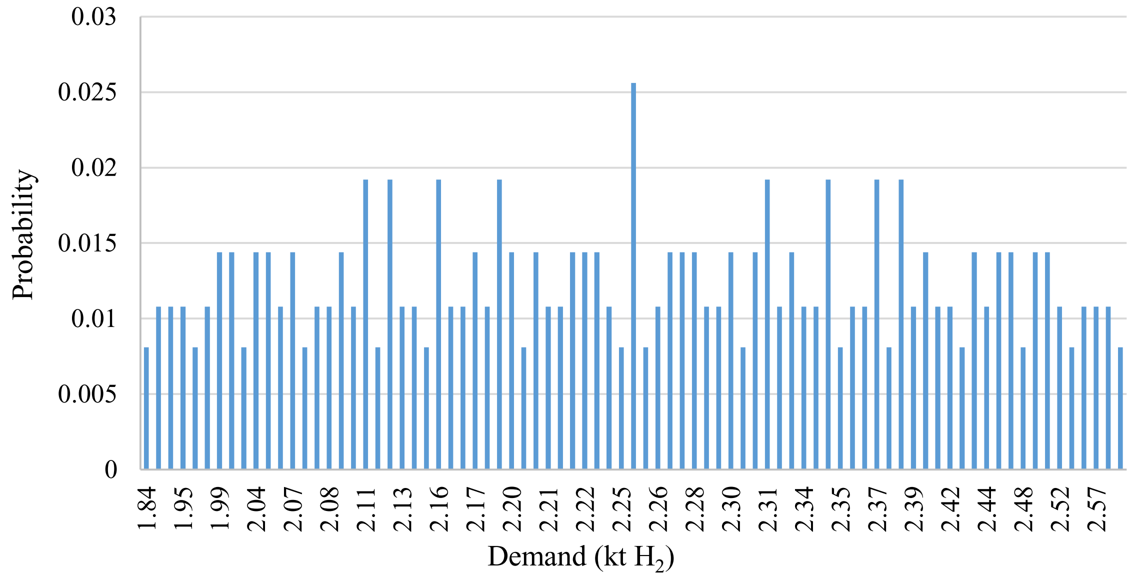

Figure 4.3 - Demand distribution. Values shown correspond to total demand for each scenario up to 2050

4.5.MATHEMATICAL FORMULATION

The objective is to minimize the total cost of the HSC network. In the following subsections the model constraints and objective function are described mathematically.

4.5.1. CONSTRAINTS

4.5.1.1. Demand constraints for a deterministic energy source

The demand for a certain energy source is calculated as follows:

$$ESD_{sc,ts,g,p,e} = \sum_{f,h} HP_{sc,ts,g,p,h,f}\,\alpha_{e,p,h}\,, \qquad \forall e,p,g,ts,sc \tag{4.1}$$

where *sc* indicates a realized scenario and *ts* is the time period. The demand must be covered by local power generation and/or imports from neighboring grid points or import from abroad as follows:

$$ESD_{sc,ts,g,p,e} \le \sum_{g''} PESAv_{sc,ts,g'',gp,e} + PES\mathrm{Im}_{sc,ts,g,p,e}\,, \qquad \forall e,p,g,ts,sc \tag{4.2}$$

4.5.1.2.Hydrogen demand constraints

The hydrogen demand by grid point can be calculated as follows:

$$HD_{sc,ts,g} = \gamma_{ts} PN_{sc,ts,g} AvD_{ts} \cdot FE\,, \qquad \forall g,ts,sc \tag{4.3}$$

The demand must be satisfied by the network and/or imports from another country:

$$HD_{sc,ts,g} \leq \sum_f \left(HD_{sc,ts,g,f} \right) + HI_{sc,ts,g} \,, \quad \forall g,ts,sc \tag{4.4}$$

The hydrogen demand in the form *f* must be satisfied by local production and/or from neighboring grid points:

$$HD_{sc,ts,g,f} \leq \sum_{t,g'} HF_{sc,ts,g',g,t,f} \,, \qquad \forall f,g,ts,sc \tag{4.5}$$

4.5.1.3.Hydrogen generation constraints.

The hydrogen production is described as:

$$HP_{sc,ts,g,f} = \sum_{p,h} HP_{sc,ts,g,p,h,f} \,, \qquad \forall g,f,ts,sc \tag{4.6}$$

The hydrogen production rate is constrained by maximum and minimum capacities as:

$$MinPCap_{p,h} NPF_{ts,g,p,h,f} \leq HP_{sc,ts,g,p,h,f} \leq MaxPCap_{p,h} NPF_{ts,g,p,h,f} \,, \quad \forall g,p,f,ts,sc \tag{4.7}$$

4.5.1.4.Hydrogen distribution constraints

It is noted that the product can only move in one direction between grid points. The product flowrate by transportation mode *t* from *g* to *g'* during time period *ts* for scenario *sc* is given as:

$$HP_{sc,ts,g,f} \geq \sum_{t,g'} HF_{sc,ts,g,g',t,f} \,, \qquad \forall g,f,ts,sc \tag{4.8}$$

The number of vehicles *t* required in grid point *g* to serve local and regional demand of hydrogen produced in the form *f* during time period *ts* is given as follows:

$$NTU_{ts,g,g',t,f} \geq \frac{HF_{sc,ts,g,g',t,f} \left(\frac{2Dis_{g,g',t}}{AvS_t} + LUT_t \right)}{MA_t \cdot TCap_{t,f}} + ExT_{sc,ts,g,g',t,f} \,, \quad \forall sc,ts,g,g',t,f \tag{4.9}$$

4.5.1.5.Hydrogen storage constraints

The required hydrogen storage is constrained by maximum and minimum capacities as:

$$MinSCap_{s,f} NSF_{ts,g,s,f} \leq HSInv_{sc,ts,g,s,f} \cdot \tau \leq MaxSCap_{s,f} NSF_{ts,g,s,f} \quad \forall g,s,f,ts,sc \tag{4.10}$$

The hydrogen inventory level at the storage facility is described as:

$$\sum_s HSInv_{sc,ts,g,s,f} \geq HD_{sc,ts,g,f} \,, \qquad \forall f,g,ts,sc \tag{4.11}$$

4.5.1.6.Time evolution constraints

As the network evolves over time, the number of production and storage facilities, and transportation units at current time period equals the number of invested units at previous time step plus the number of new invested facilities met the increased demand. This can be described as using the following constraints:

$$NPF_{ts,g,p,h,f} = NPF_{(ts\text{-}1),g,p,h,f} + InPF_{ts,g,p,h,f}\,, \quad \forall ts,g,p,h,f\!:ts \neq ts1 \tag{4.12}$$

$$NSF_{ts,g,s,f} = NSF_{(ts\text{-}1),g,s,f} + InSF_{ts,g,s,f}\,, \quad \forall ts,g,p,h,f\!:ts \neq ts1 \tag{4.13}$$

$$InTU_{ts,g,t,f} = \sum_{g'} NTU_{ts,g,g',t,f} - \sum_{g'} NTU_{(ts\text{-}1),g,g',t,f}\,, \quad \forall ts,g,p,h,f\!:ts \neq ts1 \tag{4.14}$$

where $InPF_{ts,g,p,h,f}$, $InSF_{ts,g,s,f}$ and $InTU_{ts,g,t,f}$ are the number of new invested production and storage facilities, and transportation units respectively at grid point g.

During the first period, the number of production and storage facilities, and transportation units are given as:

$$NPF_{ts1,g,p,h,f} = ExNPF_{g,p,h,f} + InPF_{ts1,g,p,h,f}\,, \quad \forall g,p,h,f \tag{4.15}$$

$$NSF_{ts1,g,s,f} = ExNSF_{g,s,f} + InSF_{ts1,g,s,f}\,, \quad \forall g,s,f \tag{4.16}$$

$$InTU_{ts1,g,t,f} = \sum_{g'} NTU_{ts1,g,g',t,f} - ExTU_{g,t,f}\,, \quad \forall g,t,f \tag{4.17}$$

where $ExNPF_{g,p,h,f}$, $ExNSF_{g,s,f}$ and $ExTU_{g,t,f}$ are the number of existing production and storage facilities, and transportation units respectively at grid point g.

4.5.1.7.Objective function

The expected total network costs of the HSC (*TotalCost*) of the HSC network is given as follows:

$$TotalCost = \min \{(PC + SC + TC + ESC + EMC + PenC)/NP\} \tag{4.18}$$

The right-hand side of Eq. (4.18) contains five parts: the costs of hydrogen production (*PC*), transport (*TC*), storage (*SC*), energy sources (*ESC*), emission fees (*EMC*), and a penalty cost (*PenC*), divided by number of time periods (NP). The objective is to minimize the total costs by finding the combination of network components that satisfies the local hydrogen demand while satisfying the constraints.

Each production plant has an associated capital- and operating cost. The total daily production cost is given by:

$$PC = \sum_{ts,g,p,h,f}\left(\frac{PCC_{p,h,f}InPF_{ts,g,p,h,f}AF_{p}}{LR \cdot OP} + \sum_{sc}\rho_{sc}HP_{sc,ts,g,p,h,f}POC_{p,h,f}\right) \quad (4.19)$$

where $PCC_{p,h,f}$ represents the capital cost of facility p size h, producing hydrogen in form f, LR is the learning rate that takes into account the cost reduction of facilities while the experience accumulates with time, AF_p is an annuity factor for facility p, OP represents the operating period, and $POC_{p,h,f}$ denotes the hydrogen production cost in form f at facility p size h, ρ_{sc} is scenario probability.

The total hydrogen storage cost is calculated as:

$$\mathrm{SC} = \sum_{\mathrm{ts,g,s,f}}\left(\frac{\mathrm{SCC_{s,f}InSF_{ts,g,s,f}AF_{s}}}{\mathrm{LR \cdot OP}} + \sum_{\mathrm{sc}}\rho_{\mathrm{sc}}\mathrm{HSInv_{sc,ts,g,s,f}SOC_{s,f}}\right) \quad (4.20)$$

where $SCC_{s,f}$ denotes the capital cost for storage facility s holding hydrogen in the form f, AF_s is annuity factor for the s storage facility, $SOC_{s,f}$ is the operating cost to store 1 kg of hydrogen in the form f at storage facility s.

The total distribution cost, calculated as the sum of the operating and capital costs, is represented as:

$$TC = \sum_{ts,g,t,f}\left(\left(TCC_{t,f}InTU_{ts,g,t,f}AF_{t}\right)\Big/OP\right) + FC + LC + MC \quad (4.21)$$

where $TCC_{t,f}$ denotes the capital cost of transport mode t for the distribution of hydrogen in form f, AF_t is an annuity factor for transport mode t, FC is the fuel cost, LC is labour cost, MC is maintenance cost.

The daily fuel cost for all scenarios and time periods is calculated as:

$$FC = \sum_{sc,ts,g,g',t,f}\rho_{sc}\frac{FP_{t}}{FET_{t}}2Dis_{g,g',t}HF_{sc,ts,g,g',t,f}\Big/TCap_{t,f} \quad (4.22)$$

where FP_t represents fuel price for transportation mode t, FET_t denotes the fuel economy for transportation mode t.

The labor cost for all scenarios and time periods is calculated as:

$$LC = \sum_{sc,ts,g,g',t,f}\rho_{sc}DW_{t}HF_{sc,ts,g,g',t,f}\left(\frac{2Dis_{g,g',t}}{AvS_{t}} + LUT_{t}\right)\Big/TCap_{t,f} \quad (4.23)$$

where DW_t represents the driver wagefor transportation mode t.

The maintenance cost for all scenarios and time periods is calculated as:

$$MC = \sum_{sc,ts,g,g',t,f} \rho_{sc} ME_t 2Dis_{g,g',t} HF_{sc,ts,g,g',t,f} \Big/ TCap_{t,f} \quad (4.24)$$

where ME_t denotes maintenance cost for transportation mode t.

The price for the energy source consumed for all scenarios and time periods is calculated as:

$$ESC = \sum_{sc,ts,g'',gp,e} \rho_{sc} PESAv_{sc,ts,g'',gp,e} (ESDis_e \, Dis_{g'',g} + ESCost_e) + \sum_{sc,ts,g'',gp,e} \rho_{sc} PES\mathrm{Im}_{sc,ts,g,p,e} ESICost_e \quad (4.25)$$

where $ESICost_e$ represents the energy source e import price, $ESCost_e$ denotes the energy source e price, generated locally, $ESDis_e$ is the delivery price for energy source e, and $Dis_{g'',g}$ is the distance between grid points.

Based on the work of De-León Almaraz [11], the total daily greenhouse gas (GHG) emission is associated with the GHG emitted during production, storage and transportation of HSC network at period ts:

$$TotalCO_{2sc,ts} = PCO_{2sc,ts} + SCO_{2sc,ts} + TCO_{2sc,ts}, \quad \forall sc,ts \quad (4.26)$$

where $TotalCO_{2sc,ts}$ is the total daily amount of emitted GHG in the HSC network during time period ts and scenario sc, $PCO_{2sc,ts}$ is the daily GHG emission from the production sites during time period ts and scenario sc, $SCO_{2sc,ts}$ is the daily GHG emission from the storage sites during time period ts and scenario sc, $TCO_{2sc,ts}$ is the daily GHG emission from distribution of hydrogen during time period ts and scenario sc.

The GHG emissions at the production sites are associated with the produced hydrogen of the form f by the each production facility p size h at grid point g during time period ts and scenario sc, and the total daily GHG emissions in production sites:

$$PCO_{2sc,ts} = \sum_{g,p,h,f} HP_{sc,ts,g,p,h,f} GEP_{p,f}, \quad \forall sc,ts \quad (4.27)$$

where $GEP_{p,f}$ is the amount of GHG emitted per kg H_2 produced in the form f in production facility p.

The total daily GHG emissions to store produced hydrogen is calculated as:

$$SCO_{2sc,ts} = \sum_{g,p,h,f} HP_{sc,ts,g,p,h,f} GES_f, \quad \forall sc,ts \quad (4.28)$$

where GES_f is the amount of GHG emitted to store kg H_2 in the form f.

The total daily transport GHG emissions are determined as via:

$$TCO2_{sc,ts} = \sum_{g,g',t,f} \rho_{sc} \cdot GET_t 2Dis_{g,g',t} HF_{sc,ts,g,g',t,f} / TCap_{t,f} \quad (4.29)$$

where GET_t is the amount of GHG emitted per km traveled distance of transportation mode t.

The final emissions fee from the HSC for all scenarios and time periods is calculated as:

$$EMC = \sum_{sc,ts} \rho_{sc} TotalCO2_{sc,ts} Tax_{ts} \quad (4.30)$$

where Tax_{ts} represents the tax for the CO_2 emissions for time period ts. It is assumed that Tax_{ts} is changing with time according to:

$$Tax_{ts} = CurTax(1 + InRate(ts - 1)), \forall ts \quad (4.31)$$

where $CurTax$ represents current value of emissions fee for 1 kg CO_2, $InRate$ represents the increasing rate.

To analyze the economic value of supply security, a penalty method is applied. The penalty is calculated as follows:

$$PenC = Pen \cdot \sum_{sc,ts,g} \rho_{sc} HI_{sc,ts,g} \quad (4.32)$$

where Pen is calculated as:

$$Pen = \sum_{sc,ts,g} \frac{\gamma_{ts} PN_{sc,ts,g} \cdot TT \cdot NetIn}{AvH \cdot HD_{sc,ts,g}} \quad (4.33)$$

where AvH represents the average number of members in one household (family), TT is the time used by a passenger transport by members of one household. $NetIn$ is the average income per household.

4.6. RESULTS AND DISCUSSION

To examine the HSC configurations, the model is setup as a MILP consisting of 5,539,256 constraints, 3,490,596 continues variables, 880,320 binary variables. The result section consists of two parts. First, the optimal hydrogen infrastructure for both configurations is discussed in more detail. Second, the effect of the demand uncertainty is analyzed and discussed.

4.6.1. THE OPTIMAL HSC CONFIGURATION

A scenario-based approach is used to model the demand uncertainty. This approach represents a collection of outcomes for all stochastic events taking place in the model with its associated probability, organized into a scenario tree (see Figure 4.4). For each of HSC configurations, three demand scenarios referred to as “high” (+20% expected demand), “medium” (expected demand), “low” (-20% expected demand) scenarios over five time periods of planning horizon are presented.

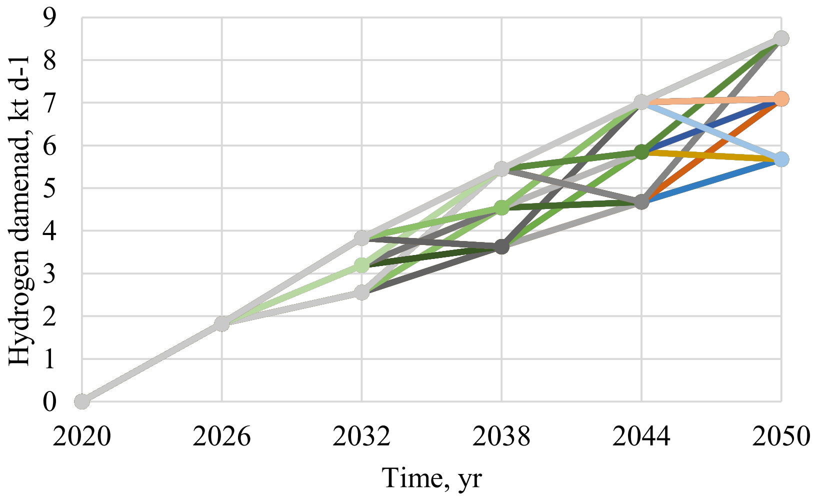

Figure 4.4 - Demand scenario tree (trajectory)

As mentioned before, the hydrogen demand is assumed to be known during first time period (2020-2026). This demand is calculated by a 6.7% penetration rate of FCEVs into passenger transport. The hydrogen demand is met by large-scale SMR-based plants located in Stuttgart, Munich, Berlin, Rostock, Mainz, Dresden and 2 large-scale SMR plants in Cologne (8 plants total). During the second time period, only three demand scenarios are examined, assumed 9.3, 11.6 and 14.0 percent penetration rate (2026-2032). The demand level is met by additional large-scale SMR plants in Stuttgart, Rostock, Mainz and by 2 large-scale SMR in Munich and Cologne (7 plants total). Nine scenarios are examined for the third time period (2032-2038), the demand level is varied from 13.3 to 19.9 percent penetration rate. Only 3 large-scale SMR plant are installed (Frankfurt, Kiel, Erfurt). For the remaining time periods there is no need for the installment of additional plants: the production capacity is enough to satisfy the hydrogen demand, which level varies between a 21.2 and 31.8 percent penetration rate. The optimal number of production plants by 2050 should be 18 large-scale SMR plants to fulfill the required demand. Hydrogen storage for 10 days requires 166 super-insulated spherical tanks installed at first time period. Additionally, 227 transportation units are required to transport the liquid hydrogen from production- to storage sites which are added in different time periods (see Table C.1). The expected total cost for the multi-stage stochastic optimization model equal 27.25 M$ per time period. Overall price of hydrogen wary from 5.11$ to 7.42$ per kg.

The second configuration of the model includes WE technology, whose current level of technological development only allows small-scale production capacity. Total number of WE-based plant equals 857 units, those are installed at the first time period at each grid points. Moreover, 214 transportation units are required to transport the liquid hydrogen to satisfy hydrogen demand. Noted, hydrogen demand is satisfied by local production. The expected total cost equal 52.97 M$ per time period. However, it was further assumed that the electricity consumption to produce 1kg of hydrogen can vary from 47.3kWh to 44.3kWh depending on the scale of plant, and all production size scales is allowed [12]. The network requires 18 large-scale electrolysis-based plants to produce liquid hydrogen to satisfy demand by 2050. During first time period hydrogen demand is satisfied by 5 large-scale WE plants (Stuttgart, Munich, Rostock, Cologne, Dresden) and 2 large-scale WE plants located in Mainz. Additional 8 large-scale WE plants(Stuttgart, Berlin, Potsdam, Rostock, Hannover, Cologne, Kiel, Erfurt) and 2 large-scale WE plants in Munich are installed at the second time period, and 1 large-scale WE located in Hannover is installed at the third time period. Moreover, the model requires 166 super-insulated spherical tanks and 270 transportation units (see Table C.2). The expected total cost for multi-stage stochastic optimization is 50.55 M$ per time period. Hydrogen cost lays between 9.49$ to 13.77$ per kg. Figure 4.5 shows of the cost assessment for both configurations. A high price of production sites and raw material of WE-based hydrogen production vs SMR-based, considering small emissions fee can be observed.

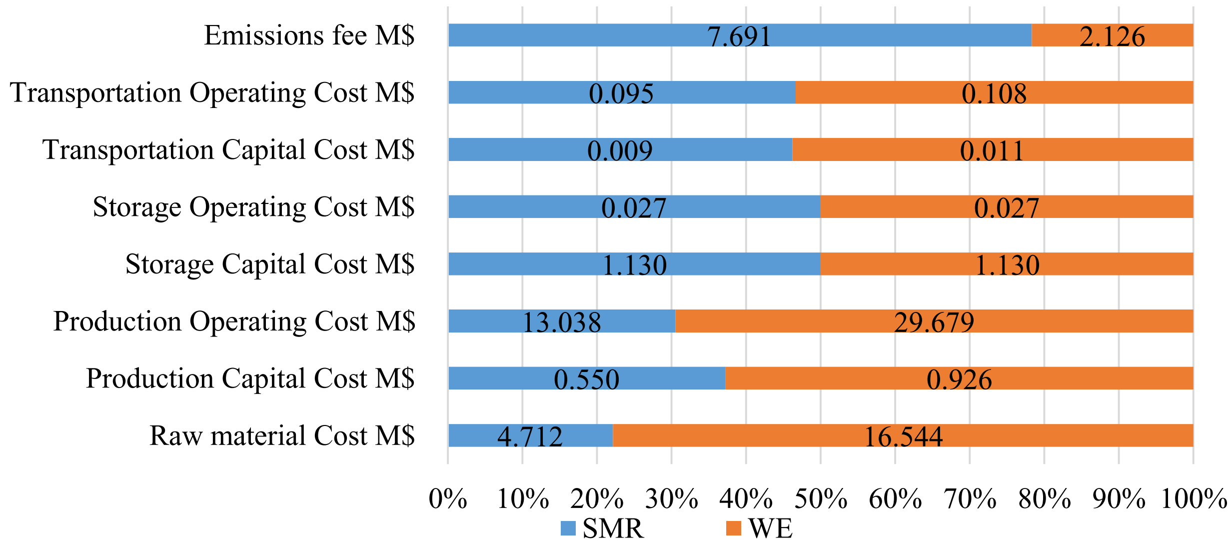

Figure 4.5 - Cost assessment of HSC: SMR vs WE technologies

4.6.2. EFFECTS OF DEMAND UNCERTAINTY

The concepts of EVPI and VSS are applied to evaluate the stochastic optimization results and compare them to their deterministic counterpart (see section 4.4). Mathematically, the EVPI is defined as the difference between the wait-and-see (WS) solution and recourse problem (RP), and the VSS is the value obtained by taking the difference between the result of using an expected value solution (EEV) and the RP. The WS solution represents the expected value of the deterministic solution that can be determined after simulation of each scenario individually, The EEV is obtained by calculating the expected value of the deterministic solution while replacing all random variables at the first-stage by their expected values and allowing a second-stage decision to be chosen optimally. In addition, the RP solution is a results of stochastic optimization. For the penalty cost that is lower than the calculated value of *PenC*, the results of the WS, RP and EEV are small because the import of hydrogen would satisfy a demand with lower costs than if hydrogen would be produced locally. However, taking into consideration the expected penalty cost, EVPIs for both configurations are more pronounced, adding up 4.2 and 6.7 M$ respectively, which are corresponding to 15-25% of the infrastructure investments. A high EVPI represents the importance of accurate projections to minimize infrastructure investments in the long run. Moreover, the VSS shows benefits of a stochastic approach for the model presented in this chapter, compared to a deterministic approach, up 7 M$ of infrastructure investments savings, corresponding 26% of total investments. Due to high cost of the second configuration, a part of the hydrogen demand is fulfilled by import, which is the cause of its lower VSS. EVPI and VSS results are presented in Figure 4.6.

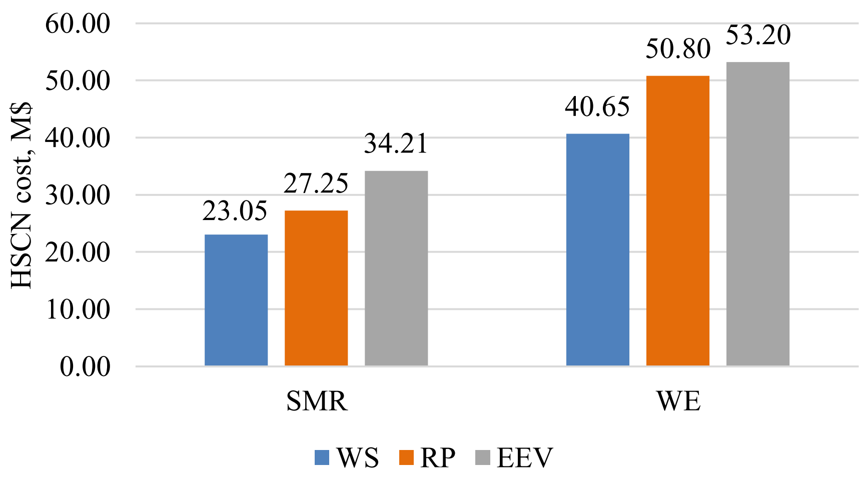

Figure 4.6 - WS, RP and EEV solutions for the evaluated network configurations

4.7.CONCLUSIONS

In this chapter, a multi-stage stochastic optimization approach is presented to assist strategic decision-making for design of a hydrogen infrastructure for the transportation sector in Germany. Based on sensitivity analysis, hydrogen demand is considered as uncertain parameter in the stochastic formulation, and its effect on the infrastructure investments is analyzed up to 2050. A scenario-based approach is applied to capture demand uncertainty over this extended period of time. Five time periods and eighty one scenarios are considered for the demand. The value of the stochastic solution for each configurations shows significant benefits were 26% of infrastructure investments savings can be made when incorporating demand uncertainty. Two configurations of a HSC are considered, which are analyzed and compared to each other according to production types. As the results show: a small emissions fee for water electrolysis is observed while the price of production sites and raw material is two times higher then steam methane reforming based technologies. However, the use of limited fossil fuels and large CO_2 emissions will shift the optimal network configuration from SMR to water electrolysis based technology according to the progress rate of technology.

4.8.NOMENCLATURE

INDICES

e	type of energy source
f	type of hydrogen physical form
g	grid points, each grid point represents German state
p	type of hydrogen production facility
h	size factor
s	type of storage facility
t	type of transportation mode
sc	demand scenarios
ts	time periods of the planning horizon

ABBREVIATIONS

BEV	battery electrical vehicles
BG	biomass gasification
CG	coal gasification
CO_2	carbon dioxide
EEV	expected result of using the expected value solution
EVPI	expected value of perfect information
FCEV	fuel cell electric vehicle
GHG	greenhouse gas
HSC	hydrogen supply chain
MILP	mixed integer linear programming
RP	recourse problem
SMR	steam methane reforming
VSS	value of the stochastic solution
WE	water electrolysis
WS	wait-and-see solution

CONTINUOUS VARIABLES

ESC	total cost for the energy source consumed for hydrogen production [$ d^{-1}]
$ESD_{sc,ts,g,p,e}$	daily energy source *e* demand by grid point *g* for production technology *p* during time period *ts* for scenario *sc* [kWh d^{-1}]

EMC	final emissions fee [$ d^{-1}]
$ExT_{sc,ts,g,g',t,f}$	continuous variable in scenario *sc* with value between 0 and 1, which is used to take an integer value for $NTU_{ts,g,g',t,f}$
FC	daily fuel cost [$ d^{-1}]
$HD_{sc,ts,g,f}$	amount of hydrogen demand satisfied by network in the form *f* in grid point *g* at time period *ts* and scenario *sc*[kg d^{-1}]
$HF_{sc,ts,g,g',t,f}$	hydrogen flowrate in the form *f* from grid point *g* to *g'* via transportation mode *t* during time period *ts* for scenario *sc* [kg d^{-1}]
$HI_{sc,ts,g}$	amount of hydrogen imported from another country to satisfy hydrogen demand in grid point *g* at time period *ts* and scenario *sc* [kg d^{-1}]
$HP_{sc,ts,g,f}$	hydrogen generation in the form *f* at grid point *g* during time period *ts* for scenario *sc* [kg d^{-1}]
$HP_{sc,ts,g,p,h,f}$	amount of produced hydrogen in the production facility *p* size *h* in the form *f* at the grid point *g* during time period *ts* for scenario *sc* [kg d^{-1}]
$HSInv_{sc,ts,g,s,f}$	inventory of product *f* in the storage facility s at grid point *g* at time period *ts* and scenario *sc* [kg]
LC	labor cost [$ d^{-1}]
MC	maintenance cost [$ d^{-1}]
PC	daily production costs[$ d^{-1}]
$PCO_{2\,sc,ts}$	daily GHG emission from the production sites during time period *ts* and scenario *sc* [kg d^{-1}]
$PESAv_{sc,ts,g'',g,p,e}$	energy source flowrate to meet demand for a certain energy source *e* in production facility *p* from the grid point *g"* to the grid point *g* during time period *ts* for scenario *sc* [unit e d^{-1}]
$PESIm_{sc,ts,g,p,e}$	flowrate importing energy source *e* to the grid point *g,* where production facility *p* is installed*,* during time period *ts* for scenario *sc* [unit e d^{-1}]
SC	the total hydrogen storage cost [$]
$SCO_{2\,sc,ts}$	daily GHG emissions from storage sites during time period *ts* and scenario *sc* [kg d^{-1}]
TC	daily distribution cost [$ d^{-1}]
$TCO_{2\,sc,ts}$	daily GHG emissions during hydrogen delivery at time period *ts* and scenario *sc* [kg d^{-1}]
$TotalCost$	total daily cost of HSC network [$ d^{-1}]
$TotalCO_{2\,sc,ts}$	total daily GHG emission of HSC network during time period *ts* and scenario *sc* [kg d^{-1}]

INTEGER VARIABLES

$InPF_{ts,g,p,h,f}$	number of new invested production facility *p* size *h* generating hydrogen in from *f* at grid point *g* during time period *ts*
$InSF_{ts,g,s,f}$	number of new invested storage facility *s* holding hydrogen in from *f* at grid point *g* during time period *ts*
$InTU_{ts,g,t,f}$	number of new invested transportation units *t* for hydrogen distribution in the form *f* at grid point *g* during time period *ts*
$NPF_{ts,g,p,h,f}$	total number of production facility *p* size *h* generating hydrogen in from *f* at grid point *g* during time period *ts*
$NSF_{ts,g,s,f}$	total number of storage facility *s* holding hydrogen in from *f* at grid point *g* during time period *ts*

$NTU_{ts,g,g',f,t}$	total number of transport mode t used for hydrogen distribution in the form f from g to g' during time period ts

PARAMETERS

AvD_{ts}	average distance travelled by personal car at time period ts [km y^{-1} $capita^{-1}$]
AvH	average number of members in one household
AvS_t	average speed of transportation mode t [km h^{-1}]
AF_p	annual factor for the facility p [%]
AF_s	annual factor for the s storage facility s [%]
AF_t	annual factor for the transport mode t [%]
$CurTax$	current value of emissions fee for 1 kg CO_2 [\$ kg^{-1}]
$Dis_{g'',g}$	distance between grid points [km]
$Dis_{g,g',t}$	distance between grid points depending of type of transport [km]
DW_t	driver wage, who drives transportation mode t [\$]
$ESCost_e$	energy source e price in year y, generated locally [\$ $unit^{-1}$ e]
$ESDis_e$	delivery price for energy source e [\$ $unit^{-1}$ km^{-1}]
$ESICost_e$	energy source e import price [\$ $unit^{-1}$]
FE	the fuel economy [kg H_2 km^{-1}]
FET_t	fuel economy for transportation mode t [unit km^{-1}]
FP_t	fuel price for transport mode t [\$ $unit^{-1}$]
$GEP_{p,f}$	GHG emitted in the production facility p to produce kg H2 in the form f [kg kg^{-1} H_2]
GES_f	GHG emitted in storage side to store kg H2 in the form f [kg kg^{-1} H_2]
GET_t	GHG emitted by transport mode t per 1 km [kg km^{-1}]
$HD_{sc,ts,g}$	hydrogen demand by grid point g during time period ts for scenario sc [kg d^{-1}]
$InRate$	increasing rate coefficient
LUT_t	load/unload time for transportation mode t [h]
LR	learning rate taking into account cost reduction of facilities as experience accumulates with time
MA_t	transportation mode t availability [h]
$MaxPCap_{p,h}$/ $MinPCap_{p,h}$	max/min production capacity for hydrogen production facility p size h[kg d^{-1}]
$MaxSCap_{s,f}$/ $MinSCap_{s,f}$	max/min capacity of storage facility s for holding hydrogen in the from f [kg]
ME_t	maintenance cost for transportation mode t [\$]
$NetIn$	average income per one household [\$ d^{-1}].
NP	number of time period
OP	operating period [d y^{-1}]
$PCC_{p,h,f}$	capital cost of facility p size h, producing hydrogen in form f [\$ d^{-1}]
$POC_{p,h,f}$	hydrogen production cost in form f at facility p size h [\$ d^{-1}]
$PN_{sc,ts,g}$	population at the grid point g during time period ts and scenario sc
$SCC_{s,f}$	capital cost for storage facility s holding hydrogen in the form f [\$]
$SOC_{s,f}$	operating cost to store 1 kg of hydrogen in the from f inside of storage facility s [\$ kg^{-1} d^{-1}]
Tax_{ts}	tax for kg CO_2 emissions for time period ts [\$ kg^{-1}]
$TCap_{t,f}$	capacity of transportation mode t to distribute produced hydrogen in form f [kg]

$TCC_{f,t}$	capital cost of transport mode *t* for distribution hydrogen in the form *f* [$]
TT	time use of passenger transport by one household [% d^{-1}]

GREEK LETTERS

$\alpha_{e,p,h}$	the ratio between energy sources *e* consumption for production facility *p* size *h* to produce 1 kg [unit e kg^{-1} H_2]
ρ_{sc}	scenario probability [%]
γ_{ts}	FCEVs penetration rate at time period *ts*[%]
τ	total product storage period [d]

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APPENDIX C

Table C.1 - Results of Configuration 1

Production stage

Time period	Grid point	Type of technology	Size	Form	Number
1	Stuttgart	Steam methane reforming	Large	Liquid	1
1	Munich	Steam methane reforming	Large	Liquid	1
1	Berlin	Steam methane reforming	Large	Liquid	1
1	Rostock	Steam methane reforming	Large	Liquid	1
1	Cologne	Steam methane reforming	Large	Liquid	2
1	Mainz	Steam methane reforming	Large	Liquid	1
1	Dresden	Steam methane reforming	Large	Liquid	1
2	Stuttgart	Steam methane reforming	Large	Liquid	1
2	Munich	Steam methane reforming	Large	Liquid	2
2	Rostock	Steam methane reforming	Large	Liquid	1
2	Cologne	Steam methane reforming	Large	Liquid	2
2	Mainz	Steam methane reforming	Large	Liquid	1
3	Frankfurt	Steam methane reforming	Large	Liquid	1
3	Kiel	Steam methane reforming	Large	Liquid	1
3	Erfurt	Steam methane reforming	Large	Liquid	1

Storage stage

Time period	Grid point	Type of technology	Form	Number
1	Stuttgart	Super-insulated spherical tanks	Liquid	23
1	Munich	Super-insulated spherical tanks	Liquid	27
1	Berlin	Super-insulated spherical tanks	Liquid	8
1	Potsdam	Super-insulated spherical tanks	Liquid	5
1	Bremen	Super-insulated spherical tanks	Liquid	2
1	Hamburg	Super-insulated spherical tanks	Liquid	4
1	Frankfurt	Super-insulated spherical tanks	Liquid	13
1	Rostock	Super-insulated spherical tanks	Liquid	15
1	Hannover	Super-insulated spherical tanks	Liquid	3
1	Cologne	Super-insulated spherical tanks	Liquid	34
1	Mainz	Super-insulated spherical tanks	Liquid	8
1	Saarbrucken	Super-insulated spherical tanks	Liquid	2
1	Dresden	Super-insulated spherical tanks	Liquid	8
1	Halle	Super-insulated spherical tanks	Liquid	4
1	Kiel	Super-insulated spherical tanks	Liquid	6
1	Erfurt	Super-insulated spherical tanks	Liquid	4

Transportation stage

Time period	Grid point	Type of technology	Form	Number
1	Stuttgart	Railway tank car	Liquid	4
1	Munich	Railway tank car	Liquid	9
1	Berlin	Railway tank car	Liquid	11
1	Rostock	Railway tank car	Liquid	22

1	Cologne	Railway tank car	Liquid	10
1	Mainz	Railway tank car	Liquid	13
1	Dresden	Railway tank car	Liquid	16
1	Kiel	Railway tank car	Liquid	3
1	Erfurt	Railway tank car	Liquid	12
2	Stuttgart	Railway tank car	Liquid	7
2	Munich	Tanker truck	Liquid	17
2	Berlin	Railway tank car	Liquid	4
2	Cologne	Railway tank car	Liquid	8
2	Mainz	Railway tank car	Liquid	1
2	Dresden	Railway tank car	Liquid	3
2	Kiel	Railway tank car	Liquid	5
3	Munich	Railway tank car	Liquid	4
3	Frankfurt	Railway tank car	Liquid	5
3	Rostock	Railway tank car	Liquid	2
3	Cologne	Tanker truck	Liquid	32
3	Mainz	Railway tank car	Liquid	3
3	Dresden	Railway tank car	Liquid	2
3	Kiel	Railway tank car	Liquid	4
3	Erfurt	Railway tank car	Liquid	2
4	Stuttgart	Railway tank car	Liquid	3
4	Munich	Railway tank car	Liquid	1
4	Frankfurt	Railway tank car	Liquid	2
4	Rostock	Railway tank car	Liquid	3
4	Mainz	Railway tank car	Liquid	11
4	Erfurt	Railway tank car	Liquid	1
5	Rostock	Railway tank car	Liquid	2
5	Cologne	Railway tank car	Liquid	2
5	Dresden	Railway tank car	Liquid	2
5	Erfurt	Railway tank car	Liquid	1

Summary	
Energy Distribution and Purchase Cost M$ d^{-1}	$4.71
Production Capital Cost M$ d^{-1}	$0.55
Production Operating Cost M$ d^{-1}	$13.04
Storage Capital Cost M$ d^{-1}	$1.13
Storage Operating Cost M$ d^{-1}	$0.03
Transportation Capital Cost M$ d^{-1}	$0.01
Transportation Operating Cost M$ d^{-1}	$0.09
CO_2 fee M$ d^{-1}	$7.69
Penalty $ d^{-1}	$0.00
Global warming potential 10ˆ3 t CO_2 d^{-1}	121.43
Total Cost M$ d^{-1}	$27.25

Table C.2 - Results of Configuration 2

Production stage

Time period	Grid point	Type of technology	Size	Form	Number
1	Stuttgart	Water electrolysis	Large	Liquid	1
1	Munich	Water electrolysis	Large	Liquid	1
1	Rostock	Water electrolysis	Large	Liquid	1
1	Cologne	Water electrolysis	Large	Liquid	1
1	Mainz	Water electrolysis	Large	Liquid	2
1	Dresden	Water electrolysis	Large	Liquid	1
2	Stuttgart	Water electrolysis	Large	Liquid	1
2	Munich	Water electrolysis	Large	Liquid	2
2	Berlin	Water electrolysis	Large	Liquid	1
2	Potsdam	Water electrolysis	Large	Liquid	1
2	Rostock	Water electrolysis	Large	Liquid	1
2	Hannover	Water electrolysis	Large	Liquid	1
2	Cologne	Water electrolysis	Large	Liquid	1
2	Kiel	Water electrolysis	Large	Liquid	1
2	Erfurt	Water electrolysis	Large	Liquid	1
3	Hannover	Water electrolysis	Large	Liquid	1

Storage stage

Time period	Grid point	Type of technology	Form	Number
1	Stuttgart	Super-insulated spherical tanks	Liquid	23
1	Munich	Super-insulated spherical tanks	Liquid	27
1	Berlin	Super-insulated spherical tanks	Liquid	8
1	Potsdam	Super-insulated spherical tanks	Liquid	5
1	Bremen	Super-insulated spherical tanks	Liquid	2
1	Hamburg	Super-insulated spherical tanks	Liquid	4
1	Frankfurt	Super-insulated spherical tanks	Liquid	13
1	Rostock	Super-insulated spherical tanks	Liquid	15
1	Hannover	Super-insulated spherical tanks	Liquid	3
1	Cologne	Super-insulated spherical tanks	Liquid	34
1	Mainz	Super-insulated spherical tanks	Liquid	8
1	Saarbrucken	Super-insulated spherical tanks	Liquid	2
1	Dresden	Super-insulated spherical tanks	Liquid	8
1	Halle	Super-insulated spherical tanks	Liquid	4
1	Kiel	Super-insulated spherical tanks	Liquid	6
1	Erfurt	Super-insulated spherical tanks	Liquid	4

Transportation stage

Time period	Grid point	Type of technology	Form	Number
1	Stuttgart	Railway tank car	Liquid	4
1	Munich	Railway tank car	Liquid	6
1	Berlin	Railway tank car	Liquid	6
1	Potsdam	Railway tank car	Liquid	11

1	Rostock	Railway tank car	Liquid	9
1	Hannover	Railway tank car	Liquid	4
1	Cologne	Railway tank car	Liquid	5
1	Mainz	Railway tank car	Liquid	26
1	Dresden	Railway tank car	Liquid	15
1	Erfurt	Railway tank car	Liquid	2
2	Stuttgart	Railway tank car	Liquid	10
2	Munich	Railway tank car	Liquid	8
2	Berlin	Railway tank car	Liquid	2
2	Potsdam	Railway tank car	Liquid	3
2	Rostock	Railway tank car	Liquid	3
2	Hannover	Railway tank car	Liquid	52
2	Cologne	Railway tank car	Liquid	2
2	Mainz	Railway tank car	Liquid	8
2	Kiel	Railway tank car	Liquid	6
2	Erfurt	Railway tank car	Liquid	7
3	Potsdam	Railway tank car	Liquid	2
3	Rostock	Railway tank car	Liquid	5
3	Mainz	Railway tank car	Liquid	1
3	Kiel	Railway tank car	Liquid	3
3	Erfurt	Railway tank car	Liquid	4
4	Munich	Tanker truck	Liquid	16
4	Munich	Railway tank car	Liquid	1
4	Cologne	Railway tank car	Liquid	7
4	Mainz	Railway tank car	Liquid	3
4	Kiel	Railway tank car	Liquid	2
4	Erfurt	Railway tank car	Liquid	3
5	Munich	Tanker truck	Liquid	1
5	Berlin	Railway tank car	Liquid	2
5	Potsdam	Railway tank car	Liquid	6
5	Hannover	Railway tank car	Liquid	2
5	Mainz	Railway tank car	Liquid	2
5	Dresden	Railway tank car	Liquid	10
5	Erfurt	Railway tank car	Liquid	11

Summary	
Energy Distribution and Purchase Cost M$ d^{-1}	$16.54
Production Capital Cost M$ d^{-1}	$0.93
Production Operating Cost M$ d^{-1}	$29.68
Storage Capital Cost M$ d^{-1}	$1.13
Storage Operating Cost M$ d^{-1}	$0.03
Transportation Capital Cost M$ d^{-1}	$0.01
Transportation Operating Cost M$ d^{-1}	$0.11
CO_2 fee M$ d^{-1}	$2.13
Penalty $ d^{-1}	$0.00
Global warming potential 10ˆ3 t CO_2 d^{-1}	33.56
Total Cost M$ d^{-1}	$50.55

5.CONCLUSION & OUTLOOK

5.1.CONCLUSION

The aim of this study was to prove that the transport sector in Germany is ready to shift from fossil fuels to hydrogen and to develop a strategy evaluating the feasibility of a hydrogen economy.

In this thesis a Mixed Integer Linear Programming (MILP) model was developed and evaluated that can be applied to solve a hydrogen supply chain (HSC) network design problem forecasting up to 2050. The formulation of this model is based on the concept of determining the best hydrogen infrastructure pathways while making decisions regarding the primary energy source, production, storage and distribution networks in Germany.

Five energy sources from different origins, four hydrogen production technologies, two hydrogen product form, four transportation modes and two storage technologies were evaluated. As a result, two configurations were proposed based on coal gasification and water electrolysis technologies. Furthermore, hydrogen production in liquid form is preferred. Germany has a well-developed railway infrastructure, i.e. the railway tank car was selected as preferred transportation mode in both configurations. It is noted that a large part of the German rail freight transport is electrified, which means that rail transport is a clean type of distribution. As hydrogen production in liquid form is preferred, super-insulated spherical tanks were used to minimize heat loss. It is noted that, renewable energy as a power source has a potential to replace commonly used fossil fuels in the near future: renewable electricity production can satisfy a hydrogen based fuel demand.

Subsequently, the MILP model has been extended considering different objectives, i.e. cost, environmental impact, safety. The ε-constraint method was applied to consider these three objectives. The optimum solution with respect to each objective was obtained first from a single objective optimization, to evaluate the lower bounds of each objective in the feasible space and upper bounds on the Pareto surface. Then, multiple solutions between these lower and upper bounds were obtained by constraining the two objectives (the environmental impact and safety) and minimizing the total daily cost. The proposed trade-off solution of the multi-objective optimization was obtained by calculation of the shortest distance between the utopia point and all points on the Pareto front. It showed the potential to build a safer HSC based on water electrolysis technology considering a decentralized configuration, where 45% of hydrogen is produced by water electrolysis and 55 % by steam methane reforming. Hydrogen costs vary between 3.95 and 10.56 $ kg^{-1}. Compared to a modern internal combustion vehicle that uses fuel with an average cost of 0.0645 $ km^{-1}, the average hydrogen cost, 0.0762 $ km^{-1}, demonstrates the feasibility of HSC network.

Subsequently a sensitivity analysis was preformed to evaluate which model parameters had the strongest impact in the total daily network cost. The sensitivity analysis showed that hydrogen demand has a very strong effect on the objective function. Including demand uncertainty in the model showed that a small emissions fee for water electrolysis is included and that the price of the production sites and raw material is three times higher as conventional lower cost hydrogen production techniques such as steam methane reforming and coal gasification. Despite economic benefits, the use of ultimate fossil fuels and large CO_2 emissions will shift the optimal network configuration from conventional hydrogen production techniques to water electrolysis. The value of the stochastic solution was applied to evaluate the stochastic optimization results, and it showed up to 26% of infrastructure investments savings.

Overall it can be concluded that the implementation of fuel cell electric vehicles powered by renewable hydrogen for the transport sector becomes feasible and actively contributes to the decarbonization of the energy system making the transport sector in Germany ready to shift to clean fuels.

5.2.PERSPECTIVES

5.2.1. MODEL EXTENSIONS

Hydrogen delivery is a critical contributor to the total daily cost, safety and emissions associated with hydrogen pathways involving centralized production configuration. The choice of the lowest-cost delivery mode depends upon specific geographic- and market characteristics such as existing infrastructure, the distance between the production site and filling station and market penetration of fuel cell vehicles (hydrogen demand). In the current optimization model, four types of transportation modes were considered namely railway tank car, tanker truck, railway tube car and tube trailer. However, the study of Robinius et al. shows that point-to-point pipeline systems are a very efficient option for transporting large amounts of hydrogen over long distances [1]. Thus, a pipelines system might be added to the model as transportation mode. Furthermore, the option of using of existing natural gas pipelines for transporting hydrogen can be taken into account.

Moreover, implementing Liquid Organic Hydrogen Carriers (LOHC) and underground storage in salt caverns might be taken into account as an option for long-term storage. The main advantage of the LOHC technology is that it enables hydrogen storage in chemically bound form under ambient conditions. In storage caverns, high amounts of hydrogen can be stored together with high injectivity and deliverability. They are characterized by low specific investment costs, long operating times for more than 30 years and low specific land requirements. As a consequence industrial hydrogen underground storage caverns and LOHC technology can be crucial for maintaining the security of hydrogen supply and can contribute to the decarbonization of the energy system [2].

5.2.2. SYNERGIES WITH OTHER POWER-TO-X SYSTEMS

As a result of the energy transition, Germany has massively invested in renewable energy production. Hydrogen will play a key role in future energy systems and can be considered as long-term renewable energy storage option. Synergies with other Power-to-X systems such as Power-to-chemicals will open the opportunity to apply renewable hydrogen to chemicals production. As conventional coal and gas-fired power plants still largely supply the German energy landscape, emitted carbon dioxide can be captured by Carbon Capture, Utilization, and Storage (CCUS) technology, which can be further used for methanol production together with renewable hydrogen. The integration of hydrogen- and carbon dioxide supply chains for methanol production can be considered as the potential option for the decarbonization of the energy system in Germany [3].

5.3.REFERENCES

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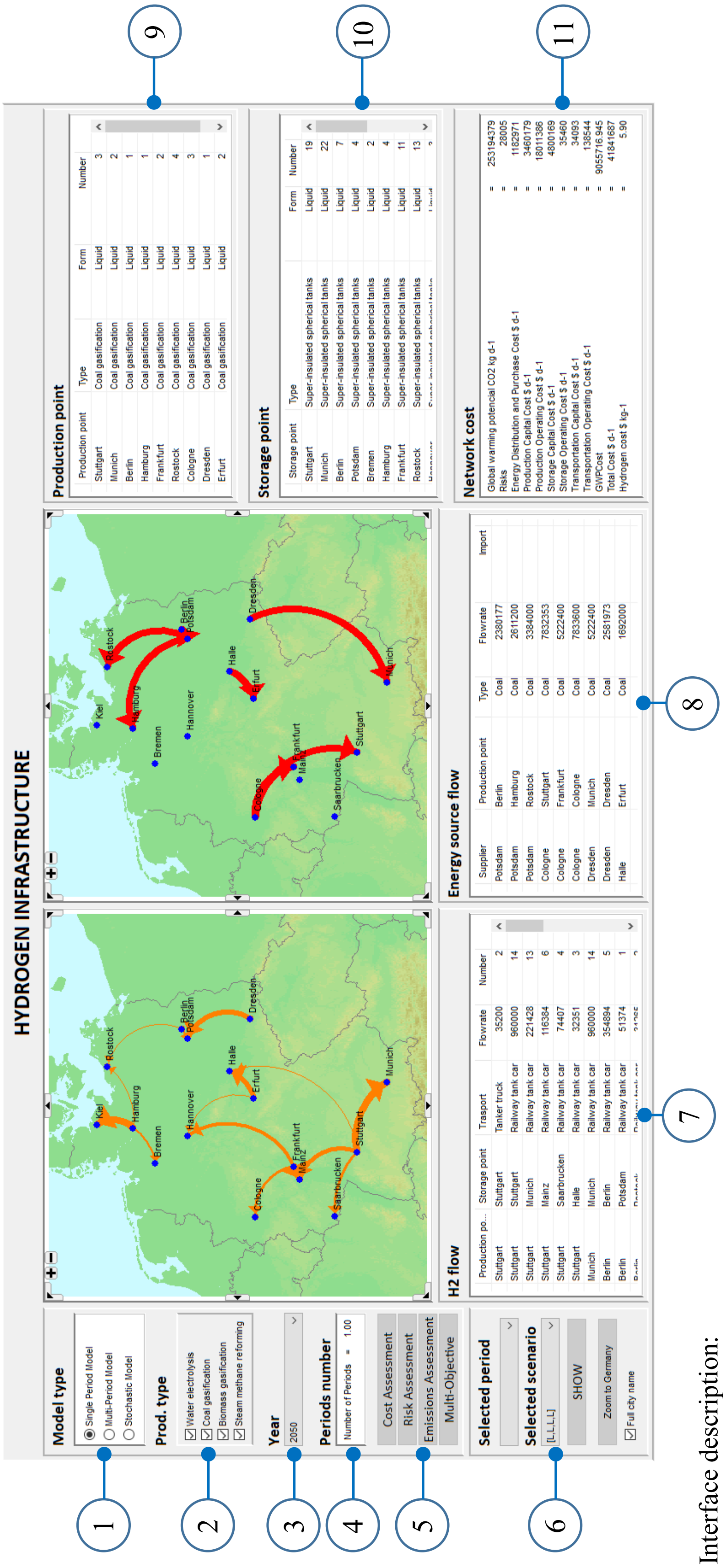
APPENDIX D

The end-user Graphical User Interface for fastest control of decision making.



Interface description:

1. Model type selection (Single period, Multi-period, Stochastic)
2. Production type selection, which will be involved into the model optimization
3. Selection of Year. The model will solve a HSC network design problem forecasting for selected year.
4. Selection of number of periods (N). This tool is available only for multi-period and stochastic model types. The model will include N time periods with time evolution constraints allowing for the transfer of production and storage plants across time periods.
5. Selection of objective function
6. Map control tools for representation of transportation links between grid points.
7. Information about hydrogen transportation from production site to costumers, and number and type of transportation units.
8. Information about energy source transportation from supplier to production site.
9. Information about location, type and number of production facilities, and form and amount of produced hydrogen.
10. Information about location, type and number of storage facilities.
11. Summary of network cost, risk and CO_2 emissions.

SCAN QR CODE FOR FURTHER INFORMATION