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ENGINEERING AND POLICY ANALYSIS

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# Exploring the acceleration of green hydrogen diffusion

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## Executive summary

Hydrogen is more and more recognized as an essential component of a sustainable future. A series of countries have issued hydrogen strategies over the past years, and climate neutral energy scenarios increasingly acknowledge a long-term need for hydrogen. Because of its versatility, hydrogen is a promising energy carrier. Hydrogen has no end-use emissions and offers possibilities for decarbonization in hard-to-abate sectors, long-term energy storage, and long-distance energy transport. Today, hydrogen primarily has a function as feedstock in refineries and chemical industry, but the possibilities for alternative purposes are extensive. In industry, it offers potential for decarbonization of steel manufacturing and chemical industry. Hydrogen can be applied in transport to power fuel cell vehicles or produce synthetic fuels. In the build environment there are options for fossil-free heating, and hydrogen can alleviate storage and transmission challenges in the renewable power sector. The applications are widespread and the potential of decarbonization is promising. However, to deploy the promising sustainable characteristics of hydrogen as a carbon-free energy carrier, hydrogen production through zero-carbon pathways is a prerequisite.

Today, the largest share of hydrogen worldwide is produced with fossil fuels, defined as grey hydrogen, which is a heavily polluting process. Coupling carbon capture and storage technology to fossil-based production, referred to as blue hydrogen, is considered to be a plausible transition step towards large-scale hydrogen adoption. The benefits of this pathway are not undisputed, and it can be argued that green hydrogen, which is hydrogen produced from water electrolysis powered by renewable electricity, is the only long-term sustainable technology.

However, the current speed of diffusion of green hydrogen is sluggish. Fundamental barriers that impede the diffusion of green hydrogen according to literature are low cost-competitiveness of green hydrogen compared to fossil-hydrogen, a lack of hydrogen infrastructure, no demand for hydrogen in end-use sectors and an absence of policies and regulations. With these barriers in place, the diffusion of hydrogen is not going to ignite spontaneously. Therefore, to enable green hydrogen to play a role in a sustainable energy future, acceleration of diffusion through the implementation of policy instruments is essential. This study investigates hydrogen diffusion and the impact of the barriers and drivers and aims to answer the research question:

*What is the impact of drivers and barriers on the diffusion of sustainable hydrogen and how can this diffusion be accelerated?*

To answer the research question, the development of green hydrogen is assessed in a quantitative manner. A system dynamics modeling approach is adopted to investigate the development of green hydrogen over time and assess the impact of policies. System dynamics allows for continuous modeling of the system behavior and provides insight in the dynamics of diffusion of hydrogen over time. A country-level perspective is depicted, with Germany as case study country. Germany is a leading country in the development of green hydrogen and has formulated a hydrogen strategy with clear and ambitious green hydrogen targets, as well as preliminary hydrogen policies. The time scope of the model is 2010 to 2050. The model is a techno-economic abstraction of the hydrogen supply chain and incorporates characteristics of each component of the hydrogen supply chain, from production to consumption. Furthermore, it endogenously models drivers of diffusion such as technological learning, investment choice behavior, and the levelized costs of hydrogen. The key performance indicators of the model are the installed capacity of electrolysis, total hydrogen demand, cumulative abated emissions, and cumulative policy costs. A series of validation tests and an uncertainty analysis have been conducted, after which the behavior of green hydrogen diffusion has been analyzed for the reference case and two scenarios. Finally, the impact of a diverse range of separately and combined tested policy levers has been examined, with the policy settings varying in strength and timing.

The base case outcome provides a picture of the current situation as reference and demon-

strates a marginal deployment of green hydrogen. No policies are implemented in this case and fossil fuel prices remain low up to 2050. It is observed that increasing carbon prices do provide slight incentive in end-use sectors to abate fossil fuels in favor of hydrogen technologies. As a result, hydrogen demand increases in heavy duty transport and steel manufacturing slightly from 2025 towards 2050. However, due to the low cost-competitiveness of green hydrogen, growing demand is supplied by an increasing capacity of blue hydrogen and green hydrogen diffusion is nonexistent. Under more progressive circumstances, with high fossil fuel prices and a strongly increasing carbon price without policies, hydrogen demand mounts to a greater extent than in the base case. Also, a slight establishment of green hydrogen diffusion is detected, with electrolysis capacity reaching 3.2 GW in 2050. Nevertheless, green hydrogen diffusion in this case initiates very late and is far from reaching the electrolysis capacity targets, 5 GW for 2030 and minimal 10 GW for 2040, from the German government. Without the introduction of policy levers, diffusion of green hydrogen will remain absent.

The examined policy levers in the model are based on existing policies, announced policies and potential policies. Eight policies were tested separately and combined, resulting in 56 different policy configurations. Of the policies supporting the adoption of green hydrogen production over blue hydrogen production, an exemption for the taxation on electricity demonstrates to be the most effective measure. It was also surprisingly found that the timing of implementation of these policies is of large influence on the effectiveness. Of the demand-side policies, carbon contracts-for-difference result in the highest increase of hydrogen demand, stimulating the adoption of hydrogen in steel manufacturing. Policies to induce the construction of hydrogen infrastructure show accelerating effects on the diffusion of both hydrogen demand and production, although very marginal. From combining the policies, it is observed that there are little amplifying effects, and that a few policy combinations show even worse outcomes than some policies activated individually. Although the individual and combined policies show in most cases positive leveraging effects, even the strongest conventional policy measures are not sufficient to meet German targets. Finally, the unconventional measure of a ban on blue hydrogen was examined. As expected, this measure drives the full share of hydrogen supply to be provided by green hydrogen production. For 2030, electrolysis targets are still not achieved, but regardless of the delayed diffusion, electrolysis capacity increases towards 11 GW in 2040 and 14.8 GW in 2050.

Several conclusions can be drawn from the model analysis and the policy examination. First, without the implementation of policy measures the future of green hydrogen will have a lack of prospect, because the barriers cannot be overcome spontaneously. Second, the acceleration of diffusion is most effectively levered with demand-side policies, as supply ultimately follows demand. Third, implementing demand-side policies without the simultaneous activation of supply-side policies results in a thriving deployment of blue hydrogen production and an absence of green hydrogen. Fourth, the timing of supply-side policies results in counter-intuitive outcomes: the effects of a delayed policy activation show larger effects than a rapid implementation in some cases, because of the relation between the policy mechanisms and variable external circumstances. Finally, without the implementation of rigorous measures, green hydrogen will not thrive, and blue hydrogen will remain the dominant hydrogen production method.

Although the model is suitable for obtaining insights in the acceleration of hydrogen diffusion dynamics, interpreting the model outcomes requires a note of caution. It must be said that the model is an abstraction of the real-world hydrogen supply chain, where real-world complexity and uncertainty are present which can never be captured comprehensively in a model. Further research could provide improvements to the model by expanding the technological scope and further examination of uncertainty and robustness. It would also be interesting to implement boundaries of growth to the model, for the assessment of limits to diffusion. Furthermore, alternative countries could be relatively easy implemented in the model for the comparison of diffusion rates. Finally, the counter-intuitive relations between timing and policy effectiveness should be examined in continuous research.

## Preface

While writing the final bits of this thesis in the library of the TU Delft, the relevance of accelerating the transition towards a sustainable future is again emphasized. A terrible war has started in Ukraine, causing a long-unprecedented geopolitical instability in Europe and a terrible humanitarian crisis. The stability of peace in Europe is in danger, and as collateral damage, the security of energy. Not only are we obliged to accelerate the energy transition and rehabilitate from our fossil fuel addiction to mitigate the long-term consequences of global warming and pollution. We must also rapidly decarbonize, provoked by the geopolitical instability, to quit our dependency on energy from unreliable, authoritarian powers. Although there are numerous hurdles to take, the potential role of hydrogen as a green substitute of incumbent fossil molecules in a sustainable future cannot be denied anymore. The field of green hydrogen is developing with the speed of light, and during this thesis process I was overtaken by actuality many times. Only the uncertain future will tell if hydrogen will live up to its promising expectations, but it is up to us to help reducing this uncertainty a little bit.

This thesis marks the final capstone of fulfilling the master's program Engineering and Policy Analysis at Delft University of Technology, and my life as a student in Delft. With great joy I look back at the master's program in The Hague, my bachelor at 3me, and the unforgettable time at 9b, in Rome, and in Rotterdam.

First of all, I want to thank Kornelis and Els for their supervision during this project. Although most meetings were digital due to Covid restrictions, you were always available when needed to support me with your much appreciated knowledge and feedback. Kornelis, I really enjoyed this process together; Thank you for sharing your enthusiasm for accelerating the energy transition and your limitless knowledge about energy technologies, leading to interesting conversations. Most of all, when I wandered about unimportant details or drifted off to the wrong direction, you were always sharp in keeping me on the right track. Els, thank you very much for sharing your System Dynamics wisdom with me, and always taking the time to check my work and model. Especially after I picked up working again after Covid, our weekly meetings truly helped me getting back on track. Also without my friends and family, I would not have come far. I want to thank Joanna, for the love and support, always and also during these months. I would like to thank my parents and Marieke, for their always right advice and encouraging words, but moreover for their warmth and gezelligheid, whether in Haarlem or in Oisterwijk. Furthermore I would like to thank Francis, for the many enlightening discussions we had during the winter months at TPM, my housemates for their feedback and nice meals, and of course all my other friends for providing distraction when needed.

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# 1 Introduction

Today, the urgency of accelerating the transition to renewable energy sources is more apparent than ever before. As part of its Sixth Assessment Report, the International Panel on Climate Change (IPCC) reports that the devastating effects of climate change are taking place faster than previously alleged, and that irreversible effects that make it impossible to adapt for nature and mankind can only be prevented through fierce action in this decade. (IPCC, 2022). To limit temperature rise exceeding 1.5 degrees Celsius, now is the time for a global transformation of the prevailing fossil-based energy system.

The grand challenge remains in finding the best pathway to abandon fossil fuels while at the same time offering energy security for an increasing world population (Sgobbi et al., 2016). Strategies for reducing greenhouse gas emissions include increasing energy efficiency, implementing carbon-capture and storage (CCS), and switching to low-carbon energy sources and energy carriers (van Vuuren et al., 2018). Much attention has been given to the power sector, with the contribution of wind and solar-PV capacity in electricity generation showing a stable increase over the past decades. Despite the sustainable progress in the electricity sector, only around 11% of the total final energy consumption (TFEC) in 2018 was produced from renewable energy sources (excluding biofuels) (REN21, 2020). According to the 1.5°C roadmap of IRENA (2021), the global share of renewable electricity of TFEC must exceed 51% in 2050 to reach climate goals. Nevertheless, exclusively concentrating on the expansion of renewable electricity has technological constraints to ensure a sustainable transformation of the entire energy system. The weather dependency of most renewable energy sources combined with the limitations for long-term storage of electrical power induces uncertainty for energy security. Furthermore, the application of electrification is not suitable for all hard-to-abate sectors (Blanco et al., 2018). The other, non-electrified share of energy in end-use sectors must therefore be provided by renewable substitutes, which requires the exploration of alternative renewable energy carriers (Den Ouden et al., 2018; Detz et al., 2019).

Because of its versatility, hydrogen is a promising renewable energy carrier. Hydrogen has no end-use emissions and offers possibilities for decarbonization in hard-to-abate sectors, long-term energy storage, and long-distance energy transport (Sgobbi et al., 2016). If produced in a carbon-free manner, hydrogen could fill the gap in the future sustainable energy system where molecules remain indispensable and abatement through direct electrification is difficult to achieve (Marchenko & Solomin, 2015; Den Ouden et al., 2018). Four sectors for application of hydrogen can be distinguished (Detz et al., 2019): In transport, hydrogen acts as fuel for Fuel Cell Electric Vehicles (FCEV), or as feedstock for synthetic fuels that can be used in aviation or maritime transportation. In buildings, hydrogen can be mixed into existing gas networks for heating. In industry hydrogen has two main applications. High-temperature industrial processes that are now provided by natural gas or coal could be fuelled with hydrogen. Furthermore, hydrogen is an important feedstock in oil refineries and for chemical production processes such as fertilizers and plastics. Lastly, in the power sector hydrogen can fulfill a role in balancing variable renewable energy supply through long-term energy storage.

Although the large scale integration of hydrogen, especially renewable hydrogen, seems only conceptual today, it might take-off in a near future. The importance of hydrogen as an energy carrier is gaining acknowledgement, leading to a momentum in politics and business (IEA, 2019). Across the globe, 19 countries have issued national hydrogen strategies in the past years, confirming the acknowledgement of potential (Hydrogen Europe, 2020). The roadmap of the European hydrogen council forecasts a 24% share for hydrogen of final energy use in 2050 in Europe (FCH-JU, 2019). Similarly, the IRENA world energy transition outlook expects a 6% share for renewable hydrogen in the global total final energy consumption for 2050 (IRENA, 2021). The International Energy Agency (IEA) (IEA, 2021) proclaims a contribution for hydrogen in the TFEC of 9.7% for hydrogen in their recent Net Zero Emissions-scenario.

To achieve the benefits of hydrogen as a carbon-free energy carrier, hydrogen production

through zero-carbon pathways is a prerequisite. According to IEA statistics, approximately 70 Mtons of hydrogen is produced annually on a global scale. The major share of hydrogen is generated from fossil fuels: approximately 76% is generated with natural gas; 22% is a product of coal, primarily in China. These so-called grey hydrogen production processes are far from sustainable and accounted for 830 Mt CO<sub>2</sub>, equally to 2.3% of total global carbon emissions in 2018 (Kakoulaki et al., 2021; IEA, 2020). Conversely, low-carbon hydrogen production in 2020 contributed a marginal 0.36 Mtons to total hydrogen production, with 0.3 GW electrolyser capacity globally installed (IEA, 2021). Green hydrogen production methods have not yet been deployed on a large scale: an estimated 5% of global hydrogen is generated from dedicated water electrolysis (IEA, 2019). Current low-carbon, or green, hydrogen production methods are not cost-competitive with incumbent grey hydrogen production methods. The price of green hydrogen varies between 3.2-7.7\$/kg, whereas costs of grey hydrogen produced with natural gas fluctuates between 1.2-2.1\$/kg (Bloomberg NEF, 2019). Determinants such as costs of renewable electricity, capital costs of electrolyzers and the path dependency of fossil-based production methods partially explain the price gap between green and grey hydrogen (IEA, 2021).

Given these points, the global energy system is in transformation, which is a complex and uncertain process. Green hydrogen production methods are in an early stage of deployment, but costs are high and market share is marginal, which makes it not yet competitive with incumbent fossil-driven technologies. Nevertheless, the urgency of quick deployment of green hydrogen as an emission reducing component in the future energy system is apparent. This research explores the impact drivers and barriers on the diffusion of green hydrogen and explores strategies to accelerate this diffusion.

## 2 Background and knowledge gap

The problem introduction emphasizes on the essential role that hydrogen could fulfill in a future sustainable energy system and the urgent need for rapid deployment of green hydrogen. This section aims to provide further background information about the diffusion of green hydrogen. Present-day literature is examined for three subjects that pertain to

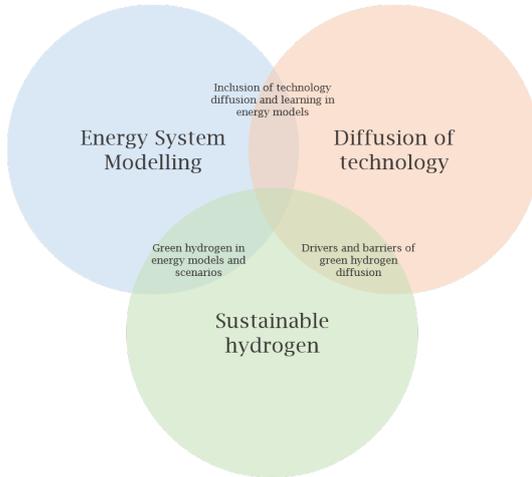


Figure 1: Three fields of literature have been examined for the background study and knowledge gap

models use a wide range of modeling tools and methods resulting in various prognoses for the diffusion of hydrogen. Hydrogen is considered in global and local energy scenarios, such as in integrated assessment models (IAM) which capture the relations within an entire energy system between environmental, economic and social factors. This allows for an evaluation of the impact of policies on decarbonization and emission targets, with the focus on cost optimization (van Vuuren et al., 2011). Integrated assessment models are often least-cost pathways that focus on the wider energy system, using comprehensive modeling tools such as MESSAGE (IPCC) and ETP-TIMES (IEA). Quarton et al. (2020) recognize an increasing trend in the implementation of hydrogen in future energy scenarios. This increasing interest in hydrogen as an energy carrier is demonstrated in the large role for hydrogen in recent renowned global energy outlooks (IEA, 2021; IRENA, 2021; BP, 2020).

An early appraisal of a future hydrogen economy was conducted by Barreto et al. (2003). They adopted a long-term perspective to quantify trends in the global energy system corresponding with the diffusion of hydrogen. An optimistic hydrogen-supportive scenario was used, technological learning of solar-pv power plants for hydrogen technologies was assumed, and international trade not incorporated. Hydrogen-based technologies were found to diffuse rapidly in this scenario and fuel cells are a major option for energy provision in transportation and electricity generation. Hydrogen generation in industrialized countries was provided by fossil-fuels long into the future, whereas hydrogen production in developing countries shifted to renewable methods more rapidly as a result of less locked-in fossil fuel infrastructures (Barreto et al., 2003). The distinction of diffusion rate of hydrogen between developing and developed countries was not corroborated by Ruijven et al. (2008). They focused on the difference between energy systems of developed and developing countries and compared hydrogen diffusion in India and Western-Europe through a system dynamics cost-based model. Model assumptions of infrastructure costs, technology learning, and energy taxation drive the diffusion of hydrogen derived from literature form the input of three scenarios, resulting in the outputs climate change, energy security, and air quality. High capital costs of hydrogen technologies and low fossil fuel prices curb the emergence

the diffusion of hydrogen. Three fields have been explored using field-related keywords and Boolean integrators: The role of hydrogen in present-day energy modeling studies and scenarios, the theory of diffusion of renewable energy technologies and hydrogen technologies and the drivers and barriers that push and obstruct the diffusion of sustainable hydrogen. The overlap of these fields is schematically displayed in figure 1. From there, a knowledge gap is defined, leading to the main research question of this thesis.

### Hydrogen in energy models and scenarios

The role of hydrogen in the future energy system is accompanied by uncertainty. A large number of studies have attempted to comprehend these uncertainties and assess the dynamics of future decarbonized energy systems. Global and local energy system

of hydrogen in the energy system in both regions, resulting in a 6% share for hydrogen in India's total final energy consumption in 2050, mostly consumed in the transport sector. Sgobbi et al. (2016) executed an integrated approach for modeling the entire hydrogen economy in Europe. They used the bottom-up TIMES model generator with the objective of providing energy security while minimising the energy costs. Two policy scenarios for the European Union were run up to 2050, a Business-As-Usual (BAU) scenario and carbon-cap scenario demanding 80% emission reduction in 2050. The stringent emission reduction target demonstrated positive impact on the deployment of hydrogen and electrolysis capacity. It is furthermore concluded in this study that the the absence of carbon capture and storage does not hamper the diffusion of hydrogen. It can be argued that forecasting the future diffusion of hydrogen in integrated energy system models has several limitations. Their focus is confined to the relation between climate and economic systems (van Vuuren et al., 2011), looking at abatement costs and excluding avoided damage or adaptation costs (Evans & Hausfather, 2018). Another limitation is the least-cost paradigm, which leads to strong focus on cost-efficiency instead of political, technological or societal dynamics and feasibility (Evans & Hausfather, 2018; McDowall & Eames, 2006). The construction of scenarios is often not transparent, allowing for unknown assumptions of the modelers choice. Models vary in scenario settings and the GHG emission targets set; the assessed policy mixes are different; the technology mix for production is not consistent, as well as the coverage of end-use applications (McDowall, 2014). Furthermore; scenarios with high ambitions for hydrogen deployment tend to have too optimistic assumptions for costs and cost reductions (IRENA, 2020; Quarton et al., 2020).

### **Diffusion of energy technologies**

The promising technological characteristics and bright-sided plausible scenarios for green hydrogen development are by no means a guarantee for a rapid growth in capacity. Diffusion of a technology is a highly uncertain process, depending on dynamics in the environment and on the uncertain evolution of the technology itself as a result of diffusion (Barreto, 2001). The diffusion of technologies and innovations is a broad field of research. It attempts to obtain insight in the determinants that affect the temporal and spatial distribution of emerging technologies (Barreto & Kemp, 2008). Early work on diffusion of innovation is provided by (Rogers, 1962), describing diffusion as a process of communication about an innovation between certain actors over time. Diffusion is measured as the adoption of a technology over time as a percentage of market saturation. The adoption rate is captured with an S-curve, prompted by early adopters that are followed by the majority and laggards before the technology reaches a maximum level of diffusion (Rogers, 1962) The S-curve for diffusion has been corroborated in the vast literature on diffusion modeling. An early introduced and widely adopted method for modeling technology adoption is the Bass model, explaining diffusion through an indicator resembling innovation, imitation and potential users (Bass, 1969). These econometric type of models were initially adopted for the analysis of consumer markets, but has seen a wider application for renewable energy technologies more recently (Söderholm & Klaassen, 2007; Usha Rao & Kishore, 2009; Wilson, 2012; Bento & Wilson, 2016). Diffusion dynamics have thus become an important aspect of modeling future energy technology deployment.

Energy technologies in general have a larger inertia of diffusion than consumer products, because of high capital cost, long lifetimes and slow capital turnovers (Barreto, 2001). Furthermore, diffusion of energy technologies is slow because of inter-relatedness between the energy system and the economic system and therefore dependent on institutional support that often lacks (Negro et al., 2012). Energy technologies are often of large scale; physically and economic, leading to slower learning and diffusion rates than granular technologies. 'Lumpy' energy technologies scale in unit size, rather than manufacturing speed and often require system integration or infrastructure decelerating diffusion (Wilson et al., 2020). In a comparative study to the duration of diffusion for different technologies including energy technologies, it was found that technologies that are non-ready substitutes for incumbent technologies show slower diffusion rates, because of the often-required new infrastructure and institutions (Bento & Wilson, 2016). Another determinant tested, unit scale, showed vari-

able results, of which the researchers concluded that diffusion can be accelerated in extreme cases and through heavy market interference of governments. Industrial manufacturing capacity is another factor that affects the diffusion rate, according to Kramer & Haigh (2009). The inertia for renewable energy technology diffusion is substantiated by Gross et al.(2018), who found a duration of 55 years for solar PV in Germany and 40 years for wind power in Denmark to diffuse to 20% of peak installed capacity, whereas consumer end-use products needed only 27 to 35 years to emerge up to 20% of ultimate market size. A positive note is given by Wilson (Wilson, 2012), who indicated an increasing diffusion rate for modern energy technologies such as wind turbines over time.

Diffusion of hydrogen technologies in specific has been subject to a number of studies. Different methodologies have been applied, such as system dynamics modeling for the uptake of FCEV (Struben & Sterman, 2008; Meyer & Winebrake, 2009; Fazeli et al., 2021). An often applied approach to study the diffusion of hydrogen technologies is the theory of innovation systems (Jacobsson & Johnson, 2000; Hekkert et al., 2007). These studies aim to provide insight in the dynamics of local innovation clusters and systemic drivers and barriers to diffusion. Suurs et al. (2009) identified drivers and barriers for the innovation of hydrogen fuel cell technologies in the Netherlands, based on the methodological framework of innovation system functions from Hekkert et al.(2007). A similar approach was conducted by Hacking et al.(2019), for the historical analysis of 60 years of diffusion of hydrogen fuel cell technologies across the UK. Andreasen & Sovacool(2015) use the seven technological innovation system functions to compare fuel cell development in Denmark and the United States. Decourt (2019) applies the framework on the diffusion of electrolyzers in Europe. Although these studies provide useful insight in the barriers of hydrogen diffusion, they assess the diffusion of hydrogen in a predominantly qualitative manner, excluding concrete measures or drivers.

### **Drivers and barriers for the diffusion of hydrogen**

Considering the different methods to assess the deployment of hydrogen, most studies set off with a number of drivers and barriers to hydrogen diffusion. Drivers to diffusion can be considered as incentives for the diffusion of green hydrogen, such as financial incentives, carbon reduction targets or policies. In contrast, barriers to diffusion are the mechanisms or phenomena that obstruct or even oppose the drivers such as high cost for green hydrogen and absence of policy directives. The different drivers and barriers described in literature can in such way be considered antonyms. The table in appendix A displays multiple barriers to the diffusion of hydrogen as described in a number of studies from a period between 2014-2020. Interestingly, the detected barriers do not largely vary in this time scope, implying the persistence of existence of the barriers to hydrogen diffusion. The barriers that are mentioned in these highlighted studies show severe overlap, and are constituted in numerous other studies to hydrogen deployment. (McDowall & Eames, 2006; Suurs et al., 2009; McDowall, 2014; Ball & Weeda, 2015; Astiaso Garcia, 2017; Maggio et al., 2019; Hacking et al., 2019; Chapman et al., 2019; Decourt, 2019; IRENA, 2020; Ren et al., 2020; IRENA, 2022).

From this preliminary literature search, the most prominent barriers to the diffusion of green hydrogen have been distinguished:

1. The high costs of green hydrogen relative to fossil hydrogen and fossil fuels
2. The absence of infrastructure for hydrogen
3. The lack of hydrogen demand in end-use sectors
4. Lack of hydrogen specific policies and regulatory incentives
5. Technological immaturity of green hydrogen technologies
6. Uncertainty about the availability of renewable electricity for hydrogen production
7. Investment uncertainty for businesses and industry

The absence of a balanced hydrogen market with interconnected production, consumption

and infrastructure can be considered a chicken-and-egg problem (Ruijven et al., 2008; Ball & Weeda, 2015; IRENA, 2022). There is large uncertainty about the market mechanisms and it remains unclear where and how levers could be implemented to overcome the barriers and stimulate green hydrogen deployment. The drivers that are mentioned in literature to propel hydrogen are found in the field of market stimulation and emission reduction goals, through the implementation of policies and sustainable energy targets. However, these are in most studies superficially touched and barely specified. Quantification of the impact of the barriers and drivers for diffusion for green hydrogen has not been conducted.

## 2.1 Knowledge gap

Hydrogen has large potential to play a versatile role in future global sustainable energy system. It is clear that sustainable energy targets benefit from a rapid diffusion of green hydrogen. However, to achieve this, a transition is needed on two fronts: first, hydrogen must be dispatched across a wider range of sectors. Conventional fossil fuel-technologies that are hard to abate through electrification must shift to hydrogen consumption. Second, hydrogen production must make the transition from the conventional fossil-based production to sustainable green production. The future of hydrogen has been assessed in several modeling studies, resulting in a range of possible hydrogen futures and scenarios (Ruijven et al., 2008; Sgobbi et al., 2016; Hanley et al., 2018; Staffell et al., 2019; Hebling et al., 2019; DENA , 2019; Energy, 2020; Gasforclimate , 2021; FCH-JU, 2019; EC, 2018a). Furthermore, vast literature is present on the speed of diffusion of renewable energy technologies (Jacobsson & Johnson, 2000; Söderholm & Klaassen, 2007; Rao & Kishore, 2010; Negro et al., 2012; Wilson, 2012; Williams et al., 2020). A number of studies assessed the diffusion of hydrogen, albeit mostly in a qualitative manner from an innovation-system perspective (Suurs et al., 2009; Hanley et al., 2018; Maggio et al., 2019; Decourt, 2019). Insights from existing research provide on the one hand qualitative knowledge about the barriers that hamper the diffusion of hydrogen, what leads to in-concrete qualitative proposals to stimulate green hydrogen diffusion. On the other hand, existing quantitative research has its limitation in scope and transparency. The scope of most integrated assessment models is geographically and technologically too aggregated to extract accurate policy recommendations on a country-scale for green hydrogen in specific (IEA, 2021; IRENA, 2022). Models focus too much on the least-cost paradigm and exclude political, technological or societal dynamics and feasibility (McDowall & Eames, 2006; Evans & Hausfather, 2018), and are often a black-box with in-transparent model assumptions(Quarton et al., 2020). Furthermore; scenarios with high ambitions for hydrogen deployment tend to have too optimistic assumptions for sustainable costs and cost reductions(IRENA, 2020; Quarton et al., 2020). To employ the potential of green hydrogen as a sustainable energy carrier in a future sustainable energy system, insight is needed how to overcome the chicken-egg situation we are in now and how to accelerate the diffusion of green hydrogen. Concrete and applicable strategies for a quicker diffusion must be defined. Thus far, the impact of drivers and barriers on the diffusion of green hydrogen has barely been quantified yet on a scope that allows for useful for policy recommendations. Similarly, a quantitative policy exploration that provides transparent, applicable strategies for the acceleration of green hydrogen diffusion is absent. This knowledge gap leads to the following research question:

**What is the impact of drivers and barriers on the diffusion of sustainable hydrogen and how can this diffusion be accelerated?**

The objective of this research is to develop insight in the dynamics of diffusion of green hydrogen and explore what measures could enhance a rapid deployment of green hydrogen. A modelling approach allows for quantitative insights in the system behavior and experimentation with policy levers. From transparent quantitative modeling with an appropriate scope, this study aims to propose a set of concrete policy recommendations to lever the acceleration of diffusion of green hydrogen.

## 2.2 Thesis structure

This thesis is structured as follows: In the next chapter, chapter 3, the research approach and subquestions to answer the main question are explained. In chapter 4, a system description is given of hydrogen supply chain in Germany. After the system description, a conceptualization of the hydrogen supply chain is given in section 5.1, and the model and its validation is described in detail in section 5.2. In chapter 6, the results are displayed. Finally, the conclusions are presented in chapter 7, after which a reflection on limitations of the model and the model outcomes is given in chapter 8.

## 3 Research approach and Methodology

This chapter explains the scope and the approach of the research, describes the subquestions, and clarifies the methodology that will be applied to answer the main research question and achieve the research objective.

### 3.1 Scope of research

Although the future of hydrogen is relevant on a global scale, this study adopts a country size-scope. Because of the geographic components of green hydrogen diffusion, such as renewable electricity availability and infrastructure, a global scale would be too aggregated to investigate. Furthermore, drivers in the shape of policies are deployed on a country level, not on a global scale. Finally, a country perspective offers the level of aggregation that is appropriate for continuous modeling of the diffusion of hydrogen and offers the availability for expansion of the model towards a global scale by reproducing the model for alternative countries. Germany is depicted as case-study country to be applied in the model. Germany is a hydrogen front-runner, with currently the largest hydrogen production and consumption in Europe (FCH2JU, 2020). Furthermore, Germany was one of the first countries to announce a hydrogen strategy in 2020, with targets for a 200-fold increase in green hydrogen production capacity of 5 GW in 2030 and minimal 10 GW in 2040 (BMW, 2020). Germany foresees a large role for hydrogen in the future energy system, in decarbonization of end-use sectors and in replacing current grey hydrogen for green hydrogen (BMW, 2020). Furthermore, Germany has large potential for a successful hydrogen future, due to the presence of infrastructure, strong regulatory environment and ambitious sustainable energy targets (Pflugmann & De Blasio, 2020).

### 3.2 Simulation technique

For the investigation of diffusion and the exploration of policy measures in a quantitative matter, a modeling approach is chosen. The definition of a model is provided by Kaplan (1964): "Any system A is a model of a system B if the study of A is useful for the understanding of B without regard to any direct or indirect causal connection between A and B". The diffusion of (energy) technologies from a system perspective can be considered as a complex, uncertain and dynamic. The complexity originates from the connection between the factors that drive and obstruct diffusion. These factors are dynamic, governed by feedback, nonlinear and history-dependent, which induce complexity (Sterman, 2000; Pruyt, 2013). Uncertainty is generally defined as limited knowledge about the future, present or past. In policy analysis, uncertainty according to Walker et al. (2012) is 'any departure from the ideal of total determinism', and is somewhere between complete certainty and total ignorance. The uncertainty in diffusion of technology lays in the inadequacy of mental capacity, or bounded rationality, about the impact of system's factors and their coherent unknown behavior on diffusion. Finally, dynamic system behavior stems from the non-linearity and feedback loops between factors, what results in an unknown behavior over time that we cannot grasp in mental models (Sterman, 2000). Simulation modeling is the only practical way to understand and test the behavior of systems of which the complexity exceeds the mental ability to understand these systems (Sterman, 2000). For complex, dynamic and uncertain problems, simulation is the only reliable way to understand the problem and evaluate the implications of policies. Simulation allows for the quantitative understanding of a complex and dynamic problem, and moreover is the only method for experimentation when experimenting in the real-world system is not possible.

For simulating a complex, dynamic and uncertain system or problem and the subsequent policy analysis, a number of simulation options can be considered. Agent-based modeling, discrete event simulation and system dynamics are often applied policy simulation techniques. Agent-based modeling has a bottom-up approach and considers the behavior of individual actors in a system from a microscopic point of view (Nieuwenhuijsen et al., 2018). Discrete event simulation (DES) simulates a system or network with individual entities,

that flow through the system. The system and the entities have a certain state that remains constant for variable periods of time and changes when discrete events occur (Hild, 2000). DES is a powerful tool for operational problems where the modelers perspective is on the complexity in details of individual model entities and views a system or problem from a close-up resolution (Lane, 2000). DES is therefore appropriate when the details of a system need to be modelled and individual states of entities must be examined (Morecroft, 1982). Thirdly, system dynamics (SD) encounters problems or systems with a continuous stock-and flow structure, where individual entities are considered as a continuous, fluid alike flow that move through the system. The emphasis is on the structure of the system and the dynamic complexity that is caused by the feedback loops in the system. In appendix B, an overview of the conceptual differences between the three simulation methods is given.

Considering the characteristics of the different modeling methods on the one hand and the characteristics of the research problem on the other hand, system dynamics is depicted as the most appropriate simulation method for this research for a number of reasons. First, SD allows for an aggregated approach of a system, in which high-level system behaviour is captured above low-level actor behaviour making a certain distance observation from the system possible (Maier, 1998). This suits the country-level perspective of the case of diffusion, for which a high level perspective is adopted and the emphasis is on the high-level system behavior instead of actor behavior. Furthermore, the behavior of technology diffusion is a complex dependent on multiple elements and their interactions (feedbacks) as stated before, and is above all continuous. SD requires a distance between the modeler and the system, through which discrete events can be regarded in a continuous matter allowing for system understanding (Richardson, 2020). Lastly, SD provides the possibility to understand a system and evaluate the impact of external factors and explore future scenarios under uncertainty, fitting the objective of this research (Qudrat-Ullah & Seong, 2010).

### 3.3 Research steps and subquestions

The modeling process of SD consists of five steps and provides the research approach of this thesis (Sterman, 2000). These phases form the entire pathway from problem formulation towards system understanding and insight in the effects of policies. The process of SD is therefore not solely a software modeling exercise, but inquires the problem from a holistic system-thinking point of view in which the real-world system is converted into a useful model. It is essential to consider the model building as an iterative process, where after each phase the previous steps are reconsidered based on insights acquired from each subsequent phase. A summarizing figure of the modeling steps is provided in figure 3. The five stages of modeling are:

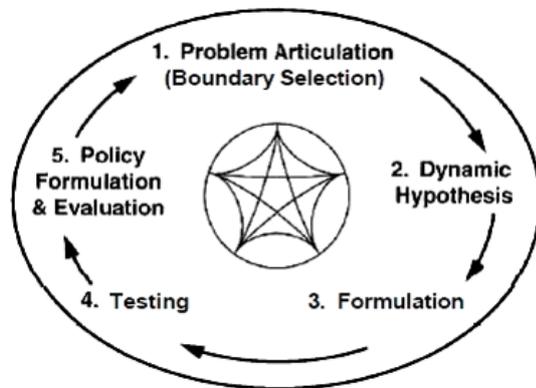


Figure 2: Representation of the SD modeling approach (Sterman, 2000)

#### 1. Problem articulation and system description

According to Sterman (2000), the problem articulation is the most important step in the modeling process. This step includes the definition of the problem and the purpose of the model. The key concepts and variables that relate to the real-world problem are examined in this step. Moreover, this step delineates the boundaries of the scope of the model by describing the real-world system and selecting the relevant factors that must be included in the model and omitting the irrelevant factors. The aim of this step is to translate the real-world situation into a system description and describe the clear problem formulation and model purpose. This step will be further indicated in this research as System description.

The subquestion that will be answered in this modeling phase is:

- What is the current state of green hydrogen in Germany and what drivers and barriers can be detected?

## 2. Model conceptualization

During the conceptualization phase the system as described in the previous phase is translated to the rough outlines of a SD-model. This step includes the abstraction of the real-world components into model subsystems or model parameters. The factors that drive and hamper the diffusion of green hydrogen are translated into submodels or model parameters. Furthermore, the relations between these factors is examined. In this step the choice is made which factors, or concepts, will be included as endogenous model parameters or exogenous factors. The purpose of this modeling phase is to construct a subsystem diagram that demonstrates the architecture of the entire model: the subsystems, model relations and external factors. From the subsystem diagram it becomes clear what factors are included in the model endogenously and what system factors are excluded from the scope. Furthermore, with the boundaries of the system and the most important subsystems defined a causal loop diagram (CLD) is constructed. In SD modeling, a CLD has a key role in conceptualizing and communicating the feedback structure of the system (Morecroft, 1982). This way, a CLD simplifies the translation of a system description into a feedback model structure. The subquestion that is addressed in this section is:

- How can the diffusion of hydrogen be conceptualized in a model?

## 3. Model formulation

After the model boundaries, submodels and the essential model parameters and variables are known, the conceptual model will be translated into a set of mathematical equations. The quantification of the conceptual model requires numerical data for the constants and external variables. When the input is adequate, the formalized model allows for simulation and experimentation of the real-world system. Therefore the main goal of this phase is to translate the conceptual model into a quantitative simulation model that simulates the diffusion of green hydrogen from a set of mathematical equations and numerical input.

## 4. Model testing

To check if the formalized model suits the purpose of the model that was stated in the first modeling phase, the formalized model will be tested. To test if the model is suitable for simulating the diffusion of green hydrogen, several methods for validation will be applied. A number of validation tests will be executed, amongst which a sensitivity analysis and extreme conditions test. Furthermore, the model will be validated based on comparison of historical diffusion to the model output and dimensional consistency. The testing phase must seek for model dimension inconsistencies and possible violations of physical laws. The aim of this step is to assess if the model is appropriate to represent and simulate the diffusion of green hydrogen in Germany. After this step, the model will be ready to use for simulation and experimentation.

**5. Policy design and evaluation** This phase comprises the application of the model. Once there is confidence about the structure and the behavior of the quantitative model, the model can be used as a tool for system exploration and policy evaluation. Experimentation will be conducted in a number of steps. First, an uncertainty analysis will be conducted to assess the impact of the range of uncertainty of external variables and the input parameters (Kwakkel & Pruyt, 2013). The uncertainty envelope of the external variables will be addressed in a scenario analysis, in which two outer possible future scenarios are examined, resulting in the uncertainty envelope of the model output based on the two scenarios. The impact of uncertainty in the parameters will be tested for a number of uncertain model constants that show diverging values in literature. Furthermore, the impact of uncertainty of several individual modeling aspects will be tested and discussed. The uncertainty will be assessed without the implementation of the policies, to obtain a full understanding of the uncertainty in the basic structure of the model. After the scenario and parameter uncertainty analysis, the policies will be implemented in the model. A number of conventional policies will

be assessed first individually and later combined. Each policy will be varied in strength and timing. After testing the conventional policies, there is room left for the exploratory assessment of more extreme, unconventional policies and their effects on the system. The aim of this phase is to discover the functioning of the basecase model and the effects of the different included system components, drivers and barriers, on the model output. Moreover, the goal is to determine the uncertainty range of the model and assess the impact of several conventional and unconventional policies on the diffusion of green hydrogen. This must answer the following subquestions:

- How do drivers and barriers affect the diffusion of green hydrogen in Germany?
- What is the potential effect of policies on the diffusion of green hydrogen?

## 3.4 Methodology

### 1. System Dynamics modeling

System dynamics modeling will be applied as method to translate a complex real-world system into a comprehensible simulation model that allows for exploration of the system behavior and policy analysis. The essence of SD modeling is in the construction of the feedback structure of the model, which determines the behavior of the model. The structure of the SD model is composed of different feedback-loops that involve non-linearities, delays and accumulation (Lane, 2008). Accordingly, the main mechanisms in SD modeling are: feedback loops, stocks and flows, and time delays (Sterman, 2002).

**Feedback loops:** A feedback loop is the essential structural element of any system. In a feedback loop, every decision is dependent on the existing condition of the system and influences that condition (Forrester, 1997). According to Forrester (1997), feedback loops impel non-linearity if the system contains a multiplication or division of a variable. Feedback loops resemble the causal relationship between factors that directly or indirectly affect each other and together determine the systems behavior. An example of a feedback loop in the field of technology development is learning by doing, in which costs reduce as a result of production experience. Another often-applied feedback loop in diffusion is the feedback loop based on potential adopters of consumer products, market saturation and word-of-mouth (Struben & Sterman, 2008).

**Stocks and flows:** Stocks and flows, or levels and rates (Forrester, 1997), represent the accumulation and dispersal of resources. Stock parameters represent the state of the system and accumulates based on the integration of flows over time. The flows, in-going or outgoing, determine the speed of accumulation or depreciation and change the value of the stocks. An often given illustration of a stock and flow structure is a bath-tub (Sterman, 2002; Pruyt, 2013). The tap is the inflow and can be regulated to allow for a water inflow of a certain amount per time unit. The bath-tub represents the stock and collects the accumulated water inflow, mathematically represented by the integral of the inflow minus the outflow. The outflow in this example is the valve, that allows water to flow out with a certain rate. Other examples of this structure are the population of species that accumulates by births and decreases through death, or a stock in a warehouse that varies through sales and production.

**Time delays:** Time delays represent the time between a decision that is made and the effects of the decision in the system. When time delays are combined with feedback loops, the system can become unstable and starts to show oscillating behavior (Sterman, 2002). An example of a time delays in the real world can be found in delivery delays in supply-chains. Firms that notice a changing demand must incorporate a time difference between allocation of orders and delivery, and beware of insufficient corrective actions between shortage and demand in case of a delay in supply to prevent overshoot or shortage in supply (Rahmandad et al., 2009).

Based on these mathematical mechanisms, SD offers a useful tool for the abstraction of the complex problem of sustainable hydrogen diffusion. It provides the possibility to simulate the

behavior of diffusion and experiment with policy levers in the system. Moreover, SD makes it possible to quantify seemingly qualitative parameters, so that the simulation exceeds a solely techno-economic perspective, but can include societal and political elements in a quantitative matter as well. For the construction and simulation of the system dynamics model, Vensim software will be used.

## 2. Data gathering

To obtain the data for the system dynamics model, desk research will be conducted. Data will be acquired from reliable sources and research institutions, such as Fraunhofer, IEA, IRENA, the EU-Joint Research Centre, and academic research papers. First, general data about the technologies for production and application of hydrogen is acquired. This consists of technological parameters that are independent of a geographical location. The next step is the acquisition of data about the status of hydrogen and the drivers and barriers of diffusion of green hydrogen in the case study country, Germany. This will include the investigation of governmental data about existing and announced policies in Germany, and technological governmental data about the existing production and consumption of hydrogen in Germany. Finally, technological and cost data will be acquired from studies that specifically focus on Germany or if not available, Europe, which will provide the input data for the SD-model.

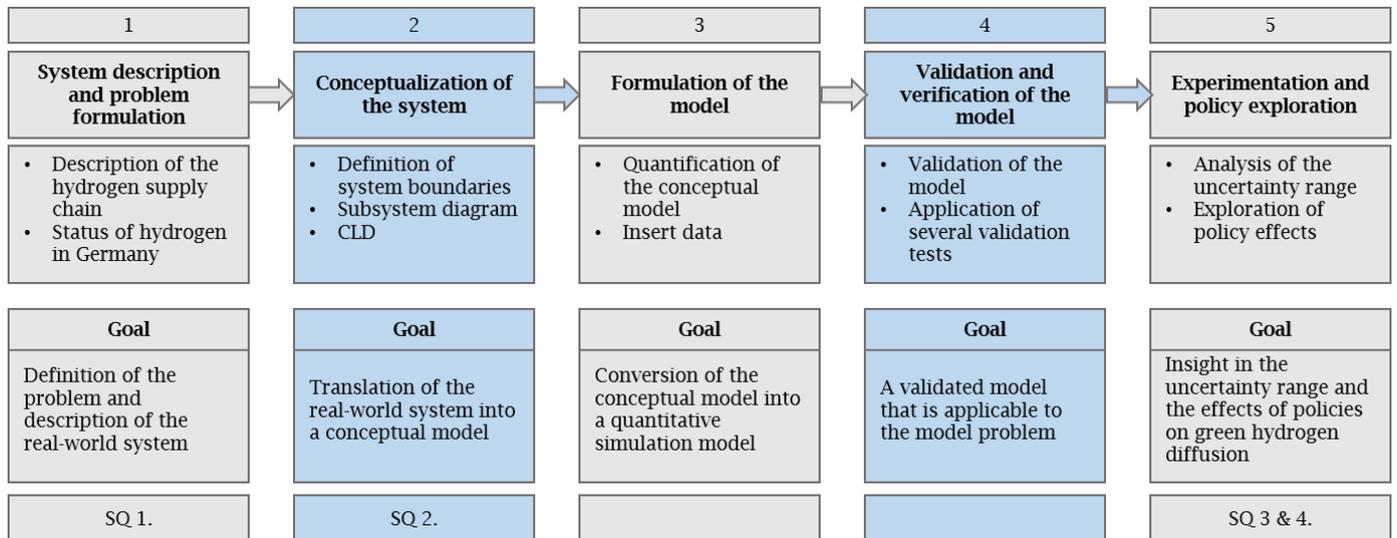


Figure 3: The five modeling steps and the goals and linked subquestions

## 4 System description

This section outlines the core technological concepts of the hydrogen supply chain from a system perspective. After a description of the hydrogen supply chain, a portrayal of hydrogen technology and hydrogen policies in Germany specifically is provided.

### 4.1 The hydrogen supply chain

The hydrogen supply chain is defined as the pathway that hydrogen follows from the source of production to final consumption. This includes a variety of production methods, transport and storage, and consumption in different end-use applications. The hydrogen supply chain is examined as a closed system in which different technologies fulfill a role as link in the value chain. A system can be defined as a set of related components that together work toward some purpose, that is considered isolated from the rest of the world, or the environment, and has both an internal structure and interaction with the environment (Kelton et al., 2012).

A schematic display of the hydrogen supply chain is provided in figure 4

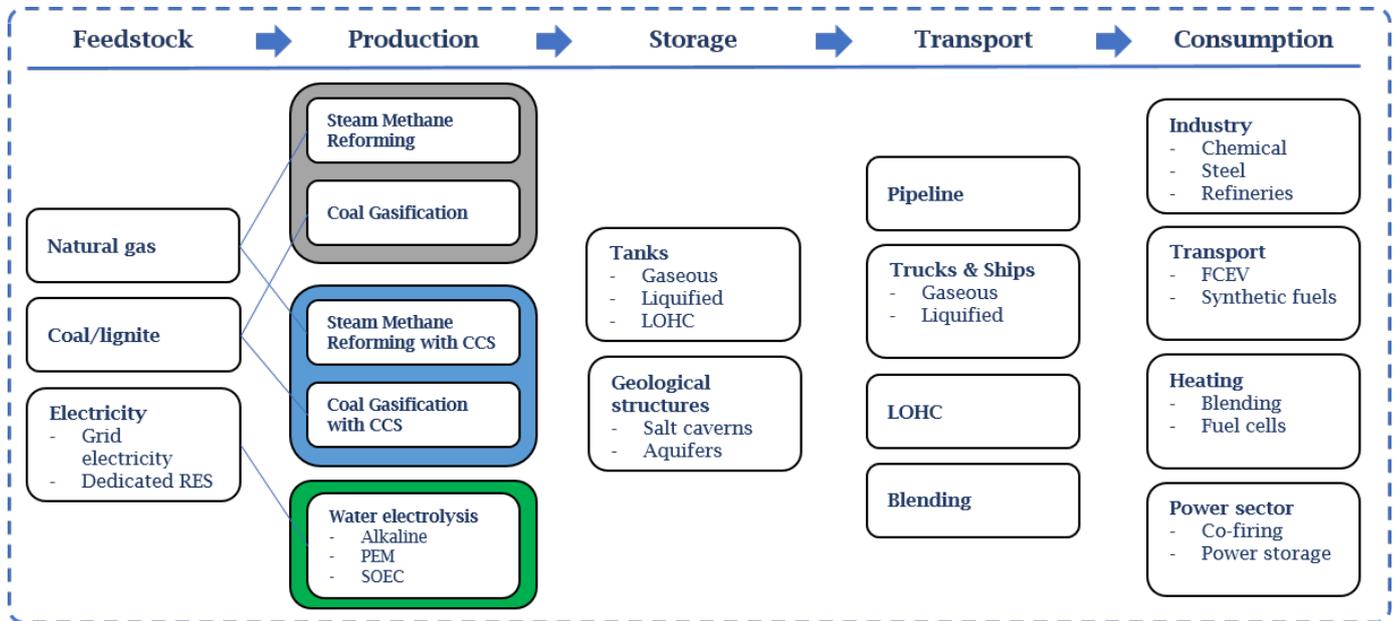


Figure 4: System perspective on the hydrogen supply chain

#### 4.1.1 Hydrogen production

From the broad assortment of production methods, the three most applied and technological mature technologies are considered in this research. These include Steam Methane Reforming (SMR), Coal Gasification (CG) and Water electrolysis (WE) (Acar & Dincer, 2019). These three dominant production methods account for almost the entire share of global hydrogen production.

Looking at global hydrogen production for a general background on production, the majority of hydrogen is produced with fossil-fuels through steam methane reforming (SMR), using natural gas as feedstock. According to IEA data, (2019), the total annual dedicated production of hydrogen in 2019 was around 70 Million tonnes, of which 75% is generated from natural gas. Approximately 205 billion cubic meters of natural gas were required for this, which is 6% of global annual natural gas consumption. Coal gasification (CG) is another common hydrogen production method, which requires coal as feedstock resulting in a large carbon footprint per kilogram hydrogen produced. Gasification of coal supplied 23%

of global hydrogen production in 2019 and required 2% of global coal consumption (IEA, 2019). These methods are broadly defined as *grey hydrogen*. Low-carbon hydrogen production methods include water electrolysis, or *green hydrogen*, or fossil-fuel based production coupled with carbon capture and storage (CCS), which is often defined as *blue hydrogen*. Water electrolysis accounted for an estimated 2% of total production in 2018. Aside the 70 Million tonnes of dedicated hydrogen produced, approximately 45 Million tonnes of hydrogen was produced in 2019 as a by-product from industrial processes. This includes hydrogen as a by-product from electrolysis in the chlor-alkali industry, from the petrochemical industry and in refineries from catalytic reforming of naphtha (Cox, 2011; Bloomberg NEF, 2019; Ball & Weeda, 2015).

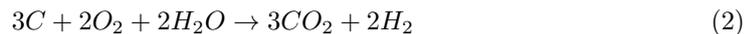
#### **Grey hydrogen: hydrocarbon reforming**

Hydrocarbon reforming is the process of generating hydrogen through the reaction of hydrocarbons with water. Hydrocarbon reforming can be applied through different production routes such as partial-oxidation, auto-thermal reforming, dry reforming and steam reforming. Of these methods, the latter is the most advanced and is conducted through the conversion of methane in the process of steam methane reforming (SMR). This endothermic process is carried out in a series of reactions, starting with methane (CH<sub>4</sub>) and water as steam (H<sub>2</sub>O). The reaction of this mixture at a temperature of 750 degrees Celsius results in syngas, a composition of hydrogen and carbon-monoxide, which is further processed through a water-gas shift reaction resulting in carbon dioxide and hydrogen. The entire process of SMR is captured in the following reaction: (Suleman et al., 2016)



According to a comparative emission assessment study by Suleman et al. (2016), SMR has a carbon-dioxide emission equivalent of approximately 12 kg per kilogram hydrogen produced.

**Grey hydrogen: coal gasification** Coal gasification is the second most used method of hydrogen production, contingent on the processing of solid carbon. Pulverized coal reacts at high temperature (800-1300 °C) in a gasifier with oxygen, resulting in a syngas mixture. This is further purified in a similar way as in SMR, resulting in a water-gas shift reaction in carbon dioxide and hydrogen (Parkinson et al., 2019). The following reaction denotes the entire process of coal gasification:



Coal gasification is a polluting process with an emission equivalent of 18 kg CO<sub>2</sub> per kilogram hydrogen produced.

**Blue hydrogen: Carbon-based hydrogen with CCS** Both steam methane reforming and coal gasification are polluting processes. To reduce carbon emissions, these production processes can be coupled with carbon capture and storage (CCS). CCS is the technique of catching the emitted CO<sub>2</sub> of the hydrogen production process and store it underground or utilize it in other chemical processes. For steam methane reforming, CCS allows for a maximum capture rate of 90% (Parkinson et al., 2019; Gasforclimate, 2021). The process of coal gasification is even more suitable for capturing emissions and has a potential capture rate of approximately 95% (Parkinson et al., 2019). At present, there are three SMR-facilities operational worldwide with CCS, producing an annual amount of 0.5 Mtons of hydrogen per year and pilot projects are under development in Norway USA, China and Canada (IEA, 2021). Blue hydrogen is however not undisputed, since there still are emissions that are not captured, as well as the fact that CCS might lock-in the use of fossil fuels and create technological path-dependence (Dickel, 2020; Azevedo et al., 2021).

**Green hydrogen: water electrolysis** The ingredients for water electrolysis are electricity, purified water and an electrolyzer. The general principle of electrolysis is based on the principle of splitting water with the use of two electrodes and a direct current and was invented by Michael Faraday in 1832 (Santos et al., 2013). Today, two types of electrolyzers

are most commonly used on a commercial scale: alkaline electrolyzers (Alk) and proton exchange membrane electrolyzers (PEM), of which alkaline electrolysis is the most established technology. The third dominant electrolysis technology is the solid oxide electrolytic cell (SOEC). However, this technology is in an early stage of development and not commercially available yet (Bloomberg NEF, 2019).

Alkaline electrolyzers requires approximately 9 liters of water per kilogram of hydrogen produced, and an electrical energy of approximately 50 to 78 kWh per kg hydrogen (Acar & Dincer, 2019). This results in an conversion efficiency for alkaline electrolysis of approximately 62% to 64%. A schematic display of alkaline electrolysis is shown in figure 5. The electrolyzer consists of an anode and a cathode placed in a liquid alkaline electrolyte. Between the electrodes is a diaphragm that allows water and charged molecules to pass, but blocks the passage of hydrogen or oxygen. When a direct current is applied to the electrolytes, water molecules are split by negative electrodes at the cathode into hydrogen ( $H_2$ ) and hydroxide ( $OH$ ). The hydroxide moves through the membrane after which the negative molecule reacts with the positive anode into oxygen and water (Dincer & Acar, 2014). The reactions in the alkaline cathode, anode and the total reaction respectively are:



The alternative conventional electrolysis technology, PEM electrolysis, follows a similar principle of water splitting through a membrane. However, a solid conductor is used instead of a liquid electrolyte. The two dominant techniques for electrolysis are often compared in literature, in which alkaline electrolysis is specified to be economically more advantageous, whereas PEM electrolysis has few technological benefits. The technical advantages of PEM are the rapid startup- and response time of the electrolyzer and the high pressure outputs (15-80 bar) (Santos et al., 2013; Saba et al., 2018; Bloomberg NEF, 2019; Proost, 2020). On the contrary, PEM requires expensive materials for the membrane such as Platinum or Iridium, which could be limiting factors in the up-scaling of this technology and increase uncertainty about this technologies' future (Kleijn & Van Der Voet, 2010).

#### 4.1.2 Hydrogen consumption

Hydrogen consumption today predominantly takes place in chemical industry. Main applications of hydrogen are the production of ammonia, and the processing heavy residual oils into higher-value products through hydro-cracking in oil refineries (Weeda & Segers, 2020). However, the versatile characteristic of hydrogen allow for application in many more end-use sectors, since it can be used as fuel for generating motion, a source of heat, and feedstock for the production of diverse materials.

#### Transport sector

The application of hydrogen in transportation is in an early stage of deployment. These days,

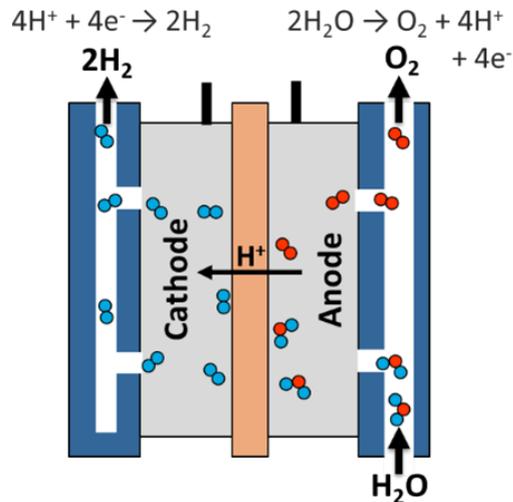


Figure 5: Schematic representation of alkaline electrolysis (EERE, 2022)

the sustainable transition in the automobile sector seems to be in the advantage of battery-electric vehicles (BEV). The most promising applications for hydrogen in road transport are in heavy-duty, long-range transportation modes, such as trucks and busses, because of the large energy storage capacity for hydrogen compared to batteries (Hydrogen Europe, 2020). Another promising application in the transport sector is the production of synthetic fuel from carbon and hydrogen feedstock. This can be easily mixed with for example kerosene, drawing on existing infrastructure.

### Industry

The first promising application of hydrogen in industry is in the decarbonization of steel manufacturing. Steel is recognized as a difficult-to-abate sector, because of the limited options for electrification in the conventional blast-furnace primary steel making route (Otto et al., 2017) Current primary steel production is based on a two-step process to transform iron ore into steel. This process consumes large amounts of coal and natural gas as feedstock and for heating. Hydrogen can be employed in this process two ways. Injection of hydrogen into the blast furnace could replace a part of the coal that is used for the chemical iron-ore processing and is relatively easy to implement in existing production facilities (Vogl et al., 2018). Another method is the production of steel through hydrogen direct reduction of iron (HDRI). Hydrogen replaces coal in this process as the reducing agent of iron ore in the blast furnace. The reduced iron is then further processed into steel in an electric arc furnace (Fischedick et al., 2014; Otto et al., 2017). The second application for hydrogen in industry lies in the chemical industry. Most urgent is the transition of grey hydrogen consumption to green consumption. Also, hydrogen can be applied as feedstock for plastics or synthetic hydrocarbons, through the methanol and methanol-to-olefins pathway, or the Fisher-Tropsch route (Weeda & Segers, 2020).

### Building sector

Hydrogen can provide an alternative of natural gas for heating buildings with hydrogen boilers. However, this is a far-fetched future as it highly dependent on the distribution availability of pipelines. Blending hydrogen into the natural gas grid is an indirect manner for hydrogen consumption in the built environment. Blending rates are experimented with and can reach up to 15% of volume depending on the technological feasibility of the natural gas grid (Melaina et al., 2013; Kanellopoulos et al., 2022).

### Power sector

The most important beneficial characteristics of hydrogen molecules over electrons are the capability for long-distance transportation without major energy losses, and possibility long-term storage. The increasing share of renewable electricity generation brings challenges for transport and storage, for which hydrogen can offer a balancing solution (Böhm et al., 2020). For example, hydrogen generation through electrolyzers in offshore wind turbines is mentioned as an option for long-distance energy transport, where stationary fuel cells ashore convert the hydrogen back to electricity (Fraunhofer IWES, 2021). Another way of utilizing hydrogen in the power sector is through the combustion of green hydrogen as replacement for natural gas in dispatchable gas turbines (IEA, 2021).

#### 4.1.3 Hydrogen storage and transport

The major challenge for storing and transporting hydrogen is a consequence of the density of hydrogen. The energy density of hydrogen at atmospheric pressure and 293 K is  $10.8 \text{ MJ}/\text{nm}^3$ , which is low compared to for example natural gas ( $31.65 \text{ MJ}/\text{nm}^3$ ) (RVO, 2020). The low energy densities lead to high costs per stored unit of energy, therefore the adjustment of the energy density of hydrogen through compression, liquefaction, or chemical conversion is needed for economically viable transport and storage (Reuß et al., 2017).

### Storage

The role of storage allows on the one hand for seasonal storage of energy when hydrogen production is accommodated by renewable energy sources, and on the other hand bridges the gap between unbalanced production and demand for hydrogen. Hydrogen can be stored in

a number of forms, of which the most common are mechanical storage in gaseous and liquid form, and chemical storage through the use of Liquid Organic Hydrogen Carriers (LOHC) (Moradi & Groth, 2019). In gaseous form, hydrogen can be stored under high pressure in tanks with pressure up to 700 bar (Ball & Weeda, 2015), which are currently deployed in hydrogen vehicles. For larger volumes and longer time spans, gaseous hydrogen can be stored in geological storage facilities such as salt caverns or depleted oil and gas fields. This is an often mentioned option for seasonal storage and has been demonstrated successfully in the UK and the US (Detz et al., 2019; Reuß et al., 2017). Similar to natural gas, hydrogen can be liquefied for storage or transport. When cooled below -252 degrees Celsius, storage as a liquid is possible under low pressure (Moradi & Groth, 2019). The cooling however requires a significant amount of energy, consuming 25 to 35% of the initial amount of hydrogen to be stored in energy. The third form of storage is through chemical conversion of hydrogen. This implies the storage of hydrogen in larger molecules entitled as Liquid Organic Hydrogen Carriers (LOHC), or as ammonia (Reuß et al., 2017). LOHC's are composed of hydrogen-lean and hydrogen-rich organic components, that through exothermic hydrogenation stores hydrogen molecules, and detaches them through endothermic de-hydrogenation (Preuster et al., 2017). Similarly, hydrogen can be chemically converted to ammonia, that liquefies at -33 degrees Celsius, demanding less energy than liquefied hydrogen. Conversion of hydrogen to ammonia might also benefit from the international infrastructure for ammonia transport and storage that is well-established. The main disadvantage of chemical converted hydrogen storage and transport is the requirement of a conversion plant on both sides of the transport route, demanding large capital investments and high energy consumption (Preuster et al., 2017).

### **Transport**

Transportation is an essential link in the supply chain, when consumption is located elsewhere than hydrogen production. Also, long-distance transportation of molecules results in less energy losses than electricity transportation, indicating the promising role for hydrogen in the power sector. In January 2022, the first intercontinental shipment of liquefied hydrogen was executed from Australia to Japan (Reuters, 2022). Long-distance seaborne transport of hydrogen is most viable as liquefied hydrogen, LOHC, or as ammonia (Baufumé et al., 2013). Transportation over land currently occurs mostly with gaseous storage tanks on trucks, however this is a very costly activity. Large-scale transmission and distribution over land over a distance is more feasible with hydrogen pipelines. Currently, roughly 5000 km of dedicated hydrogen pipelines are available globally, of which the large share connecting industrial sites (IEA, 2021). Hydrogen pipelines can be newly constructed, or, less costly, be retrofitted from existing inoperative natural gas pipelines (Cerniauskas et al., 2020). The final method for transport is the mixing of hydrogen into the natural gas grid (Melaina et al., 2013; Ogden et al., 2017). The natural/gas hydrogen blend can be directly combusted in end-use applications, or the hydrogen can be separated from the natural gas at location of demand for separate use.

## 4.2 Hydrogen in Germany

This section provides background information on the current role of hydrogen in Germany, and applies the framework of drivers and barriers to diffusion to the German hydrogen system. Furthermore, it explains shortly the ambitions and plans of the German government, what projects are in the pipeline and how the governance around hydrogen in Germany is organized.

### 4.2.1 Current status of hydrogen in Germany

#### Hydrogen production

Germany is the largest producer and consumer of hydrogen in Europe. With an estimated annual demand of 58 TWh hydrogen (1.65 Mtons, 208 PJ), Germany accounted for 21% of the total European hydrogen production in 2018 (FCH2JU, 2020). The current hydrogen production and consumption in Germany predominantly consists of on-site production for direct use industrial purposes, 85% of total production, according to the FCHJU(FCH2JU, 2020). On-site production implies that this hydrogen does not enter the national hydrogen market or supply chain. The large share of the on-site production is conducted in oil-refineries and chemical industry, which account for 92% of total on-site hydrogen production. A share of the on-site production is categorized as by-product hydrogen. This type of hydrogen is the derivative of industrial processes such as oil refining and the Chloralkali process. The other 15% of hydrogen produced is so-called merchant hydrogen, which is produced for selling purposes to industrial clients or the retail market. The conventional production pathway for hydrogen in Germany is Steam Methane Reforming (SMR), accounting for 71% of total production. Coal gasification provides 18% of the total hydrogen, whereas water electrolysis contributes a humble 0.25% with a production capacity of 0.00769 Mton (0.915 PJ) per year(FCH2JU, 2020). For comparison, the annual total energy consumption of the German transport sector in 2019 was 2379 PJ (IEA, 2020). The average capacity of electrolyzers is currently in the range kilowatts to a few megawatts, with the largest electrolyzer installed in 2021 having a peak capacity of 10 MW (Refhyne, 2018). The other share of production methods consists of the industrial feedstock by-products. In figure 6 the locations of hydrogen production sites are displayed, showing a concentration of fossil-based production near the existing industrial clusters such as the Ruhr-area, Leipzig and München in the left map, whereas the electrolyzer facilities on the right map are more spread throughout the country as these are rarely on-site production plants.

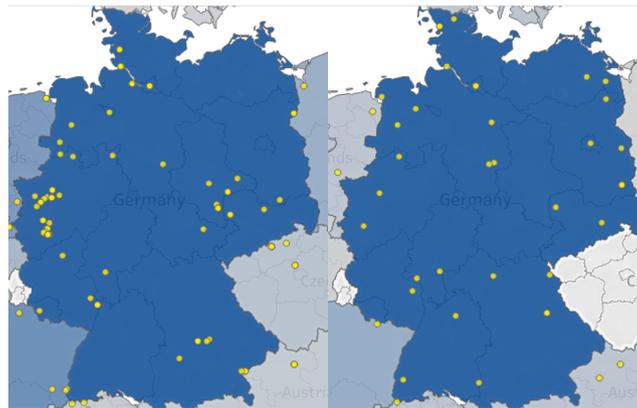


Figure 6: Fossil-based (left) and electrolysis (right) hydrogen production sites in Germany, 2021

#### Hydrogen consumption

Approximately 85% of the hydrogen demand originates from the chemical industry and refineries (FCH2JU, 2020). In oil-refineries, hydrogen is an essential feedstock for desulfurization of crude oil and hydro-cracking. In the chemical industry, hydrogen is predominantly

used for the production of ammonia, which is the feedstock for fertilizers, and methanol. Hydrogen consumption in other sectors than industry and refineries today can be found in transport, where 9.1 TJ was consumed in 2018 (FCH2JU, 2020). Hydrogen consumption in transport comes from a scarce number of hydrogen vehicles. 312 fuel cell vehicles are found on the German roads in 2020, with a hydrogen refuelling network comprising of 83 refuelling points (ACEA, 2021). The small merchant produced hydrogen share is currently transported and distributed in compressed state via trucks. The initiation of hydrogen distribution networks with pipelines can be found in the Ruhr-area connecting Köln, Dusseldorf, Essen and Dortmund over a length of 240 km. This pipeline is operated by Air Liquide and connects industrial hydrogen producers and consumers. The other major hydrogen pipeline is located near Leipzig, which is operated by Linde gas and spreads over 135 km (Lambert & Schulte, 2021).

### 4.3 The German hydrogen policy landscape

Over the past years, Germany has put itself on the forefront of hydrogen development in Europe and aims to be a leader in the deployment of hydrogen and development of electrolyzers. In the context of climate neutrality for 2050 that Germany has committed to in the Paris Agreement, and the recent reformulation of ambitions to climate neutrality in 2045 (Bundesregierung, 2021), Germany acknowledges the role that hydrogen can and must play in a future sustainable energy system. The national ambitions for hydrogen and guidelines for action are defined in the National Hydrogen Strategy, that was issued in June 2020 as one of the world's first national hydrogen strategies (BMW, 2020).

#### 4.3.1 Hydrogen strategies

##### The German Hydrogen Strategy

The main objective of the Hydrogen Strategy is to provide a directional framework that indicates the steps that are required to meet German climate targets with the assist hydrogen, and guides innovation and investments for the generation, transport and use of hydrogen. It aims for the development of a sustainable and competitive hydrogen market, international cooperation and trade, infrastructure, and hydrogen adoption in end-use sectors. Furthermore, the Strategy states that the only form of long-term sustainable hydrogen is hydrogen based on sustainable energy. The pathway towards the sustainable hydrogen economy is translated into required actions in five main areas (BMW, 2020):

1. Boost green production capacity up to 5 GW by 2030 for a production of 14 TWh hydrogen per year, accompanied by the required renewable electricity capacity. The electrolyzer capacity must scale up at least another 5 GW by 2040.
2. Create reliable hydrogen demand in end-use sectors, emphasizing on sectors where green hydrogen is close to cost-competitiveness and that are otherwise difficult to decarbonize. Total hydrogen demand for 2050 is expected to lay between 110 and 380 TWh.
3. Scale-up hydrogen infrastructure through investments in new hydrogen pipelines and the re-purposing of phased-out natural gas pipelines.
4. Expand knowledge and innovation through the establishment of long-term research and innovation programs, to achieve technological maturity across the supply chain in 2030.
5. Establish international ties for cooperation and trade, on a regional scale around the North-sea area and on a global scale with bilateral and multilateral hydrogen trading partnerships.

##### The European Hydrogen Strategy

The European Hydrogen Strategy was published in late 2020 by the European Commission, recognizing green hydrogen development as a pillar of achieving the targets of the EU Green Deal (EC, 2020b). The priority of the strategy is in line with the German Hydrogen Strategy and emphasizes the development of green hydrogen, the rapid up-scaling of electrolysis capacity, and creating a demand for hydrogen. The integration of hydrogen into the energy system is divided in two phases: The first phase up to 2024 attempts to decarbonize current

grey hydrogen production through equipping factories with electrolyzers or CCS, scale up of electrolysis manufacturing, and stimulate early demand. Furthermore, the objective is to install 6 GW of electrolyzer capacity connected to renewable power sources. The focus of policies in this phase is on a regulatory framework for green hydrogen substituting grey, facilitating demand for leading markets such as chemical industry and heavy-trucks, and early planning for hydrogen infrastructure. The second phase from 2025-2030 consolidates hydrogen in the energy system, where green hydrogen becomes cost-competitive with blue and grey hydrogen. Hydrogen will be integrated with the power system and largely deployed in industry and transport. To accommodate this rapid uptake, the construction of a dedicated hydrogen infrastructure must be scaled-up. In 2030, a minimum of 40 GW of electrolysis capacity must be installed. Policies in this phase aim for demand stimulation through investments, the completion of an international hydrogen market and the unroll of infrastructure.

### 4.3.2 Active and announced policies in Germany

Aside from the National and the European hydrogen strategies that provide guidance and targets for a hydrogen future, a number of announced and implemented measures are already in operation to steer the future of hydrogen. On top of hydrogen measures that specifically support hydrogen, there are a number of general sustainable energy policies in play that directly or indirectly have an effect on the diffusion of green hydrogen.

- **European Emission Trading Scheme:** The most influential policy measure is the European Emission Trading Scheme (ETS) that is active since 2005, when almost all allowances were provided to business for free and the non-compliance penalty was 40 Euros per tonne CO<sub>2</sub> (EC, 2020c). In 2021 however, the price hit 90 euros per tonne CO<sub>2</sub> (BNEF, 2021). Also, the fourth phase of the ETS program started, with an increases pace of cutting emissions at an annual rate of 2.2% from 2021 onwards, compared to 1.74% before. Regarding the hydrogen sector, the ETS has implications on the costs of hydrogen production with fossil fuels and in the chemical industry and steel making sector.
- **Coal phase-out:** In 2020, the German parliament voted in favor of the Coal Exit Law which marks the phase-out of coal-fired electricity generation before 2038 and disallows the installation of new coal-fired plants. Regarding hydrogen, this law implies that a future for hydrogen production through coal gasification (with or without CCS), is far-fetched (Clean Energy Wire , 2020).
- **Fossil-fuel taxation:** Since 2021, the German government has, parallel to the European Emission Trading Scheme, enforced a carbon tax on fossil-fuels use for transportation and heating. This carbon tax builds up from 2021 from a fixed price towards 2026, where it ends at a value of 60 Euros per tonne CO<sub>2</sub> and is auctioned from then (Bundesministerium der Justiz, 2019; Clean Energy Wire, 2021). This policy is not particularly designed to promote the use of hydrogen, but might have stimulating effects on the demand growth of hydrogen in the transport sector. Diesel is becoming slightly more expensive, with approximately 15 ct/L at a price of 60 Euros per tonne CO<sub>2</sub> for this policy, and might force several end-users to abate Diesel trucks and choose for sustainable alternatives amongst which FCEV-trucks trucks.
- **Fuel blending quotas:** Influential overarching renewable energy targets are issued in the Fit-for-55 package of the European Commission, which proposes a green hydrogen share in industry of at least 50%, and a quota for a synthetic fuel share in aviation of 28% in 2050 (EC, 2020a), these however are only targets and not yet converted into concrete policy measures. The Renewable Energy Directive (RED II) of the European Union states that "Member States must require fuel suppliers to supply a minimum of 14% of the energy consumed in road and rail transport by 2030 as renewable energy" (EC, 2018b). Since 2007, Germany has had a binding quota for biofuels, which has a current share of 6% and must increase 25% by 2030 according to the new legislation.

Synthetic fuels that are produced from hydrogen are since 2021 included in this scheme as biofuels and will be mainly contributing to sustainable aviation, heavy duty road transport and shipping (BMU, 2020; Clean Energy Wire , 2021).

- **Tax exemptions:** Levies on electricity are high in Germany, but there are policies alleviating the burden for some. Already incorporated in the electricity taxation scheme in Germany is the exemption of the regular electricity tax (Stromsteuer). According to article 9 of the Stromsteuergesetz (Bundesamt für Justiz, 1999), electricity that is used for electrolysis is excluded from the payment of regular Stromsteuer. This tax amounted 1.54 ct/kWh in 2020 (BDEW, 2022), and accounted for approximately 10% of electricity costs for electricity consumers of the largest scale in 2021 (Band IG, (Eurostat, 2021)). An additional step in reducing the cost of producing sustainable hydrogen has been enforced in the in 2021 reformed German Renewable Energy Act (EEG), which is a taxation on grid electricity for the financial support of renewable energy expansion and grid modernization. Internationally competing companies with a high energy use, such as ThyssenKrupp and ExxonMobil are exempted from this levy (Schultz, 2019). Nevertheless, for non-global operating companies, albeit with a high energy consumption of over 100 GWh per year (approximately equals an 11 MW electrolyzer with a 100% capacity factor), the energy level is still a cost factor on the energy bill. In 2021, the levy was 6.5 ct/kWh accounting for roughly 40% of the total electricity cost (BDEW, 2022). The reformed German Renewable Energy act from 2021 alleviates the costs for producers of green hydrogen and states that electricity dedicated for green hydrogen production is discharged from the EEG surcharge on the electricity bill (Akat & Göss, 2021).
- **Subsidies:** Direct financial support for green hydrogen equipment is guaranteed in several forms. One type of funding of the EU is the arrangement of IPCEI (Important Projects of Common European Interest) for hydrogen. In this scheme, projects that contribute to hydrogen innovation on European level and the European hydrogen targets can submit a request for public funding (EC, 2020c). The German government has already guaranteed a public support fund of 9 billion Euros to boost green hydrogen production projects and sustainable steel industry (BMW i , 2021). On top of that, the H2Global investment fund, established by the German Ministry of Economy and Energy, was introduced in June 2021 and supports private investments for a total of 500 MW in electrolysis capacity (BMW i , 2021).
- **International agreements:** Finally, to impel international collaboration in the field of renewable hydrogen, Germany has already established several bilateral agreements with Australia, Canada, Chile, Morocco and Saudi Arabia for innovation partnerships and potential green hydrogen production import. These countries have favorable characteristics for the large-scale production of green hydrogen, and might benefit from hydrogen export in the future (IEA, 2021) (the geopolitical implications of hydrogen will be slightly touched upon in the discussion section of this study).

Germany demonstrates active progress in the design of policies to stimulate the adoption of sustainable energy in general and to some extent hydrogen in particular. The policies that particularly stimulate the growth of the hydrogen sector are currently limited. Although the Hydrogen Strategies denote a vast amount of ambitions and guidelines to impel the deployment of green hydrogen, these are not yet translated into policies and not yet visible in the current package of active policies. When considering the current state of the hydrogen sector in Germany and the observed barriers that are still active, it is apparent that there are only limited policies that directly address these challenges. The cost-gap between green and fossil hydrogen is slowly converging through the electricity tax exemption and direct funding of green hydrogen equipment. Hydrogen demand is supported with the quota for biofuels and the emission taxation of fossil-fuels in transport. Infrastructure is however not addressed with existing policies. Regarding the currently active policies and the existing barriers to green hydrogen diffusion, it can be questioned if these policies are sufficient for a rapid diffusion and able to provide enough leverage to overcome the diffusion barriers.

### 4.3.3 Optional hydrogen policies for Germany

Regarding the current status of hydrogen in Germany and the active barriers, it is obvious that on top of the active policies described in the previous paragraph, additional measures are required to overcome these barriers and induce a rapid deployment of green hydrogen. Costs can come down through technological learning, innovation expenses and unit scaling, but these mechanisms do not ignite spontaneously. The abundant availability of hydrogen outlooks, forecasts and roadmaps provides a source of additional policy options for hydrogen development (BMW<sub>i</sub>, 2020; Agora Energiewende, 2020; DENA, 2019; IRENA, 2020). Policies which focus on hydrogen specifically can be divided in three categories (Agora Energiewende, 2020): First, policies to stimulate the production of green hydrogen and close the cost gap between green and grey hydrogen production are policies that are active on the supply side. Second, policies to create a market for hydrogen and stimulate demand are implemented on the demand side of the supply chain. Thirdly, the integration of the hydrogen supply chain can be achieved through overarching policies that focus on infrastructure and storage, or cover other aspects than hydrogen in particular but are expected to have effect on hydrogen. The following additional policies for the support of green hydrogen as described by IRENA and Agora Energiewende (2020; 2020), are included in this research:

- **Carbon Contracts for Difference:** Demand side policies must push consumption and stimulate end-users to adopt hydrogen technologies over fossil technologies. Carbon Contracts for Difference (CCfD) are a promising policy to stimulate carbon abatement in end-use sectors such as chemical industry and steel factories. Therefore this policy is also highlighted in the German Hydrogen Strategy (BMW<sub>i</sub>, 2020). The carbon contract is an agreement between the government and a producer about a fixed carbon price over a certain time period, approximately 15 years. This fixed price, or so-called strike price is based on the difference between the abatement costs and the conventional fossil-based production costs including carbon costs. The strike price is fixed, but the costs of carbon vary. Therefore the financial support that is received from the government fluctuates as well and diminishes when the carbon price increases. The government closes the gap between the carbon price and the strike price to finance abatement. However, if the carbon price exceeds the strike-price, the producer pays the government (Gerres & Linares, 2020; Agora Energiewende, 2020).
- **Gas grid blending quota:** Quotas for biofuels amongst which hydrogen and derivatives are already active for road transportation, but could be applied in a wider range of sectors. Hydrogen injection into the natural gas grid, or blending, could be promoted through the enforcement of a blending quota. Currently, the maximum technological feasible blending rate for the German gas grid is 15% in some sectors of the grid (Melaina et al., 2013; Kanellopoulos et al., 2022). The German government could consider the implementation of hydrogen blending into the national gas grid, to alleviate the consumption of natural gas in various sectors that are grid connected.
- **Subsidies for hydrogen infrastructure:** The absence of a hydrogen infrastructure is considered as one of the largest barriers to hydrogen diffusion. Hydrogen could be transported through newly constructed transmission and distribution pipelines, or retrofitted natural gas pipelines. Plans and consortia are already active in Europe to sketch a rough silhouette of a border-crossing hydrogen network (Gasforclimate, 2021). In Germany, plans are made by a consortium gas transmission grid operators under the umbrella organisation FNB Gas (FNB Gas, 2021). This plan consists of a preliminary network of approximately 5000 km of new and retrofitted pipelines for 2030. Currently however, there are no concrete measures for governmental support of hydrogen infrastructure. To achieve expansion of the infrastructure network, governmental funds and the facilitation of capital flows could be the key to acceleration (IRENA, 2020).
- **Ban on CCS for hydrogen production:** Finally, a very preliminary policy might be supportive to increase the share of green hydrogen production over grey and blue

hydrogen. The new German government already preliminary announced a governmental ban on the support for blue hydrogen, excluding blue hydrogen from subsidy and tax reduction schemes (EurActiv, 2022). This measure expands the costs of blue hydrogen per unit of hydrogen produced, and might be the solution to close the gap between green and blue hydrogen.

## 5 Modeling the hydrogen supply chain

The German hydrogen supply chain is simulated in with the System Dynamics model that is constructed for this research. Based on the steps from Sterman (2000) as described in section 3.3 the model is constructed through the following phases: conceptualization, formalization, model testing and policy exploration. This chapter illustrates each step of the translation of the real-world hydrogen supply chain system into the system dynamics model.

### 5.1 Model conceptualization

The dynamic behaviour and transformation of the hydrogen supply chain will be captured in a simulation model, to comprehend the system and facilitate a tool for investigation of the system. Conceptualization of the system is the first step of the System Dynamics model building process. During the conceptualization, the most important question the modeler must ask himself is: "What is the purpose of my model?" (Sterman, 2000). Departing from this question, this section addresses the purpose of the model, the model boundaries and components, key variables, time horizon and causal loop diagram.

#### 5.1.1 Model purpose

Modeling the hydrogen supply chain originates from the problem formulation described in chapter 2. The relationship between the model and the problem definition and research questions must be considered carefully, since the model is solely the tool for problem solving rather than the goal of research itself. In short, according to Sterman (2000), a good model models a problem, not a system. With regards to modeling a problem instead of a system, the problem is the chicken-egg situation between demand and supply as described in the literature gap. The purpose of this model is therefore to understand the dynamic behaviour of the hydrogen supply chain system and gain quantitative insight in the effects of barriers and policies on the diffusion of green hydrogen over time.

#### 5.1.2 Model boundaries and components

The model purpose translates into the model composition which is delineated by model boundaries. This is illustrated by the distinction between endogenous, exogenous and excluded components of the hydrogen supply chain. Setting the model boundaries must be done with caution; choosing for modeling too few components and details might result in an oversimplified representation of the real-world system. The model might resemble the modeler's input too much in that case. On the other hand, including too much or irrelevant components and endogenous variables can make the model too complex. Hence, it might miss its purpose of simplification of a real-world system, or worse, become too detailed and become incomprehensible.

The core of the system dynamics model represents the technological structure of the hydrogen supply chain as described in the system description. This structure consists of the production, transport and demand of hydrogen, and the feedback between these elements. The inclusion of other relevant components is based on the drivers, barriers and policy objectives that have been found in literature as described in section 4.2. System factors such as learning of technology, investment incentive and behavior and political drivers which are main drivers that affect the hydrogen supply chain are translated to accompanying submodels. An overview of the model structure and linkages between submodels is denoted in figure 7. The composition of hydrogen supply chain model is derived from the XLRM-modeling framework of Lempert et al. (2003). The blocks within the grey shaded area represents the core of the model; the three stages of the hydrogen supply chain. The factors that affect the supply chain and that are modeled in separate submodels, levelized cost of H<sub>2</sub>, investment in production and learning-by-doing, are displayed around the hydrogen supply chain. All model components within the dotted area are endogenously modeled interdependent components through the system relations (R). The building blocks outside the dotted area are

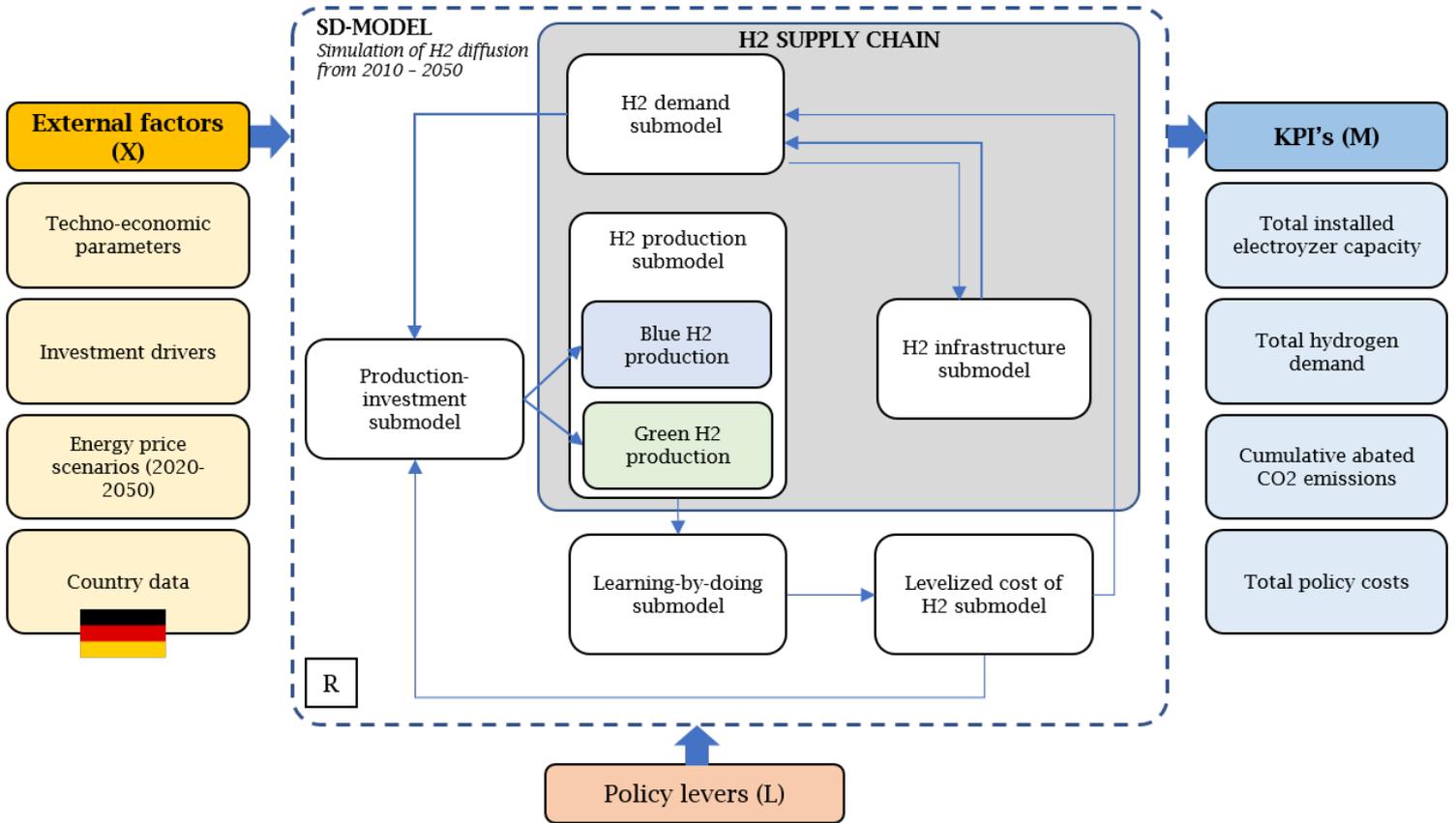


Figure 7: Overview of the model structure and model components, with the external factors (X), policy levers (L), system relations (R) and key performance indicators (M).

exogenous variables and parameters (X). The red box below represents the impact of the policy levers (L) on the system. The model outputs are the key performance indicators (M) and are displayed on the right. In more detail, the following six system components are included as submodels:

**H2 production submodel:** The production submodel calculates the hydrogen production capacity of each production type and the share of each production method. In this submodel, the three most conventional hydrogen production methods are included: existing grey hydrogen production, blue hydrogen in the form of steam methane reforming and coal gasification, both with carbon capture and storage, and green hydrogen as alkaline water electrolysis, schematically displayed in the green and blue blocks in figure 7. The capacity of grey hydrogen cannot be expanded in this model, but only depreciates. The share of production investment of green and blue hydrogen is determined by the output of the *Production investment submodel*. Investment in new capacity is driven by the gap between demand and supply, making the investment in new production capacity demand driven. Furthermore, the production component is connected with the *Demand submodel*, in which the total hydrogen demand is simulated. The production submodel is furthermore connected to the *Learning-by-doing submodel*, for which the input is the cumulative installed capacity of electrolyzers.

**H2 demand submodel:** Hydrogen demand is modeled for three sectors: heavy duty trucks, steel manufacturing and gas blending into the grid, as described in section 4. Each sector is modeled separately and includes investment behaviour in new technologies based on the total cost of ownership and feedstock costs. The relative price difference between the fossil-based conventional technologies and the new hydrogen technologies determines the investment share. This incorporates that the demand for hydrogen in each end-use

sector is endogenously affected by the price of hydrogen (calculated in the *Levelized cost of H2 submodel*), relative to fossil fuels. Fossil fuel prices are external factors. Furthermore, the hydrogen demand for fuel cell heavy-duty trucks is dependent on the availability of infrastructure from the *H2 infrastructure submodel*. Steel making and gas blending into the grid are centralized technologies and therefore independent of the infrastructure submodel. The output of the demand submodel is the total hydrogen demand, which is of influence on the *H2 infrastructure submodel*, and the *Production investment submodel*.

**Infrastructure submodel:** Infrastructure is included in a separate submodel and is connected through a feedback loop with the *H2 demand model*. Hydrogen infrastructure installation is positively affected by the growth of hydrogen demand, since investments in infrastructure increase when demand for hydrogen is increasing. Vice versa, the increasing hydrogen infrastructure has a reinforcing effect on the demand for hydrogen in the *H2 demand model*. The model incorporates new hydrogen pipelines as well as retrofitted natural gas pipelines.

**Levelized cost of H2 submodel:** Cost of production is determined for the different production methods through the operational and capital expenditures and is expressed as the levelized cost of hydrogen. This submodel calculates the costs of the green and blue hydrogen. Affected by the *Learning-by-doing submodel*, the capital cost of green hydrogen production equipment decreases. The levelized cost expresses the price per unit of production and provides the incentive for the investment decisions in each type of hydrogen production method. When demand grows and there is a shortage in supply, the output of the levelized cost of H2 submodel determines the division of investment for each production type in the *Production investment submodel*. The external input for the levelized cost calculation are technological and cost parameters for each production technology derived from literature.

**Learning-by-doing submodel:** The concept of learning-by-doing is captured in the model through a feedback loop between cumulative installed electrolyzer capacity and capital costs of electrolyzers. The cumulative installed electrolyzer capacity is an output of the *Production submodel* and determines how fast the capital costs of electrolyzers decline. The dynamic capital costs are subsequently included as input for the *Levelized cost of H2 submodel*.

**Production investment submodel:** This submodel calculates the investment share of each production method in the *H2 production submodel*. The investment share is based on the relative costs of hydrogen from each production method, which is the output of the *Levelized cost of H2 submodel*. The production method with the lowest costs of production per unit of hydrogen results in the largest profit for the investor or producer, and therefore gains investment share over the other less cost-competitive methods of production.

### 5.1.3 Key model variables

Each submodel of different model parameters, and have inputs in the form of constants, and variables. Model constants have fixed values that are independent of time, whereas model variables are dynamic and change over time. Model parameters are the system components that are calculated endogenously in the model. The model outputs, or key performance indicators, are all endogenously determined and therefore never directly the result of exogenous input variables. A few variables are inserted in the model as exogenous input variables, meaning that the dynamics of the variable over time is adopted from literature or assumed. In table 1, the most important endogenous and exogenous model variables are displayed. The endogenous variables, or model parameters in this list are all calculated in the model, whereas the exogenous model variables are adopted from literature. The listed endogenous variables are the most important variables that indicate the state and behavior of the hydrogen supply chain system, and moreover represent the drivers and barriers that are described in section 2. The listed exogenous variables are all external factors that are modeled exogenously and time dependent. Further elaboration on the model variables will be provided in section 5.2.

Table 1: Fundamental endogenous and exogenous model variables

Endogenous model variables	Exogenous model variables
Total hydrogen production capacity	Price of fossil fuels
Investment share green hydrogen	Price of carbon emissions
Investment share blue hydrogen	Price of electricity
Levelized cost of hydrogen	Efficiency of electrolysis
Hydrogen demand	Energy demand in end-use sectors
Technological learning by doing	Cost reduction in end-use sectors
Investment hydrogen end-use sectors	
Available infrastructure capacity	
Total abated carbon emissions	
Total cost of policies	

#### 5.1.4 Key performance indicators

In regards to the model purpose, several endogenous model variables are of interest to examine the system behaviour and output and appraise the diffusion of green hydrogen. The performance metrics, or key performance indicators are derived from the green hydrogen objectives of the German government and mirror the status of sustainable hydrogen over time and show the progress of the green hydrogen targets. These performance metrics are denoted in the right column of figure 7. The following key performance indicators are distinguished:

1. Installed electrolysis capacity: the main objective of the German Hydrogen Strategy is to amplify the share of hydrogen in the energy system to achieve carbon abatement and reduce emissions. Electrolyzer capacity specifically looked at on the production side, since the hydrogen production can also be supplied by grey or blue production capacity. Electrolyzer capacity demonstrates the status of green hydrogen production capacity and represents the gauge for sustainable hydrogen diffusion.
2. Hydrogen demand: the chicken-egg stalemate is a gridlock of both the supply side and the demand side. Since the demand side is modeled endogenously and is affected by the dynamics of the levelized cost of hydrogen relative to the costs of fossil fuels, the hydrogen demand indicates a counterbalance of the production side in the model signalling the growth of the entire hydrogen sector. Furthermore,
3. Cumulative abated CO<sub>2</sub> emissions: not only does the German government pursue to abate fossil fuels in the hydrogen sector by replacing the current conventional grey hydrogen production by more sustainable green production, it also targets for hydrogen to indirectly reduce emissions in end-use sectors such as industry and transport and replace fossil fuels. This variable measures the cumulative carbon abatement from the transition within the hydrogen production sector and hydrogen adoption in end-use sectors combined.
4. Policy costs: the implementation of policies is primarily at public expenses. To examine the feasibility of policies, the policy cost is included as output variable.

#### 5.1.5 Policy levers

In figure 7, the policies levers are displayed in the red block below the system. From the described policy landscape in section 4.3, a number of existing and potential policies are included in the model. The following policy levers will be included as policy levers:

1. Electricity tax reduction: this policy represents the tax exemption for the electricity that is used for electrolysis. The policy reduces the costs of electricity and therefore the levelized costs of green hydrogen and will be implemented in the *Levelized costs of H2 submodel*.
2. Electrolysis equipment subsidy: this policy includes the subsidy scheme for green hydrogen production equipment. Investors for green hydrogen can through this measure receive a financial support to alleviate the capital costs of electrolyzers, which in the model will be represented in the *learning-by-doing model*.
3. Carbon Contracts for Difference: this policy is implemented on the demand side of the hydrogen supply chain. The CCfD closes the cost gap between incumbent fossil-based steel production and hydrogen-based steel production, to increase the incentive in the steel production sector to make the transition to sustainable hydrogen production. This policy is will be conceptualized in the *H2 demand submodel*.
4. Grid blending quota: this policy supports the mixing of hydrogen into the grid and is implemented in the *H2 demand submodel*.
5. Infrastructure investment support: this measure supports the acceleration of construction of infrastructure. This policy will be at play in the *H2 infrastructure model*.
6. Coal phase-out: the announced phase-out of coal can have serious consequences for the supply of hydrogen, since 18% of German hydrogen is currently produced with coal gasification through coke-oven gas. Quitting coal has also large consequences for the hydrogen sector, since new investments in coal gasification plants will be banned and existing coal-fired plants will be closed, even if they are equipped with CCS. In the model, this has policy will be affecting the *Production investment submodel*.
7. Fossil-fuel tax: this policy increases the costs of Diesel trucks via the emission scheme for fossil-fuels in transport and heating and is implemented in the *H2 demand submodel*.
8. Ban of CCS: this preliminary policy announcement will affect the supply side of the model through the *Production investment submodel*. Because of its preliminary nature, this measure will be examined separately from the above described policies.

### 5.1.6 Causal loop diagram

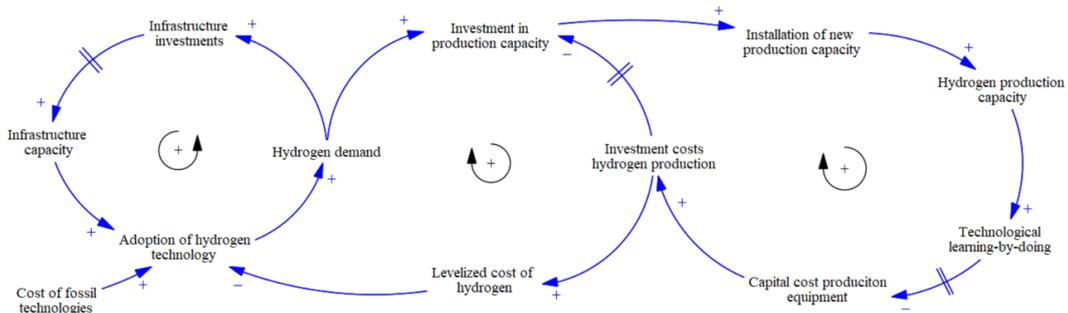


Figure 8: Causal loop diagram of the conceptualized hydrogen supply chain system

Finalizing the model conceptualization, a highly aggregated causal loop diagram of the system is constructed (Morecroft, 1982; Forrester, 1997). The CLD consists of three feedback-loops that determine the behavior of the system. The first loop is the left reinforcing feedback loop between infrastructure and demand. There is a causal relation between the increase in demand and the installation of infrastructure. It is assumed that when the market for hydrogen grows and the adoption in end-use sectors increases, the demand for transportation accessibility increases as well. Similarly, considering the fuel infrastructure dependency of hydrogen vehicles, the demand for hydrogen in the transport sector will grow when the availability of infrastructure increases. This reinforcing feedback loop mimics the

chicken-egg paradigm; as long as neither of the parameters increase, the loop remains motionless. The second loop is the most right loop, demonstrating the effect of learning by doing of the electrolyzers. The increase of installed production capacity has a positive effect on the phenomena of learning by doing. The capital costs of the green hydrogen production equipment decreases with a delay, and decreases the levelized costs of green hydrogen. This has a positive effect on the investment in green hydrogen production capacity, reinforcing the decrease of the green hydrogen costs. The third loop is the large reinforcing feedback loop that entails almost the entire system from demand to production to levelized costs of hydrogen. This loop comprises the reinforcing loop of learning-by-doing, but moves from the investment costs of hydrogen production past the investment in new capacity. Instead, it increases the demand for hydrogen, because of the increased cost-competitiveness of hydrogen with fossil-fuels in end-use sectors. Although there are three reinforcing feedback loops, the system does not immediately initiate growth and does not grow endlessly. The combination of the second and the third feedback loop result in an archetype structure for an S-shaped growth (Sterman, 2000). This model structure is the combination of two basic structures of exponential growth (third loop), and goal seeking (second loop). The outcome is a model behaviour that grows exponentially at first, but reaches a point of equilibrium. The reinforcing structure of the system does however not instigate out of nowhere. Because of the chicken-egg structure in the first and second feedback loops, the equilibrium must be disturbed (for example by a policy lever) to start the feedback mechanism. The limit to growth in this case is the bounded by the demand for hydrogen, that cannot grow limitless and prevents the system from expand endlessly.

## 5.2 Model formulation

As described in the model conceptualization section, the diffusion of green hydrogen will be considered in the model structure of the hydrogen supply chain from production to consumption and vice versa. This section describes the formulation phase of the model building process. The formulation consists of translating the rough model outline from the conceptualization phase into mathematical equations and parameters. From a subsystem diagram and CLD, the model is converted from a qualitative concept into a quantitative simulation model. The model is formulated with Vensim Software (Ventana systems inc. , 2022). The formulation description follows the line of reasoning of the hydrogen supply chain and for each submodel, the structure as well as the most important equations and main input parameters are explained. For several submodels, a simplified display of the abstraction in SD are shown. An overview of all simplified submodel structures is provided in appendix L, and all model equations are listed in a random order in appendix ??.

### 5.2.1 H2 production submodel

The production of hydrogen and installation of new production capacity is modeled in the H2 production submodel. This submodel comprises the investment in new production capacity that is driven by demand and calculates the required new production capacity as a consequence of plant depreciation. The most important outputs of this subsystem are the installed capacities of each production technology and the share of sustainable hydrogen production of total production.

Three types of production technology are included: coal gasification (CG), steam methane reforming (SMR) and alkaline water electrolysis (WE). CG and SMR are the prevailing production technologies and are prospective sustainable candidates in combination with carbon capture and storage (CCS) (Dickel, 2020). Electrolysis is the leading technology for sustainable hydrogen production, with alkaline electrolysis being the most mature type of electrolysis technology. Considering alkaline electrolysis solely is a simplification, since PEM-electrolysis is a promising technique with a large market share. Because of large uncertainty about the future share of adoption of PEM-electrolysis versus alkaline-electrolysis, and the key performance indicator is total installed electrolysis capacity, alkaline electrolysis is assumed the only possible type of water electrolysis technologies. Emerging sustainable production alternatives such as biomass gasification and thermochemical water dissociation are not included based on technology immaturity and uncertainty of future deployment (Acar & Dincer, 2019). Furthermore, hydrogen production from oil is excluded from the model scope, given that this method is only applied for on-site production and consumption in refineries and therefore is not enacted in the merchant hydrogen supply chain (Hydrogen Europe, 2020). Installation of new capacity is driven by the investment in new production capacity. The total investment is driven by the gap between supply and demand. This implies that the supply side of the hydrogen supply chain responds to the demand side of the chain. Which type of production methods are subsequently installed, or the investment share of each production method, is calculated in the *Production investment submodel*.

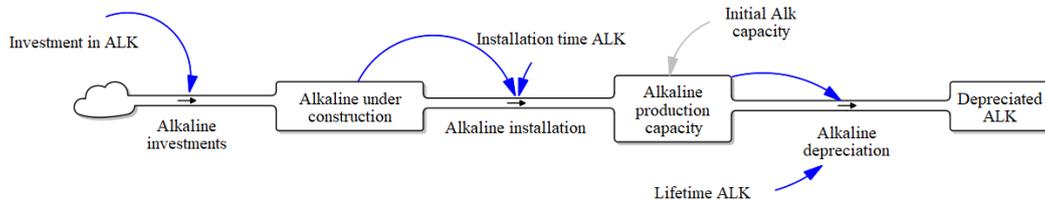


Figure 9: SD structure of construction and depreciation of alkaline electrolysis production capacity

The installation of production capacity model structure is denoted in figure 9. This figure displays the installation of alkaline electrolysis, but resembles the structure of CG and SMR

as well. The installation, depreciation and production capacity is modelled with a stock-flow structure. In SD, the flows denote a rate per unit of time, whereas the stocks are accumulations. The installation of new capacity is therefore continuously modelled: the installation rate is expressed in [MW/year] and the stock of installed capacity in [MW]. The accumulation in the stocks of construction and installed capacity as a function of the integrated flows for each of the production methods is mathematically expressed with the following equations [MW]:

$$Under\ construction_J = \int_t (Investments_J - Installation_J) dt \quad (6)$$

$$Production\ capacity_J = \int_t (Installation_J - Depreciation_J) dt \quad (7)$$

Where  $J$  represents the three different hydrogen production options. To account for the time intervals, or delays, between investment and installation, and installation and depreciation, first-order delays are used. The delay time determines the duration of stay, or accumulation time, in the stocks. The delay times are expressed as *Installation time* and *Lifetime* per production technology. A first order delay is expressed as:

$$Depreciation_J = \frac{Production\ capacity_J}{Lifetime_J} \quad (8)$$

Where  $J$  represents the three different hydrogen production options. Finally, the share of alkaline electrolysis capacity of the total installed hydrogen production capacity is finally calculated as [%]:

$$Share_{J|Alk} = \frac{Capacity_{Alk}}{\sum Capacity_J} * 100\% \quad (9)$$

Where  $J$  denotes the different hydrogen production methods, and *Alk* represents alkaline electrolysis.

### 5.2.2 Learning-by-doing submodel

The learning-by-doing mechanism is captured in a reinforcing feedback loop connecting the cumulative installed capacity of electrolyzers with the cumulative installation of technology. For alkaline electrolysis technology, the installation rate of electrolysis capacity of the *H<sub>2</sub> production submodel*, accumulates into this submodel into Cumulative experience Alk (see figure ??). Cumulative experience affects the investment costs through a technology-specific learning rate. The learning rate indicates the rate of cost reduction for each doubling of cumulative installation. The cost reducing dynamics of learning-by-doing are described as follows [\$ /kW]:

$$C_t = C_0 * \left(\frac{P_t}{P_0}\right)^{-\alpha} \quad (10)$$

Where  $C_0$  denotes the initial capex of alkaline electrolyzer per kW capacity,  $C_t$  is the capex at time  $t$ .  $P_t$  denotes the total installed capacity of electrolysis at time  $t$  and  $\alpha$  is the dimensionless learning coefficient derived from the learning curve, derived from  $LR = 1 - 2^{-\alpha}$ . Therefore,  $\alpha$  is calculated with [dmnl]:

$$\alpha = LOG_2(1 - LR) \quad (11)$$

Where  $LR$  is the learning rate, indicating the cost percentage change caused by the doubling of installed capacity. A learning rate of 18% results in a price reduction to 82% of the previous costs when cumulative capacity doubles (Söderholm & Klaassen, 2007). The model structure of cost reduction through learning in Vensim is shown in figure 10. The stock *Cumulative experience Alk* contains the total installed capacity of alkaline electrolyzers.

Vast literature is available about the learning rates of renewable energy technologies, but the field of study to the learning potential of hydrogen technologies is comparably juvenile.

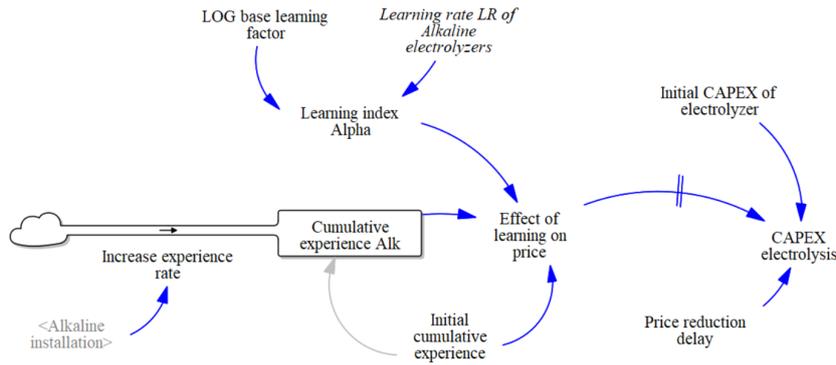


Figure 10: System dynamics structure of CAPEX dynamics through technological learning

In 1998, Rogner pioneered in detecting the learning rate of alkaline electrolyzers and concluded on a value between 7-12% (Rogner, 1998). Schoots et al. (2008) analyzed hydrogen production technologies and found a learning rate for electrolysis equipment of 18% with an error margin of 13%. This learning curve was updated through an extensive expert elicitation by Schmidt et al. (2017), confirming the LR of 18% and curtailing the uncertainty margin from 13% to 6%. Krishnan et al. (2019) found a learning rate of 16% with an error margin of 6%, but recognized a poor fit of the experience curve with gathered data. An assessment of learning rates of different components of electrolyzers was conducted by Bohm et al. (2020) resulting in a system learning rate of 13%, dependent on the technological configuration of the alkaline electrolyzer system. This study adopts the learning rate of 18% as stated by Schmidt et al. (2017). A crucial assumption in adopting this learning rate is the geographical scope. The model only considers capacity increase and learning in Germany, whereas the above described studies adopt a global scope or European scope for learning by doing. This assumption implies that the cost reduction through learning-by-doing in the model is less than it would be in the real-world. Another important initial parameter in this submodel is the initial capex (cost in 2010) of alkaline electrolyzers. Determination of this value is also not undisputed and has a range of 600 - 2000 \$/kW in examined literature (Schmidt et al., 2017; Böhm et al., 2020; Nguyen et al., 2019; Bloomberg NEF, 2019). In appendix G, a more elaborate overview of literature on capital costs of alkaline electrolyzers is provided. The large range can be contributed to diverse system configurations, location of manufacturing and system scale. Based on the diverse values in literature, an initial capex for alkaline electrolysis in 2010 of 1000 \$/kW is adopted in the model.

The price reduction from learning-by-doing does not happen instantly, a third order delay is incorporated in the model to account for this transfer of information and has a duration estimated at 1 year. Furthermore, unit size growth and efficiency improvement which are considered to be phenomena provoked by learning as well (Wilson, 2012), are not included in the model.

### 5.2.3 Production investment submodel

To simulate the investment behaviour choice in new capacity mathematically, a multinomial logit function is used. The multinomial logit function is often applied human choice behavior modeling, which concerns the choice behavior of individuals and originates from economics. If discrete choice modeling of separate actors is not feasible, it is necessary to adopt the choice behavior of individuals based on the observations of choices in a population (McFadden et al., 1973). For this, the multinomial logit function can be applied, as it models the choice of individuals in a population, assuming heterogeneity of choice behavior amongst this population (Yoo & Ready, 2014). Thus, the multinomial logit function determines the choice between multiple similarly available options of a product or technology, based on a single criteria such as cost feasibility or utility (Kauffmann, 1998). In this model, the investment choice between blue hydrogen or green hydrogen can be considered as an

investment decision between equally available alternatives based on economic feasibility of the production technology. It is assumed that the criterion for investment choice is the cost of production, or levelized cost of hydrogen, since the production methods with the lowest LCOH returns the highest profit. To illustrate, the logit function to determine the share of investment  $IS$  of alkaline electrolysis  $alk$  of the total investment in the three production technologies  $J$  is as follows[dmnl]:

$$IS_{Alk} = \frac{e^{-\lambda C_{Alk}}}{e^{-\lambda C_{Alk}} + e^{-\lambda C_{SMR}} + e^{-\lambda C_{CG}}} \quad (12)$$

Where:

$\lambda$  = Logit parameter for investments in production capacity [dmnl]

$C_{Alk}$  = Levelized cost of hydrogen from alkaline electrolysis [\$/kg]

$C_{SMR}$  = Levelized cost of hydrogen from steam methane reforming [\$/kg]

$C_{CG}$  = Levelized cost of hydrogen from coal gasification [\$/kg]

In the multinomial logit function, the share of investment for each technology is determined by the logit parameter  $\lambda$ . For the installation of new production capacity, this parameter is determined at -1. This value of the logit parameter and the implications for the model are further discussed in section 6.2.4.

#### 5.2.4 Costs of hydrogen production

One of the main drivers of the model is the cost of hydrogen. To assess the cost of production and compare different production methods, the cost is expressed in Levelized cost of hydrogen (LCOH). This factor expresses the cost per unit of production based on the discounted total cost over the lifetime of the plant, divided by the total discounted production during the lifetime of the plant. The levelized costs is widely applied in energy-economics and is the conventional method to evaluate hydrogen production costs (Tlili et al., 2019; Cihlar et al., 2020; Fazeli et al., 2021). The levelized costs for each production method  $J$  is expressed as follows [\$/kg] :

$$LCOH_J = \frac{\sum_{t=0}^n \frac{CAPEX_J + OPEX_{J_t}}{(1+r)^t}}{\sum_{t=0}^n \frac{P_{J_t}}{(1+r)^t}} \quad (13)$$

Where:

$CAPEX$  = Capital investment cost per unit of capacity [\$/kW]

$OPEX$  = Variable and fixed operational cost of production per unit per year [\$/((kW\*year))]

$Pt$  = Total production per kW over plant lifetime [kg]

$n$  = Project lifetime

$r$  = Discount rate

$t$  = Year

The total costs as well as the total production are discounted over the lifetime of the production plant, with a discount rate of 8%. This is a common discount rate in energy projects (Tlili et al., 2019). The net present value (NPV) represents the present value of the total future net cash-flow. Since there is no expected return of investment incorporated in the calculation of the LCOH, the cash-flow only consists of costs. As seen in equation 13, the LCOH is composed of three elements: capital costs, operational costs and total production. The SD-model structure for the calculation of alkaline LCOH is displayed in figure 11

#### Capital costs

Capital expenditures are the initial investment cost per unit of capacity. The capital costs for CG and SMR are adopted from literature, having values of 2680 and 1680 \$/kW respectively and are assumed not to transform over time (IEA, 2019). The capital costs for alkaline electrolysis is debated in a vast amount of literature leading to a range of costs from \$600 to \$2000 (Schmidt et al., 2017; Nguyen et al., 2019; Tlili et al., 2019; Bloomberg NEF, 2019),

as debated in appendix G. This study adopts a reasonable assumed initial investment price of 1000 \$/kW for 2010. The implications of the choice of initial capex are further discussed in section 6.2.3. The capex of electrolysis is expected to decrease over time as a consequence of the output of the *learning-by-doing submodel* and is therefore endogenously calculated with the previously described model mechanism.

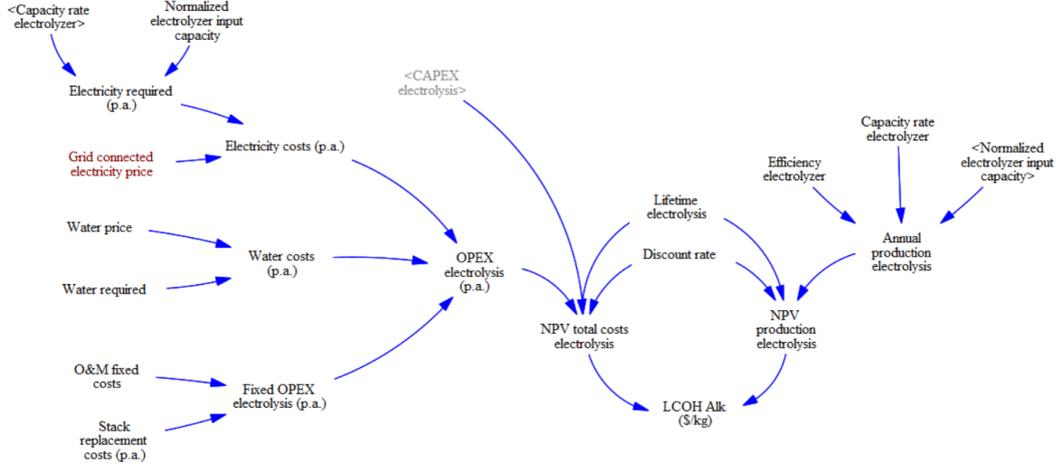


Figure 11: System dynamics structure for the levelized costs of hydrogen from alkaline electrolysis

### Operational costs

Operational expenditures include the fixed operational costs, which are the annual expenditures independent of the operation hours per year, and the variable costs, that depend on the annual operation hours. For electrolysis, the fixed opex comprises the O&M costs with an annual cost of 3% of capex, and the stack replacement costs. The electrolyzer stack components have a lifetime of approximately half the electrolyzer system lifetime (IRENA, 2018). Stack costs are calculated as a fixed share of the system capex and included as operational costs. The variable opex for electrolysis is based on electricity costs and water costs required per unit of hydrogen produced. Feedstock consumption refers to the power or input capacity of the plant; efficiency is therefore not included in the opex equation for electricity consumption (1 kW plant consumes 1 kW feedstock). Following the model structure in figure 11, the annual operational cost for alkaline electrolysis before discounting is described with the following equation in [\$/ (kW\*year)]:

$$OPEX_{Alk} = (C_{Electricity} + C_{H2O}) * CF_{Alk} + C_{O\&M} + C_{Stack} \quad (14)$$

Where:

$C_{Electricity}$  = Annual electricity costs per kW of capacity [\$/MWh]

$C_{H2O}$  = Annual water costs per kW of capacity [\$/kg]

$C_{O\&M}$  = Annual O&M costs per kW of capacity [\$/year]

$C_{Stack}$  = Annual stack costs per kW of capacity [\$/year]

$CF_{Alk}$  = Capacity factor of electrolyzers [hours/year]

Electricity consumption is based on the power or input capacity of the plant. Electricity costs are based on the price for large industrial consumers (band IG, >150000 MWh per year) including taxes and levies adopted from historical data from 2010 to 2021 (Eurostat, 2021). The future electricity costs are included exogenous and adopted from the STEPs and NZE-scenario of the IEA (IEA, 2021). Water is utilized for feedstock and cooling, estimated at 9L H<sub>2</sub>O per kg hydrogen produced (Böhm et al., 2020). The capacity factor of electrolysis is set at 90% (roughly 7884 full load hours p.a.), with the electrolyzers are assumed to be grid connected (IEA, 2020).

For CG and SMR, fixed opex solely consists of O&M costs calculated as a fixed share of capex per year (Böhm et al., 2020). Elements included in the variable opex for CG and SMR are the costs for feedstock - coal and natural gas, additional electricity, water, carbon capture and storage and emissions of non-captured carbon. The equations for the annual operational costs for SMR and CG can be denoted as follows [\$/ (kW\*year)]:

$$OPEX_{SMR} = (C_{NG} + C_{Electricity} + C_{H2O} + C_{CCS} + C_{CO2}) * CF_{SMR} + C_{O\&M} \quad (15)$$

$$OPEX_{CG} = (C_{Coal} + C_{electricity} + C_{H2O} + C_{CCS} + C_{CO2}) * CF_{CG} + C_{O\&M} \quad (16)$$

Where:

$C_{NG}$  &  $C_{Coal}$  = Annual cost of natural gas and coal per kW of capacity [\$/MWh]

$C_{H2O}$  = Annual water costs per kW of capacity [\$/kg]

$C_{CCS}$  = Annual costs of carbon capture and storage per kW of capacity [\$/ton CO<sub>2</sub>]

$C_{CO2}$  = Annual costs for non-captured emissions [\$/ton CO<sub>2</sub>]

$C_{O\&M}$  = Annual fixed O&M costs per kW of capacity [\$/]

$CF_{Alk}$  = Capacity factor of electrolyzers [hours/year]

The costs of natural gas and coal are obtained from Eurostat (Eurostat, 2021), and IEA (IEA, 2019) respectively. The economic parameters for carbon capture and storage are adopted from Parkinson et al. (2019) and GasforClimate (2021) and are estimated at 50\$/ton CO<sub>2</sub> for SMR and 43.9 \$/ton CO<sub>2</sub> for CG with capture rates of 90% and 95%. The annual costs for non-captured carbon is calculated through the carbon price as determined in the European Emission Trading Scheme, with historical data obtained from (Eurostat, 2021). The capacity factors for SMR and CG are both 95% (IEA, 2019).

### Production

The factor of total production in the LCOH equation comprises the total amount of hydrogen produced during entire the lifetime of a plant per unit of capacity. The structure of this equation is shown in the right part of figure 11. The formula for the total production is given as follows in [kg/(kW\*year)]:

$$Production = \eta_J * Cf_J * NCV_{H2} * 8760 \quad (17)$$

Where  $\eta_J$  is the efficiency of the production method J and  $Cf_J$  the capacity factor of production method J.  $NCV$  is the net calorific value, or lower heating value (LHV), of hydrogen with a value of 33.29 [kWh/Kg]<sup>1</sup>, 8760 is the number of hours per year.

The efficiency  $\eta$  of alkaline electrolysis is included as an exogenous lookup variable, with an increasing efficiency from 62 to 75% from 2010 to 2050 (Schiebahn et al., 2015). The efficiency of SMR is 0.69% (IEA, 2019) and of CG is 0.58% (IEA, 2019).

### 5.2.5 Demand for hydrogen

The model incorporates hydrogen demand for three end-use sectors: Heavy-duty fuel cell trucks (HDT), hydrogen-direct reduced iron (HDRI) and hydrogen injection into the natural gas grid (Blending). These three sectors are included based on their paramount and promising characteristics to be the first sectors for the large-scale adoption of hydrogen as concluded in a number of studies (BMW, 2020; Gasforclimate, 2021; Hydrogen Council, 2021).

Hydrogen consumption in each sector is simulated through the choice behavior model structure with a multinomial logit function. The share of investment in each technology for each sector is driven by the relative costs of the technology, which incorporates the fuel costs. Consequently, if the price of hydrogen decreases relative to alternative fuels, the investment share of the hydrogen technology will increase.

<sup>1</sup>For energy conversion calculations, the lower heating value (LHV) is used in this research

### Demand in heavy duty transport

To assess the development of hydrogen consumption in heavy duty transport, three types of technologies (HDT) are considered: Conventional diesel trucks, battery electric vehicle trucks (BEV) and hydrogen based fuel cell electric trucks (FCEV). Trucks defined as HDT have a weight  $>3.5$  tons with a total truck stock of 840.326 trucks in 2010 and an annual growth rate of 1.5% (ACEA, 2019). The truck lifetime is 9.5 year, with an annual mileage of 140.000 assumed similar for each technology (Ruf et al., 2020). Since the investment share of each technology in the multinomial logit function is fully cost-based, the total cost of ownership (TCO) per truck type is assessed to allow for a comparison of lifetime costs for different technologies. This assumes a like-for-like truck performance, implying that the experience for end-users is similar for each technology (Roland Berger, 2020). The TCO for each technology is composed of the endogenously calculated fuel price and an exogenous factor for fixed costs. This is calculated as follows for each truck type  $T$  in [\$/truck]:

$$TCO_T = Lifetime * Mileage_{p.a.} * Fuel\ consumption_T * C_{fuel_T} + TCO\ excl.\ fuel_T \quad (18)$$

Where the lifetime and annual mileage are assumed similar for each truck type (Roland Berger, 2020). The fuel consumption in [kWh/km] and fuel costs in [\$/kWh] calculate the total lifetime expected fuel costs  $C_{fuel_T}$ . The factor  $TCO\ excl.\ fuel$  includes the cost parameters for the capex and fixed opex and is expressed per truck in [\$/truck]:

$$TCO\ excl.\ fuel_T = CAPEX_T * LR_T + OPEX\ fixed_T \quad (19)$$

$LR_T$  is effect of technological learning on the capex. This factor is inserted as exogenous parameter based on the expected capital costs for FCEV trucks and BEV trucks in 2050 as reported by (Roland Berger, 2020). This learning rate results in an expected capex in 2050 of 612679 \$ and 560000 \$, and an annual price reduction of 0.833 % per year 1.34 % per year for FCEV and BEV respectively (IEA, 2020). Diesel trucks are assumed to remain constant in capital costs.

Subsequently, the share of investment, or probability of purchase, per truck type is calculated with the multinomial logit function. The logit function is commonly applied to assess purchase probabilities in transport modeling, and has been demonstrated for hydrogen vehicles by Struben & Sterman (2008) and subsequently by Meyer et al. (2009). The relative costs expressed in TCO per truck are expressed in [\$/truck\*km]. For illustration, the investment share  $IS$  of FCEV trucks of total investment in heavy duty trucks is shown as example. The equation is similar for other modes of heavy duty trucks and is expressed as [%]:

$$IS_{FCEV} = \frac{e^{-L_{HDT} * C_{FCEV}}}{e^{-L_{HDT} * C_{Diesel}} + e^{-L_{HDT} * C_{BEV}} + e^{-L_{HDT} * C_{FCEV}}} \quad (20)$$

Where:

$C_{FCEV}$  is the cost per kilometer for FCEV-trucks

$C_{BEV}$  is the cost per kilometer for BEV-trucks

$C_{Diesel}$  is the cost per kilometer for Diesel trucks

$L_{HDT}$  is the logit parameter for heavy duty transport.

The base value for the parameter in transport is set to -1.5, indicating a flexible market that is sensitive to price fluctuations. Identification of the logit parameter is difficult, since it expresses a number of qualitative factors that determine the choice of individuals. The function responds differently to high and low logit parameters. A high parameter (-0.5) indicates a very low response of consumers or investors to decline of costs, whereas a low parameter (-5) results in a very high price-demand elasticity (McFadden et al., 1973). In a modeling study to the adoption of different types of passenger vehicles, Struben & Sterman (2008) adopt a elasticity rate of -1.5, which is regarded moderately elastic according to the authors. Khan et al. (2020) found a price elasticity coefficient for different types of passenger vehicles of -1.3. This study adopts a moderate price elasticity in the heavy duty

truck sector and uses the logit parameter of -1.5. More discussion on the value of the logit function is provided in section 6.2.4.

### ***Effect of infrastructure on FCEV trucks***

Aside from the TCO as criterion for investment, it can be argued that the availability of refuelling infrastructure has significant influence on the probability of purchase. The absence of infrastructure is, as mentioned earlier, one of the primary obstacles to hydrogen diffusion. For FCEV, the absence of hydrogen refuelling infrastructure hampers the uptake of hydrogen vehicles (Hanley et al., 2018). Correspondingly, the construction of hydrogen refuelling infrastructure can be considered to be in a positive feedback loop with the purchase of hydrogen vehicles (Meyer & Winebrake, 2009). The presence of refuelling infrastructure is not a constraint for diesel trucks, and is assumed not to be a constraint for BEV trucks.

To simulate the effect of limited hydrogen infrastructure as a constraint on the uptake of FCEV trucks, the factor *supporting impact of infrastructure on FCEV* is defined. This factor normalizes the hydrogen infrastructure available assuming a linear relation between infrastructure on the purchase rate of hydrogen trucks. Moreover, this parameter closes the positive feedback loop between infrastructure and vehicle adoption. The upper limit of the *supporting impact of infrastructure on FCEV* is indicated with the constant *max. pipeline for full capacity*, with a value of 40.000 km. This value is adopted from Reuss et al.(2017), according to whom a covering infrastructure grid in Germany consists of 40.000 km of pipeline, leading to an unconstrained growth of 50% FCEV trucks of total. Reuss et al. (2017) estimate this figure based on a 50% share of FCEV of total. Regarding solely HDT, this might be a high estimation. In case of complete absence of hydrogen infrastructure, *supporting impact of infrastructure on FCEV* is equal to zero and restrains the adoption of FCEV trucks.

It can be argued that this could be improved by following the modeling procedure of (Meyer & Winebrake, 2009), who assess the number of required refuelling stations per number of FCEV and the relative distance between the refuelling stations. However, for the matter of simplification, this step is bypassed which results in the total pipeline infrastructure as an indicator for hydrogen adoption.

### **Steel & Iron industry**

For the steel sector, three routes of production are modeled: Conventional blast furnace-basic oxygen furnace (BF-BOF) steel; Hydrogen injected blast furnace (H2-BF), and hydrogen direct reduced iron (HDRI). Annually, Germany produces 29.5 Mtons of steel per year with BF-BOF. The annual growth of steel production capacity is assumed to be zero, leading to steel plant replacement solely driven by plant depreciation. The lifetime of a steel factory is not unambiguously determinable, because of the numerous components in steel making facilities. Nevertheless, the median lifetime of a blast furnace is examined by Vögl et al.(2021) and is estimated at 17 years. Investment in steel production capacity is modeled as a continuous flow normalized to Mtons per year. In reality however, the transformation of the steel sector would follow a more stepwise pathway caused by the discrete conversion of separate steel plants.

The investment decision for each technology is driven by the total production cost per ton steel. Costs for each production pathway consist of different components dependent on the feedstock and emissions. Conventional BF-BOF uses coal as primary feedstock and makes other costs for electricity and carbon emissions. The costs for H2-BF with CCS consist of costs for coal, electricity, hydrogen, emissions and CCS. Finally, HDRI steelmaking has costs for hydrogen and electricity consumption (Fischedick et al., 2014; EPRS, 2021). The total costs per tonsteel for each production pathway  $S$  can be expressed as [\$/ton steel]:

$$C_S = C_{feedstocks} + C_{electricity} + C_{emissions} + C_{CCS} + C_{fixed} \quad (21)$$

Where  $C_{fixed}$  are the fixed costs per ton steel, including capex and fixed opex. The values for  $C_{fixed}$  are adopted from (EPRS, 2021). Today, HDRI steel is not employed on a large scale and is not yet available for large-scale steel making. It can be argued that the large scale

availability of green hydrogen is, similarly to the feedback loop between infrastructure and transport, quelling the upscaling of HDRI-steel making. This feedback loop is attempted to be simulated through the dependency on hydrogen price. Nevertheless, technology readiness for HDRI is incorporated with a *technology readiness* switch, allowing HDRI-steel making to grow after 2025 (Gasforclimate , 2021).

After determination of the production cost per tonsteel of each technology route, the investment share of each steel technology is also calculated with the multinomial logit function. The investment share in HDRI steel production is determined as follows [dmnl]:

$$IS_{HDRI} = \frac{e^{-L_{steel} * C_{HDRI}}}{e^{-L_{steel} * C_{BF-BOF}} + e^{-L_{steel} * C_{H2-BF}} + e^{-L_{steel} * C_{HDRI}}} \quad (22)$$

Where:

$C_{HDRI}$  is the cost per ton steel from hydrogen reduced iron production

$C_{BF-BOF}$  is the cost per ton steel from the conventional blast-furnace production route

$C_{H2}$  is the cost per ton steel from blast-furnace production with hydrogen injection

$L_{steel}$  is the logit parameter for new steel production investments

The value of the logit parameter  $L_{steel}$  is initially set to -1.5, similar to the transport sector, which implies a low demand-price elasticity in this market. There is no research available in which the multinomial logit function is applied to adoption of new technologies or investors behavior in the steel sector. Determination of the logit parameter for the steel sector is therefore an uncertain process. The method for the logit parameter estimation of van Vuuren (van Vuuren, 2007) is followed for this case. He suggests to fit the logit function to historical data of investments, or otherwise adopt a (somewhat arbitrary) value for the logit parameter that seems legitimate. There are only six steel production sites in Germany, which indicates a very slow and inelastic price fluctuation response and thus a very high logit parameter (Eurofer, 2021). On the other hand, the margins in the steel sector are thin and competition is high, indicating a high price elasticity and thus a low logit parameter. The value -1.5 is chosen as a moderate value, since no valid value can be adopted from earlier research or historical validation. The demand for hydrogen in the steel sectors is finally calculated as the sum of hydrogen consumption in HDRI steel production and H2-BF steel production.

### Blending

The third end-use sector for hydrogen demand in the model is mixing hydrogen into the grid. This technology is controversial, because of safety concerns and lack of regulation (Melaina et al., 2013; Kanellopoulos et al., 2022). Nevertheless, when safety obstacles are overcome and regulations for blending are in place, blending might become a large instigator of hydrogen demand.

The amount of hydrogen per energetic part of gas mixture depends on two factors (Kanellopoulos et al., 2022). Firstly, the volume share or mix ratio of hydrogen and natural gas determines the amount of hydrogen injection into the gas grid. The possible volume share depends on the technological characteristics of the gas grid and varies per region or distribution grid. Secondly, hydrogen consumption depends on the percentage of natural gas infrastructure that is employed for blending. Hydrogen injection is currently in a pilot stage in which the hydrogen is injected at the capillaries of distribution grids. This occurs in local projects in which the blended gas reaches only a limited number of end-users (IEA, 2019).

In the model, the hydrogen demand for blending is driven by the cost gap between conventional pure natural gas and the blended mixture per unit of energy. This entails that the hydrogen consumption for blending is dependent on the hydrogen price. The volume rate for blending is assumed constant at 15% of volume, which is technologically possible in Germany according to (Hydrogen Europe, 2020; BMWi, 2020). The capital costs of blending per unit of energy are included at a value of 0.2 \$/MWh (Melaina et al., 2013). Furthermore, the blending share is a measured percentage of the entire natural gas consumption of Germany,

which assumes that all natural gas consumed is centrally distributed through the grid. With the multinomial logit function, the percentage of natural gas grid that is subject to blending is calculated, resulting in a proportion of the total natural gas consumption that is replaced by hydrogen.

$$IS_{mix} = \frac{e^{-L_b * C_{mix}}}{e^{-L_b * C_{NG}} + e^{-L_b * C_{mix}}} \quad (23)$$

Where:

$C_{mix}$  is the cost per  $nm^3$  of mixed gas

$C_{NG}$  is the cost per  $nm^3$  of 100% natural gas

$L_b$  is the logit parameter for blending

The logit parameter  $L_b$  is initially set at -4. This considerably high volatility is chosen for the adaptability of hydrogen injection as soon as technological constraints have diminished. Similarly to the steel sector, there is no previous research found about the adoption of a choice behavior model for hydrogen blending. Regarding the model basecase outcomes, -4 is a reasonable estimation done by the author. If the grid is suitable to accommodate hydrogen blending and injection equipment is in place, the share of blending can easily be adjusted dependent on the relative prices of natural gas and hydrogen. The major "if" in this assumption is the readiness of the grid and mixing equipment (Quarton & Samsatli, 2018). To account for this, the model contains a technology readiness switch for hydrogen blending that is initially set for 2025.

### 5.2.6 Hydrogen infrastructure

The connecting link between supply and demand is transport of hydrogen. The availability of infrastructure is one of the drivers that will accommodate the transformation from on-site production for local consumption, towards an integrated hydrogen market on a national level. One of the key challenges of the research questions is to quantify the effects of seemingly difficult-to-quantify drivers. The effect of infrastructure availability is often mentioned as an obstacle to market deployment, however only few studies attempt to quantify this causal relationship (Reuß et al., 2017; Cerniauskas et al., 2020).

Several studies have assessed scenarios for hydrogen transport and the economic feasibility of different transport modes in Germany based on geospatial modeling. These scenarios assume, similar to this study, centralized hydrogen production for merchant purposes where demand clusters and production clusters must be connected with infrastructure (Baufumé et al., 2013; Reuß et al., 2017; Robinius et al., 2017). The spatial characteristics of infrastructure make it complex to simulate the construction of infrastructure in an appropriate way with system dynamics. Infrastructure construction simulation is therefore drastically simplified, based on estimations from literature. A simplified SD-model structure of the infrastructure submodel is shown in figure 12.

The construction of infrastructure in the model is driven by the expected demand for hydrogen via the parameter *Infrastructure response to demand*. This parameter estimates the expected hydrogen demand with the Vensim *Forecast* function, which is a simple trend extrapolation forecast of the future hydrogen demand based on historic behaviour. This simplified model structure resembles the real-world upfront planning of infrastructure based on expected demand. A planning horizon of 5 years is chosen, based on the planning and construction time of infrastructure.

To couple the expected hydrogen demand with the investment of infrastructure, the constant *KM pipeline required per TJ demand* is included in the model. The value for this parameter is estimated from the geospatial findings of Baufumé et al.(2013), Reuss et al. (2017) and Robinius et al. (2017). Each study calculates an optimal transmission and distribution network of hydrogen pipelines based on demand scenarios. Their findings are translated to 0.035 Km transmission pipeline and 0.12 Km distribution pipelines per TJ hydrogen

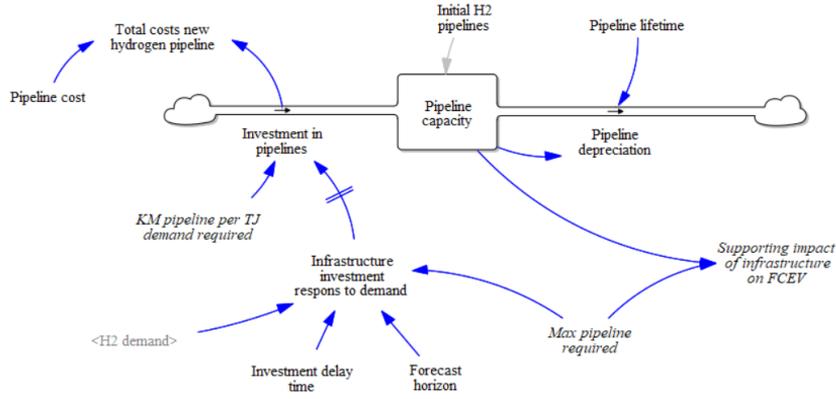


Figure 12: System dynamics structure for the construction of new hydrogen infrastructure

demand, with pipeline diameters fixed between 100mm and 300mm for distribution and transmission respectively (Robinius et al., 2017).

The potential for retrofitting natural gas pipelines is included in the model in *share of retrofitting*. Retrofitting existing natural gas grid to hydrogen pipelines is considerably cheaper than building new hydrogen pipelines, but can not be applied to all natural gas pipelines. An estimation was made by Cerniauskas et al.(2020), who found an optimistic value of 49% of the future hydrogen pipelines to be retrofitted natural gas pipelines. This is significantly lower than the estimation of a retrofitted share of 69% in European hydrogen pipelines from Gasforclimate (2021). Because of the scope, this study adopts the value of Cerniauskas et al.(2020).

The investments in pipelines are driven by hydrogen demand. However, the pipeline grid density might at a certain point become saturated compared to the increasing demand. From that moment solely the pipeline capacity is at issue. This point of saturation is assumed to be 40.000 km of total pipeline, adopted from (Reuß et al., 2017), and is modeled as *max. pipeline for full capacity*. The effect of the grid saturation on the adoption of FCEV is explained in section 5.2.5. 40.000 is a fairly low estimation compared to the German natural gas grid, with a length of over 507.000 km (BMW, 2020), but hydrogen can be transported by other means as well, and produced at any location across the country.

The total costs for the pipelines are based on the capital costs and fixed operational cost of construction over a lifetime of 40 years, as provided by Gas for Climate (2021). The opex of the pipeline are estimated at 1% of capex per year. The cost of compressors and refuelling stations are excluded from the cost calculations. Aside from the length, the capital costs of pipeline also depends the flow capacity, or diameter of the pipelines. Three types of pipelines have been included which are divided for a fixed share each according to (Robinius et al., 2017). The share and diameters of the pipelines are 45% of small diameter (100 mm), 35% of medium diameter (100mm > d < 300mm) and 20% large (>300mm).

According to Reuss et al. (2017), who conducted a spatial optimization study to a future hydrogen distribution network in Germany, the most viable transportation option is transmission with pipelines and distribution with gaseous-hydrogen trailers. In case the hydrogen demand density and the FCEV penetration rate is high (>75%), distribution by pipeline becomes feasible over truck-distribution.

### 5.2.7 Carbon emissions

One of the key model objectives is the carbon emission from hydrogen production. Derived from hydrogen emissions is the emission abatement in end-use sectors as a result of hydrogen adoption. The abated carbon emissions consist of two components: the direct emissions that are abated by the transition from grey to green or blue hydrogen, and the emissions

that are reduced in the end-use sectors from the abatement of fossil-fuel technologies. The calculations are a simplified representation of the real-world emissions. First, the carbon intensity of hydrogen production is calculated. The annual emissions from each hydrogen production method are evaluated, which sum up to the *Total annual carbon emissions hydrogen production*. For grey hydrogen, the emissions are derived by the multiplication of *production capacity* with the *emission per kg hydrogen*. For blue hydrogen, the calculation is similar, however the carbon capture rate is added to the equation. The emissions from electrolysis are not assumed to be zero, since the electrolyzer capacity is presumed to be grid-connected. Therefore, the carbon intensity of hydrogen from electrolysis is dependent on the carbon intensity of the electricity grid. The emission from grid electricity in Germany in 2017 was 485 grams per kWh (Umwelt Bundesamt, 2021). The future carbon footprint of grid electricity is assumed to be in accordance with the share of renewable electricity based on historical data. Thus, a linear relation between the share of renewable electricity and the carbon footprint is assumed. The share of renewable electricity is modeled with a lookup-function and is based on the sustainable electricity targets for 2030 and a net-zero electricity supply in 2050 (Fraunhofer ISE, 201). The grid emission intensity  $E$  at time  $t$   $E_t$  is calculated as follows in [kg CO<sub>2</sub>/kWh]:

$$E_t = \alpha * S_t + \beta \quad (24)$$

Where  $S_t$  is the variable share of renewable at time  $t$  from the lookup function,  $\alpha$  is the emission coefficient which represents the slope of the linear emission function calculated as:

$$\alpha = \frac{-E_{2010}}{S_{2050} - S_{2010}} \quad (25)$$

Where  $E_{2010}$  denotes the grid emission factor in 2010.  $S_{2050}$ ,  $S_{2010}$  are the shares of renewable electricity in Germany for 2010 and 2050, with values of 17% and 100% respectively. The y-intercept coefficient  $\beta$  is derived from the two equations using the initial values.

From the annual emissions per production method, the carbon intensity of hydrogen  $Ci_{H_2}$  is calculated through [kg CO<sub>2</sub>/kg H<sub>2</sub>]:

$$Ci_{H_2,t} = \frac{\text{Total annual carbon emissions H2 production}_t}{\text{Total annual H2 production}_t} \quad (26)$$

The abated carbon emissions for hydrogen production relative to the initial emissions from grey hydrogen entirely  $Ca_{H_2}$  is calculated as [Mtons/year]:

$$Ca_{H_2,t} = \text{Carbon emissions H2}_{2010} - \text{Carbon emissions H2}_t \quad (27)$$

Aside from the direct emissions from hydrogen production, the annual and cumulative carbon emission reduction caused by the transition to hydrogen technologies in end-use sectors is examined. The abated carbon emission per sector are calculated as the difference between the emissions from the sector without any endorsement of hydrogen technologies, and the emissions from the sector including hydrogen technology implementation. The sum of the sectors defines the total carbon abatement per year, and cumulatively, on account of the adoption of hydrogen technologies. Finally, the total abatement is calculated as the sum of direct emission reduction in hydrogen production and the emission reduction in end-use sectors in [Mtons CO<sub>2</sub>/year].

### 5.2.8 Policy implementation and policy costs

The policies described in section 4.3 and 5.1.5 are implemented in the model and are linked to the submodels where each policy is of influence. The modeling of policies is rather straightforward, as it comprises the inclusion of a switch in the form of a pulse-, ramp- or step-function, with a certain height and duration. A few of the modeled policies contain direct cost elements that require financing, or indirect expenditures through the reduction of tax income. The net costs are calculated in Vensim for each policy separately and ultimately

combined to assess the total annual costs and the total cumulative costs of each policy combination. The policies are adopted from (DNA , 2019; Agora Energiewende, 2020; IRENA, 2020; BMWi, 2020).

**Electricity tax reduction:** The electricity tax discount is assumed to be a discount on the levies that are in place for grid electricity consumption in Germany (BDEW, 2021). In the model, this policy applies to the cost of electricity for electrolysis solely. The costs are calculated as the reduced tax income [\$/year]:

$$PC_{Eta} = E_{costs} * tax_{discount} * E_{consumption} \quad (28)$$

Where  $tax_{discount}$  is the share of electricity price reduction for electrolysis.

**Electrolysis equipment subsidy:** The subsidies for the capital investments in electrolysis capacity are calculated as a share of the electrolyzer capital costs. This supply side policy is suggested by (Agora Energiewende, 2020). The exact values of the policy levers will be described in the section experimental setup 5.5. The total policy cost of the subsidies for alleviating the costs of electrolyzer equipment is calculated through [\$/year]:

$$PC_{Alk_{subsidy}} = Alk_{capex} * Alk_{subsidy} * Alk_{investments} \quad (29)$$

Where  $Alk_{subsidy}$  is the share of the capex in [\$/kw] of water electrolyzers that is subsidized.  $Alk_{investments}$  represents the total investment in electrolysis per year in [kW/year].

**Carbon Contracts for Difference:** Carbon contracts for difference (CCfD) are modeled for the steel industry and provide economic support for investment in HDRI steel plants and is recognized as a powerful demand-side policy (Agora Energiewende, 2020; IRENA, 2020; BMWi, 2020). The concept of the CCfD is that the government closes the cost gap between the carbon abatement costs and a pre-determined carbon price of the ETS. The pre-determined carbon price is set at a height at which the production of steel through the BF-BOF process including emission costs is expected to be equivalent to the costs of low-carbon HDRI steel. The translation of the policy is translated to a price reduction for HDRI per unit of steel produced as follows [\$/ton steel]:

$$Discount_{HDRI} = CCfD_{strikeprice} - BFBOF_{carboncosts} \quad (30)$$

The policy costs of the CCfD are equal to the  $Discount_{HDRI}$  times the annual installation of HDRI steel production capacity. An increasing carbon price limits the costs of the policy. The inclusion of the pre-arranged and fixed nature of  $CCfD_{strikeprice}$  implies that when the carbon price exceeds the CCfD price, the policy costs will become negative. This is at expense of the involved companies and results in a profit for the national government.

**Grid blending quota:** A blending quota is implemented in the model as a compulsory share of the natural gas grid that is subjected to hydrogen injection (Kanellopoulos et al., 2022). This policy acknowledges the technology readiness of 2025, as discussed in section 5.2.5, but assumes no further constraints to the implementation of blending on large scale. The policy adopts a volume blending rate of 15% into the grid, but the policy is expressed as the share of the total grid that is used for blending at a volume blending rate of 15%. The expenses for the policy consist of the cost gap between the conventional full natural gas distribution, and the additional expenses for hydrogen blending per unit of energy.

**Infrastructure investment support:** If the government decides to initiate the roll-out of the hydrogen infrastructure, upfront investments are modelled as an artificial financial injection in infrastructure per year that is independent of the hydrogen demand or production (IRENA, 2020). In the model, this is formulated as the direct construction of a fixed amount of pipelines and retrofitted pipelines in km per year. This implies that the quantification of this policy is not expressed in costs, but in km pipeline per year, and that costs are calculated afterwards. The costs for the upfront investments in infrastructure are assumed to be at expense of the government and are calculated in a similar matter as costs for the regular market-originated infrastructure.

**Coal phase-out:** The coal-phase out (Clean Energy Wire , 2020), is implemented in the *Production investment submodel*, where the market share for investments in coal is artificially diminished in the time frame that is the input for the policy. This is conducted through an artificial price increase of coal gasification resulting in zero investments in this technology. This policy solely impedes the investment in new coal gasification production capacity, and therefore no costs are made with this policy lever.

**Fossil-fuel tax:** In 2021, Germany announced a carbon emission price for transport and heating, expanding carbon pricing to sectors that are not included in the ETS. The so-called *Brennstoffemissionshandelsgesetz* (Bundesministerium der Justiz, 2019) is incorporated in the model as a fixed carbon price for fossil-based transport emissions. The profits of this tax scheme are calculated through the emissions from the entire Diesel truck fleet [\$/year]

$$PC_{Fuelex} = C_{Emission} * KM_{Total} * Emission \quad (31)$$

Where  $C_{Emission}$  is the predetermined carbon price for transport,  $KM_{Total}$  the total annual mileage of the entire diesel truck fleet, and  $Emission$  the carbon emission per truck per kilometer.

**Ban on CCS:** There are no costs made for the activation of this policy lever. The policy is implemented in the model on the supply side, and increases the costs of CCS artificially to an extreme height. This excludes blue hydrogen from the investment option, resulting in a ban on CCS.

### 5.3 Main model assumptions

This list includes the main assumptions that were adopted for modeling the hydrogen supply chain. The assumptions are categorized per submodel but can be considered non-exhaustive. The implications of the most significant assumptions on the model outcomes will be discussed in the discussion in chapter 8.

#### Production submodel:

1. In reality, the supply chain consists of countless more technologies in each stage of the chain. The high-level aggregation system allows for the exclusion of small-scale technologies that currently have a marginal share of contribution in the supply chain and are not expected to scale up in technology readiness on a short term.
2. The development of green hydrogen is assumed independent of the differences in technological and economical characteristics between alkaline and PEM electrolyzers. The study solely considers alkaline electrolysis.
3. The technological performance of all considered technologies are assumed not to deteriorate during the lifetime.
4. Electricity supply for electrolysis is assumed to be grid-connected. The carbon footprint of green hydrogen is calculated through the footprint of electricity generation in Germany.
5. Carbon capture and storage technological performance and costs are assumed to remain unimproved up to 2050. CCS technology is assumed to have access to unlimited storage capacity.

#### Demand submodel:

1. All hydrogen produced is assumed to be accessible for purchase as merchant hydrogen.
2. Fossil fuel end-use technologies do not technologically improve or decline over time.
3. Annual steel production is assumed to remain stable and the adoption of HDRI-steelmaking is assumed to be independent of infrastructure.

#### Infrastructure submodel:

1. The relationship between the availability of hydrogen pipeline infrastructure and the attractiveness of FCEV-trucks is assumed to be linear, and is saturated at a pipeline reach of 40.000 km.
2. Geo-spatial characteristics for infrastructure construction are excluded from the scope.

#### Other submodels:

1. The total levelized costs of hydrogen do not include the costs for transportation, storage, and further processing.
2. The electricity generation in Germany is assumed to be carbon neutral in 2050, and is assumed furthermore to have a linear relationship with the share of renewable electricity generation of the total electricity production capacity, derived from the carbon intensity and share of renewable energy sources in 2020.
3. The learning rate for learning on a global scale is adopted, but the learning of technology is assumed to be a national event.
4. All expenses that result from the implementation of policies are included in the total cost of policies, even if these costs are not directly at the expenses of the government.

## 5.4 Model testing

The step of validation and verification is often considered as a process of confirming that the model is correct or that it resembles reality and replicates historical data. However, this conception might lead to a limited analysis of the model’s behavior, robustness and limitations. Therefore model testing is not about whether the model is ‘right’, but rather if the model serves its purpose (Sterman, 2000). In other words, objective demonstration of the truth is impossible (Pruyt, 2013). Nevertheless, model testing through validation and verification is a crucial step in SD model building, since it reveals and confides the usefulness of the model. As stated by Senge & Forrester (1980), the ultimate objective of validation is to obtain confidence in a model’s soundness and usefulness as a policy tool. With the model purpose in mind, several validation procedures have been conducted to gain insight in the model behavior, usefulness and its limitations.

Validation methods in SD can be divided in two main categories. Structural validation checks if the model structure and parameters correctly illustrate real-world structure and values. Behavioral validation checks whether the model outcomes are plausible. This study adopts a series of validation methods as described in literature by Senge & Forrester (1980), Barlas (1989), Sterman (2000) and Qudrat-Ullah (2012).

### 5.4.1 Direct structure tests for structural validity

#### 1. Boundary adequacy test

Boundary adequacy tests if the model boundaries and submodels are accurately chosen in line with the model purpose. It compares the real-world structure to the model structure and assesses if important real-world concepts are modelled endogenously. This qualitative assessment is conducted through comparison of the subsystem diagram (figure 7) and the input parameters with the components of the real-world hydrogen supply chain. It could be argued that the list of excluded variables and subsystems is inexhaustible for any model, however, the relevancy of the included and excluded concepts for the model purpose is what is at issue.

All key performance indicators are a product of endogenously modelled systems. As shown in the subsystem diagram (figure 7), the entire hydrogen supply chain is modeled endogenously. One variable that is modeled as exogenous variable but could also have been included endogenously is the *efficiency of electrolyzers*. Similarly to the decrease of capital costs as a consequence of learning-by-doing, the efficiency of the electrolyzers is expected to increase with technology adoption (Schmidt et al., 2017). Efficiency increase rates are however adopted from literature and not modelled endogenously. Likewise, *capital cost reduction of FCEV and BEV*, and *capital cost reduction of HDRI steel* are exogenous variables adopted from literature (IEA, 2019), but could have been modelled endogenously as a result of technology adoption and learning-by-doing. Significant real-world concepts that are modeled as exogenous components are the costs for electricity and the costs of fossil fuels. Comprehending these markets in the model would be a challenging task and is not executed, but the interference between the market growth of hydrogen and the costs of electricity and fossil fuels cannot be ignored.

#### 2. Structure verification

Structural validation examines the aggregation level of the model compared to reality (Qudrat-Ullah & Seong, 2010). In line with the boundary assessment, the subsystem and causal diagram is used for this verification. The high-level aggregation of the model does suit with the model purpose and moreover with the model scope. The geographical scope of Germany requires a high level overview, since the hydrogen system and policies are considered on the national level and comprises a system of large quantities. The exclusion of several components of the real-world hydrogen system might have delivered a slight deviation between the model outcomes and real-world behavior, albeit this discrepancy might be small, if not negligible, regarding the scope of the study. Aside from the aggregation level, the model structure does not lead to unwanted, unexpected, or physically impossible behavior.

A behavioral salience is seen in the parameter *Supply-demand gap*, which shows a cyclical behavior. This behavior is not uncommon in system-dynamics and is traceable to the feedback loop between the *Investments in new capacity* and *Total installed capacity* (Forrester, 1997). The delay between the signalling of a supply shortage and the actual finishing of new production capacity is reinforced by this loop, causing the oscillating behavior of the *Supply-demand gap* and *Investments in new capacity*. The implications of this behavior are elaborated upon further in this research.

### 3. Dimensional consistency

The dimensional consistency can automatically be tested with the built-in Vensim unit check tool. All units are in place, what means that for each equation the units match on both side of the equations. Aside from the automatic unit tests, the model is checked for arbitrary units that are incompatible with real-world units, which are not included in the model.

### 4. Parameter verification

Parametric validity evaluates the value and the meaning (i.e. if the model parameter has a clear, real life counterpart (Sterman, 2000)) of each model parameter. To translate real-world concepts into simplified mathematical concepts, the use of fabricated parameters or variables is inevitable. The *logit parameters* attempt to capture the concept of demand elasticity and willingness-to-pay and therefore reflect a simplification of an intangible real-world concept. The significance of the value of the logit parameters is further discussed in section 6.2.4. Likewise, the *supporting impact of infrastructure on FCEV* is a nonphysical factor that is embedded to translate the normalized effect of infrastructure availability on the investment in FCEV trucks.

#### 5.4.2 Structure-oriented behavior tests for behavioral validity

### 5. Extreme conditions test

The extreme condition test evaluates the behavior of the system under extreme circumstances for a number of input parameters. This validation procedure is effective for two reasons. First, it discloses model behavior and model flaws that the modeler can hardly grasp in the expected behavior of a single equation (Senge & Forrester, 1980). Second, it reveals the model's ability to behave outside normal or expected patterns (Qudrat-Ullah, 2012). Moreover, this test reveals possible faults in model equations because the modeler can check the credibility of the model outcomes under extreme conditions and compare them to real-world expected behavior. The extreme condition test is evaluated for the model KPI's *electrolysis capacity* and *hydrogen demand*. The table with input for the extreme condition test as well as the visualisation of the outcomes are displayed in appendix C.1.

The extreme settings for energy prices are expected to lead to very low, or very high adoption of the type of hydrogen production that is reliant on that type of energy. In other words, an extremely high natural gas price might lead to zero adoption of steam methane reforming and an increase of electrolysis, whereas very high electricity costs will minimize the installation of electrolysis. Similarly, when initial demand is tested for extreme values, a high initial demand will lead to large and rapid growth of electrolysis. The initial capex of electrolyzers affects the adoption of electrolyzers, but when the price of electrolyzers is extremely low a rapid increase might not by definition take place. The installation of electrolysis is dependent on numerous other factors, that might offset the low capital costs.

The outcome graphs for the extreme condition tests are collected in figure 33 in appendix C.1. The following behavior is detected in this test:

1. An extremely high capex for electrolyzers leads to zero installation of electrolyzers.
2. Extreme values for electricity costs correspond with an extremely high, or zero installation of electrolyzers.
3. A high coal price results in large electrolysis capacity, and in strong demand growth because of the rapid abatement of conventional coal-based steel making.

4. Similar to the coal price, the influence of gas price corresponds with the expected uptake of electrolysis.
5. When the existing demand is artificially enlarged, the electrolysis capacity expands rapidly to satisfy this extreme demand. Analogously, no demand means no installation of production capacity.

The model behavior from the extreme condition tests corresponds with the expected behavior of the real-world system and obeys physical laws. Not only can be concluded from this test that the model remains stable and behaves accordingly even under extreme conditions, this test also provides useful preliminary insight in the model behavior. Pushing model inputs to extreme values reveals where possible bypasses may be for affecting the model objectives and confirm the effects of the barriers to diffusion. For example, a radical demand growth forces acceleration of diffusion for green hydrogen and, high electricity prices and capital cost of electrolyzers obstruct its capacity completely. These insights will contribute to further assessment of the system and policy design.

Table 2: Sensitivity analysis input variables, BC values and upper and lower tested limits

Tested model parameters	BC value	Lower	Upper
Initial CAPEX electrolyzer	1000	900	1100
Learning rate electrolyzer	0.18	0.16	0.2
Capacity factor electrolyzer	0.9	0.81	0.99
Pipeline required	0.071	0.0639	0.0781
Logit parameter investment	-0.5	-1.5	-0.25
Logit parameter steel	-1.5	-3	-0.5
Logit parameter HDT	-1.5	-3	-0.5
Logit parameter blending	-4	-6	-2

## 6. Sensitivity analysis

A sensitivity analysis is conducted as part of the behavioural validation. A sensitivity analysis examines the numerical and behavioral sensitivity of the model outputs to a set of model input parameters and variables. In SD, it is not common to include policies in the sensitivity analysis, because the response of the system to policies is investigated in the policy testing phase of modeling (Sterman, 2000). The aim of the sensitivity analysis is to detect which parameters are most strongly moving the model. From there, it provides insight in which model parameters are most important and demand thorough attention of the modeler (Sterman, 2000). The sensitivity analysis is conducted for the parameters denoted in table 2. The values are tested for the basecase input with a range of plus and minus 10%. This range is similar for each parameter to allow for comparison of the influence. For the logit parameters however is deviated from this range and is a wider range of values tested. This is done because of the large uncertainty of the values of the logit parameters. The wide uncertainty envelope allows for an amplified lens on the effects of the logit parameter uncertainty. As a consequence of deviating from the  $\pm 10\%$ , the outcomes of the logit sensitivities cannot be used for sensitivity comparison with the other parameters, and are the logit parameters excluded from the multivariate sensitivity analysis. The effects of the sensitivity analysis are evaluated for the KPI's *electrolysis capacity* and the *hydrogen demand*.

First, a univariate sensitivity analysis is executed for the parameters in described in table 2. The output graphs are displayed in appendix C.2. The electrolyzer capacity shows most significant numerical sensitivity to the capacity factor, as is highlighted in figure 13, with a range of about 112 MW for a  $\pm 10\%$  input envelope. This high influence of the capacity factor is due to the effect this constant has on the levelized cost of hydrogen. The costs

increases strongly when the capacity factor decreases, since a lower utility rate results in less production for the same capital costs. The price increase has a declining effect on the investment share of green hydrogen, explaining the high sensitivity of electrolysis capacity to the capacity factor. Pipeline required showed the largest impact on the demand, due to the direct feedback between the infrastructure construction and demand. Considering the most to least influential parameters on electrolysis capacity, the following order is observed from most to least effect: *Capacity factor electrolyzer - Learning rate electrolyzer - Initial CAPEX electrolyzer - Total pipeline required*. The logit parameter reveals large numerical asymmetric sensitivity on both assessed model outputs. This can be clarified by the amplifying effects of the feedback loops in the SD model. Higher input numbers cause larger amplification of behavior. Therefore, the upper sensitivity envelope of some parameters is larger than the lower range. For the logit parameters, this is inverted, since this comprises negative values, as can be seen for the electrolysis capacity sensitivity to the logit (appendix C.2).

Second, a multivariate sensitivity analysis is carried out, with the input of all parameters for a range of  $\pm 10\%$ . Because of the uncertain characteristic of the value logit parameters, these are excluded from the multivariate sensitivity. A multivariate sensitivity evaluates the sensitivity of *electrolysis capacity* and *hydrogen demand* to a combined set of input parameters over the sensitivity space and reveals the cumulative influence of the set of parameters, indicating the maximum sensitivity of the tested model objective. The results of the multivariate analysis can be found in Appendix C.2. Because of the dominance and uncertainty of the logit parameters, which are examined separately later in this research, the logit parameters are not included in the multivariate sensitivity analysis. The outcome shows no behavioral sensitivity, and numerical sensitivity is predominantly present in the electrolyzer capacity. The hydrogen demand shows a small margin of numerical sensitivity, as can be seen in Appendix C.2.

Numerical sensitivity was detected for the two tested model outputs. The sensitivity is foremost visible for the electrolyzer capacity, which is heavily affected by the capacity factor and indirectly the price of hydrogen. The multivariate sensitivity demonstrated not very significant diverging and unexpected numerical influence. Aside from insight in the effects of important parameters, the sensitivity teaches more. Similar to the extreme condition test, this analysis is an exploration to gain insight in the system behavior, such as the influence of leveled costs on the capacity of green hydrogen, and discover potential buttons that lever the system which can be utilized for the implementation of policy interventions.

## 6. Comparison with alternative scenarios

A common method of behavioral validation is historical validation. Historical validation compares the outcome of the model with real-world behavior of the system from the past. This method can easily be applied if the model covers a part of history and the system showed dynamic behavior in that slice of the past. Although the hydrogen supply chain model starts in 2020 and thus comprehends 10 year of the past, historical validation is in this case not of use. Because of the relative static state of the system, where demand and supply pertained in equilibrium, there is no historical motion of factors to be examined. As a variant on the historical behavior test, the model outcomes are compared to alternative scenarios and outlooks for the development of hydrogen in Germany. Although each study has its own numerical inputs, structure, and policy assumptions and must therefore be interpreted with caution, the alternative studies might offer an insight in the range of viable

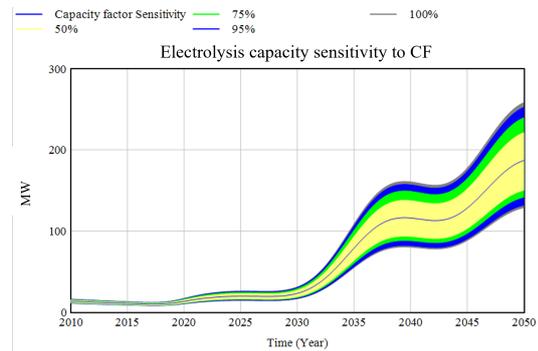


Figure 13: Univariate sensitivity of the electrolyzer capacity to the capacity factor under a  $\pm 10\%$  input range.

scenarios. Since historical validation is not possible and an expert elicitation is not employed, this test provides some form of comparison with the view of experts in the field.

Table 3: Comparison of hydrogen demand per sector of with alternative hydrogen scenarios for Germany and Europe (Hebling et al., 2019; DENA , 2019; Energy, 2020; Gasforclimate , 2021; FCH-JU, 2019; EC, 2018a)

Scope of scenario	H2-SD model	Germany		EU		Germany (1/4 EU)	
		Lower	Upper	Lower	Upper	Lower	Upper
Output parameter							
Total (TWh)	x	250	900	698	2300	174	575
Power sector	x	10	200	43	650	26	162
Industry sector	x	220	330	125	675	31	169
Modeled sectors total (TWh)	158	110	760	306	1592	76	398
Transport: FCEV-trucks	85	42	500	85	850	21	212
Buildings: blending	0.2	30	200	81	579	20	145
Steel sector	15	38	60	140	163	35	41

Only a few studies exclusively investigate the future of hydrogen in Germany. Therefore a number of studies with Europe as scope are included as well, from which the rough estimation is made that Germany comprises approximately 1/4th of the total hydrogen consumption. The studies are divided in three categories based on scope: Germany, and 1/4th of Europe. Three hydrogen scenario from Fraunhofer ISI, DENA, and Greenpeace with Germany as the scope were assessed (Hebling et al., 2019; DENA , 2019; Energy, 2020). Three studies that composed scenarios for hydrogen in Europe were examined from GasforClimate, FCHJU and the European Commission (Gasforclimate , 2021; FCH-JU, 2019; EC, 2018a). From these studies, the scenarios that were most in line with the basecase of this research regarding future energy prices, policies, modeled technological components and timeline were depicted for comparison. Because of the wide assortment of hydrogen production methods, a valid comparison for electrolysis capacity could not be made. Expected hydrogen demand is however estimated in each of the included scenario studies and therefore used as comparison criterion. Per sector, the outer ranges of forecasted hydrogen demand in 2040 or 2050 are summarized in table 3 in TWh, that were found across the scenarios ("modeled sectors total" is not equal to the sum of the sectors, since existing hydrogen demand is excluded from the table). Compared to the other studies, the base outcomes for hydrogen of this research are rather conservative and end up in the low spectrum of the demand range. The transport demand of this study is well within margins of the compared range, but steel and blending- compared with building sector in other studies - are lagging. Although the steel and blending sector hydrogen for 2050 are out of range of comparable scenario studies, that does not mean this model is inadequate. Firstly, the divergence can be attributed to a number of model decisions. The SD model assumptions might simulate the consumption in these sectors too moderate and conservative. Otherwise, it could be ascribed to the input variables for future energy prices that are more conservative in this study than used in the other scenarios. In response to the low basecase results, this research includes an alternative on the system on the hydrogen system through the inclusion of a more progressive scenario. This scenario embodies more impelling model settings and outputs, which will be discussed in the following chapter.

### 5.4.3 Conclusions and implications from model testing

Structural and behavioral tests provided the confidence that the SD-model can be used for further experimentation. The model boundary is adequately chosen for the aggregation level and scope of this study, and includes the relevant components of the hydrogen supply chain. The structure resembles the real-world supply-chain structure, parameters are adopted from

validated an reliable sources, and the dimensions of the units are correct. Furthermore, the model shows reasonable behavior that is in line with physical laws under extreme conditions, and is not severely disturbed, behaviorally nor numerically, by the alteration of influential input parameters. The logit parameters might distress model behavior if chosen inappropriately, but that is covered in section 6.2.4. Furthermore, the oscillating behavior that was found in the structure verification must be taken into account when interpreting the model outcomes. This oscillation will be extensively discussed in section 6.2.5. Finally, the model outcomes are low relative to comparable hydrogen scenarios, however, the inclusion of a progressive scenario in this research provides the answer to the low basecase scenario.

## 5.5 Experimental setup

To evaluate the impact of external factors and policy levers and improve insight in the model behaviour under uncertainty, a range of model experiments are conducted. The following section describes the experimental setup that is applied work towards the conclusion of this study.

### Simulation settings

The model runs from 2010-2050. A large time scope fits the continuous characteristics of SD-modeling. Moreover, the duration of diffusion is uncertain, but is not an overnight process. To assess the full trajectory without interruption due to a too narrow time scope, the model adopts a timeline towards 2050. Furthermore, the final time is chosen in line with the net zero emission ambitions of Germany and the Paris Agreement. The model output is in years. The Vensim model uses Euler integration method with a timestep of 0.03125, which is the equivalent of approximately 11 days. This timestep is chosen through halving the timesteps and observing when model output does not change. This is the largest timestep for which model output does not show significant differences compared to a smaller timestep.

#### 5.5.1 Basecase analysis setup

First, the basecase is analyzed to understand the fundamental dynamic behavior of the system. The basecase represents the reference of the model output. The basecase adopts the central values of the range of uncertain technological and economic parameters, and assumes conservative energy prices and carbon costs. The exogenous variables are predominantly in line with the conservative STEPS-scenario of the IEA (IEA, 2021) and resemble the conservative scenario as discussed in the following section (5.5.2). The results of the basecase analysis are presented and discussed in section ??

#### 5.5.2 Uncertainty analysis setup

Where the real-world behavior of the hydrogen system is very uncertain, the model that resembles the system is also subject to uncertainty. To obtain an understanding of the role of uncertainty in the model behavior and outcomes, an uncertainty analysis is conducted. Uncertainty is considered on two aspects: parametric uncertainty of the model input parameters and constants, and scenario uncertainty, which is caused by the uncertainty in exogenous variables that include future values. Following Kwakkel et al. (2013), the cumulative uncertainty ranges of parametric and scenario uncertainty results in the final scenario space. An uncertainty analysis is not to be confused with a sensitivity analysis. According to Pruyt (2013), an uncertainty analysis is a means to virtually explore plausible real-world effects of assumptions over their plausible uncertainty ranges, while a sensitivity analysis is conducted to explore the sensitivity of a model to small parameter disturbances.

##### 1. Parametric uncertainty

The input parameters are gathered from data in literature. However, literature is not in all cases consistent about technological and economic values resulting in an uncertainty range for some constants. Parametric disalignment in literature appears on the one hand because a number of parameters are collected from research that does not study Germany in particular but have a wider geographical scope, resulting in the inclusion of geographical dimensions in the parameter range. On the other hand because several inputs for this model are assumed constant and independent, whereas in reality this might be a variable fluctuating over time, such as capacity factors or the costs of technologies. To assess the uncertainty range of the model output, the model conducts 10.000 multivariate runs in which random values are picked for each parameters within the limits of the parameter's uncertainty envelope. The experiment is conducted with a random normal distribution. The upper and lower limits are obtained from literature. If literature did not provide a range, a reasonable deemed range is depicted, dependent on the parameter. This analysis results in an uncertainty range the model outcomes in the basecase. The inputs for the parametric uncertainty analysis are per

submodel provided in the tables in appendix E. The outcomes of the analysis are presented in appendix F.

## 2. Scenario uncertainty

To assess the uncertainty envelop created by the exogenous model variables, two scenarios are evaluated. These scenarios represent a disadvantageous hydrogen conservative scenario, and progressive hydrogen supportive scenario, which are further referred to as the conservative and progressive scenario. The scenarios determine the input values for the exogenous variables of the supply chain model, which are the costs for electricity, natural gas, coal and the carbon price from 2020 to 2050. The input values for the two scenarios are extracted from the estimated future costs in the Stated Policies scenario (STEPS) and the Net Zero Emissions scenario (NZE) from the IEA (IEA, 2020). The conservative STEPS scenario resembles the future direction of carbon emissions and energy demand based on the current and announced policies of countries worldwide. This exploratory scenario does not aim for specific abatement goals, but provides a picture of the future based on today’s pathway and results in a fossil based future in 2050. Alternatively, the progressive NZE scenario is a normative scenario that creates a trajectory to limit global temperature rise to 1.5 degrees Celsius. This scenario stools on innovation and energy efficiency, emergence of new technologies and a transformation of the energy sector. It describes the requirements for a limited temperature rise, including the recognition of sustainable hydrogen as imperative element. The model adopts the prices of the scenarios with no ‘strings attached’, leaving other model assumptions of the IEA out of scope. The STEPS-scenario presumes relatively high energy prices and low carbon prices, whereas the NZE scenario forecasts all prices to decrease and carbon prices to increase significantly. Electricity price input is determined with the project size of electrolysis in mind. A 10 MW electrolyzer that is grid connected and has a capacity rate of 90% consumes approximately 80.000 MWh per year. Based on the expected unit size growth of electrolysis plant size (100 MW electrolyzers are not exceptional in the current electrolysis project pipeline of Germany (Radowitz, 2022)), the electricity price range is chosen for large industrial consumers. For Germany, this range above 150 GWh/year (Band IG, (BDEW, 2021; Eurostat, 2021)). In table 4 the values for variables over time in the two scenarios are presented. A visual representation of the variables is presented in appendix D.

Table 4: Scenario inputs for the exogenous variables

<b>Conservative scenario</b>	<b>Unit</b>	<b>2010</b>	<b>2020</b>	<b>2030</b>	<b>2040</b>	<b>2050</b>
Electricity costs (grid)	\$/MWh	98,4	121,4	114,0	123,0	123,0
Natural gas costs	\$/MWh	39,9	28,9	29,2	30,4	31,5
Coal costs	\$/MWh	12,9	7,0	8,2	8,6	9,0
Carbon costs	\$/ton CO2	17,3	30,1	65,0	75,0	90,0
<b>Progressive scenario</b>	<b>Unit</b>	<b>2010</b>	<b>2020</b>	<b>2030</b>	<b>2040</b>	<b>2050</b>
Electricity costs (grid)	\$/MWh	98,4	121,4	54,5	40,0	30,0
Natural gas costs	\$/MWh	39,9	28,9	14,8	14,2	13,7
Coal costs	\$/MWh	12,9	7,0	7,5	6,9	6,3
Carbon costs	\$/ton CO2	17,3	30,1	130,0	205,0	250,0

## 3. Additional uncertainty analyses

The previous experiments cover the uncertainty of parameters and exogenous variables, but it noteworthy to address the impact of three alternative types of uncertainty separately. Therefore, the implications of uncertainty on the model for the three following subjects is analyzed and discussed in more detail:

1. Uncertainty in the CAPEX of electrolyzers
2. Uncertainty in the multinomial logit function parameters
3. Uncertainty in the model structure of investment in new production capacity

The findings of these separate uncertainty analysis are presented in section 6.2.3, 6.2.4, and 6.2.5 respectively.

### 5.5.3 Policy analysis setup

The policies that will be tested in this research are denoted in section 5.1.5. The effects of the different measures on the diffusion of hydrogen will be tested for diverse implementation times and strengths of the policies. In appendix I, the input settings for the tested for policy configurations are displayed. Each policy will be tested in four different configurations, where the strength, or value of the policy and the implementation time are the varying factors. These are denoted as *LowSlow*, *LowFast*, *HighSlow* and *Highfast*. First, each policy is examined individually for all policy settings. This provides insight in the effects of each separate policy on the system and the four KPI's. Second, the different policies are combined for the different configurations to assess the system behavior to the combined policies and moreover the relation between policies. Finally, an assessment is conducted with unconventional policies, which will be combined with the tested conventional policies. This must provide insight in the potential of acceleration and the response of the system to more rigorous policy levers.

## 6 Results

This chapter outlines the outcomes of the model analysis. The steps of the analysis process are outlined in section 5.5. First the outcomes of the basecase are discussed, after which this section presents the results and implications of the uncertainty analysis. Following, the effects of the policies on the system and the KPI's are explained. Finally, the implications of the policy implementation on the diffusion of hydrogen is elaborated on.

### 6.1 Basecase results

The baserun represents a conservative scenario for the exogenous variables, and no policies are functioning. This results in a picture of the expected hydrogen diffusion pathway when no hydrogen policies are active. For hydrogen production capacity and total demand, the basecase outcome is shown in figure 15. The red line shows the expansion of the total demand, whereas the other lines, with the color corresponding to the type of production, show the dynamics of the hydrogen production capacity. What is most striking from this case is that the basecase indicates an increase of hydrogen demand, regardless of the absence of any form of policy support. The initial hydrogen demand of 58 TWh from chemical industry and refineries is relatively stable until 2025, after which starts to expand following an S-shaped pathway towards a demand of approximately 160 TWh in 2050. For comparison; the total natural gas consumption of Germany in 2020 was approximately 840 TWh (BP, 2021). The growth of total hydrogen demand represents the cumulative adoption of FCEV-trucks, HDRI-manufacturing and blended hydrogen into the grid, whereas demand for the chemical sector and refineries is assumed to remain constant. The largest contribution to total demand comes from FCEV-trucks. As depicted in figure 14, the total costs of ownership for FCEV trucks (green line) and Diesel trucks (blue line) converge as a result of technological learning of FCEV trucks, and intersect around 2030 to achieve cost parity. Ultimately, this cost competitiveness results in a market share for FCEV-trucks of 26% in 2050, even without policy stimulation. The increase in market share for FCEV is however relatively moderate due to the even more competitive costs of electric trucks (green line in figure 14, to which also the stagnation of demand growth towards 2050 can be attributed. Demand is furthermore boosted from 2025 through the introduction of HDRI in the steel sector, of

which the investment share converges to the traditional BF-BOF steel production pathway, and blending, that starts on a small scale in 2025. The interestingly increasing demand without policy support can be mainly contributed to two model mechanisms. First, the expected increase in carbon price towards 2050 enlarges the costs of conventional fossil-based technologies and drives investments in hydrogen based steel making (HDRI) and blending

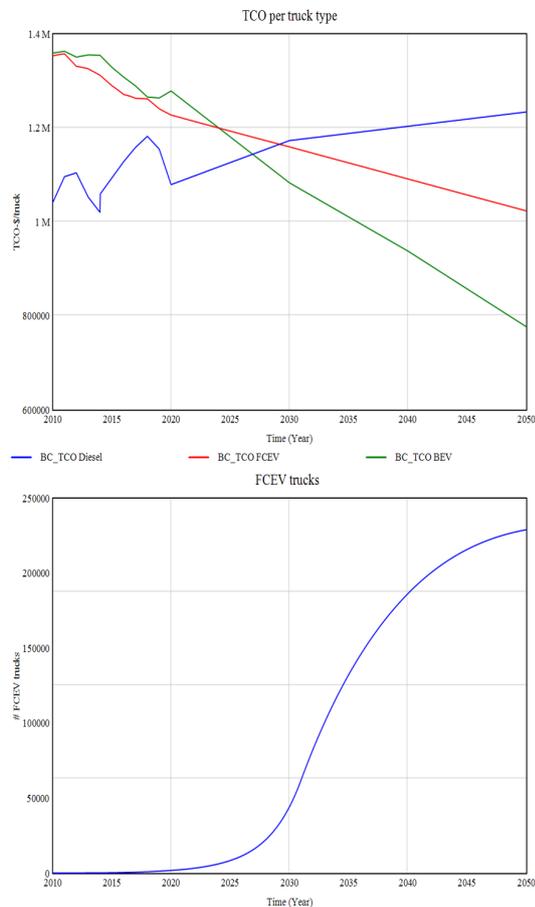


Figure 14: (A) TCO of three modeled types of power-trains for heavy duty trucks: Diesel, electric, fuel cell. (B) Diffusion of FCEV-trucks in the basecase.

hydrogen into the grid. Second, as depicted in figure 14, the total cost of ownership of alternative fuel vehicles is decreasing relative to cost of Diesel-trucks due to expected technological learning, what motivates the deployment of FCEV-trucks. Hydrogen demand in each end-use sector is modeled with the multinomial logit-function. However, the value of the logit parameter is of minor influence here; a range for the logit in transport of -4 to -1 results in a numerical range of total demand of 158-162 TWh in 2050 respectively and shows negligible behavioral variation. Further analysis of the impact of the logit parameters on the model outcome is provided in section 6.2.4. The share of hydrogen demand in the transport sector is high compared to the demand share in steel making and blending not because of the value of the logit parameter, but due to the more rapid diverging cost-gap between Diesel- and FCEV-trucks than the cost competitiveness of hydrogen technologies in the other sectors.

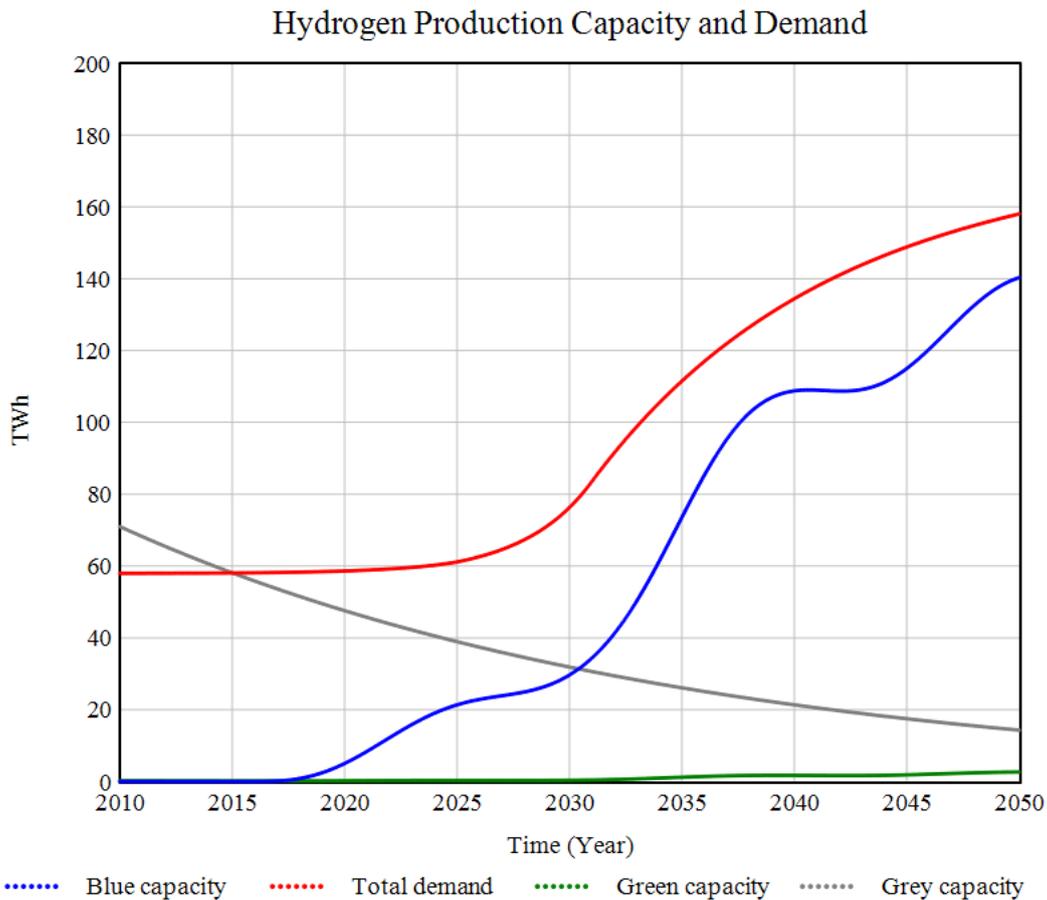


Figure 15: Basecase: Hydrogen production capacity for each type of hydrogen and total demand in TWh

Observation of the production capacity firstly shows the grey line representing the decline of grey hydrogen capacity. Grey hydrogen is not newly installed in the model and decreases as a consequence of depreciation. The decreasing fossil-based hydrogen capacity is primarily replaced by blue hydrogen (blue line). The installation of blue hydrogen capacity is slightly delayed relative to the decline of grey hydrogen, caused by the construction time of the blue hydrogen facilities. Because investments in new production capacity in the model do not incorporate the construction delay of new plants, there is a slight overshoot of investment each time the supply cannot meet demand. Consequently, the supply-demand gap shows oscillating behavior and the diffusion of hydrogen production (blue line in figure 15) displays not a smooth growth pathway. This model behavior and its consequences for the outcomes is further elaborated on in section 6.2.5. What furthermore stands out in the basecase is

the very limited uptake of green hydrogen. The total installed electrolyzers reach an annual output of 2.7 TWh with a capacity of approximately 190 MW in 2050. Whereas the cost of production is the primary driver for investment behaviour in new production capacity, a thriving diffusion of green hydrogen is unattainable for the basecase and demand is primarily met by blue hydrogen. The cost-gap between blue and green hydrogen is too large for green adoption, and remains existent up to 2050. The cost gap fluctuates between approximately 2.5 to 5 \$/kg, what restrains investments in electrolysis. Subsequently, the low adoption of green hydrogen prevents the reduction of the electrolysis costs from learning by-doing in this case: the slightly decreasing capex strands at 660\$/kW in 2050. The low diffusion of electrolysis clearly reflects the current deficient circumstances and absence of driving policies, and results in a flourishing future for low-cost but polluting blue hydrogen production. Now looking at infrastructure in the basecase, it is detected that the infrastructure is increasing caused by the growing hydrogen demand. Infrastructure increases rapidly between 2025 and 2030, leading to completion of the elementary hydrogen transmission grid around 2032. This result is surprising, since literature denotes the absence of hydrogen infrastructures as one of the major barriers to green hydrogen diffusion. In this case, no policies are required to instigate infrastructure development what not mirrors the observations from other studies. Possibly, the design of the model causes this growth to occur and is reflected upon in chapter 8. Finally looking at the carbon intensity of hydrogen in the basecase it is seen that this reduces strongly, from 11.0 kgCO<sub>2</sub>/kgH<sub>2</sub> in 2010 to approximately 2 kgCO<sub>2</sub>/kgH<sub>2</sub> in 2050. This is a result of the shift away from polluting grey hydrogen production to carbon capture and storage for blue hydrogen. Consequently, the total annual direct emissions from hydrogen production reduce from 24 Mtons/year to 9.5 Mtons/year. Even with the of the increase in demand and production capacity. Considering this footprint reduction in the perspective of the total annual carbon emission abatement, including the emission reduction in end-use sectors as a result of hydrogen adoption, the abated emissions per year increase to 54 Mtons/year in 2050 with respect to 2010 hydrogen emissions. This is approximately 7.1% of total CO<sub>2</sub> emissions in Germany in 2010. The cumulative amount of total abated carbon emissions increase up to 882 Mtons in 2050 relative to 2010. Policy costs are not relevant for the basecase since no policies are active.

The basecase represents the development of the hydrogen sector without policies, conservative energy prices and an increasing cost of carbon. Regardless of the conservative environment, hydrogen demand increases slightly and subsequently the hydrogen supply of blue hydrogen production takes-off. Green hydrogen is not a factor of play in this case. The basecase illustrates to some extent the presence of the barriers to diffusion found from literature and described in section 2: (1) High costs of green hydrogen averts electrolyzer installation and push the required production towards blue hydrogen. (2) Infrastructure absence is initially reducing the deployment in the transport sector but is as described not a dominant barrier in the basecase outcomes. (3) Lack of hydrogen demand is also not a barrier of significant presence, since demand is nevertheless growing because of the increasing carbon price. (4) Finally the lack of policies can be considered a present barrier in the basecase outcomes, since the diffusion of green hydrogen clearly will not take place without policy interventions. Considering the green hydrogen targets of Germany, these are not closely met under the circumstances of the basecase. Electrolyzer capacity in 2030 and 2040 reaches 33 MW and 176 MW respectively, while the targets for electrolysis in the German hydrogen strategy are 5 GW and 10 GW for these years. The findings of the basecase substantiate the necessity of accelerating the green hydrogen transition with policy measures to reach the German green hydrogen targets.

## 6.2 Uncertainty analysis results

System Dynamics modeling comprises the complexity of the system and enables the generation of plausible future scenarios (Eker & van Daalen, 2015). However, the future of hydrogen is intrinsically uncertain, suggesting that the abstraction of the hydrogen system incorporates uncertainty as well. Uncertainty in model outcomes is a consequence of uncertainty about the exogenous variables such as future gas costs, and the model input parameters such as capital costs of electrolyzers. An uncertainty analysis is not a sensitivity analysis, since the outcome of sensitivity provides insight in the weight of parameters on the model outcome, while the uncertainty analysis provides insight in the possible range of outcomes as an effect of uncertainty in the parameters. This section elaborates on the consequences of these types of uncertainties in the model. First, the uncertainty in exogenous variables is assessed through the design of two outlying scenarios for energy and carbon prices. Second, the parametric uncertainty is tested through manually assessing the uncertainty range of key input parameters and the combined effects of these ranges on the model outcomes (Kwakkel & Pruyt, 2013). Furthermore, this section explores the implications of uncertainties in the model that might influence final outcomes, such as the electrolyzer capex, logit parameters and investment behavior structure.

### 6.2.1 Scenario uncertainty

For the scenario analysis, the exogenous variables that are used as input for the energy costs and carbon costs are varied. The future expected costs for electricity, natural gas, coal and carbon are derived from the STEPS- and NZE-scenarios of the IEA. The input values for the exogenous variables for 2010 and 2050 are provided in section 5.5 and table ???. Similar to the basecase, policies are not active in this analysis. The goal of the scenario analysis is to compare two possible versions of the future and create some insight about how the hydrogen supply chain might develop in the coming decades under different circumstances.

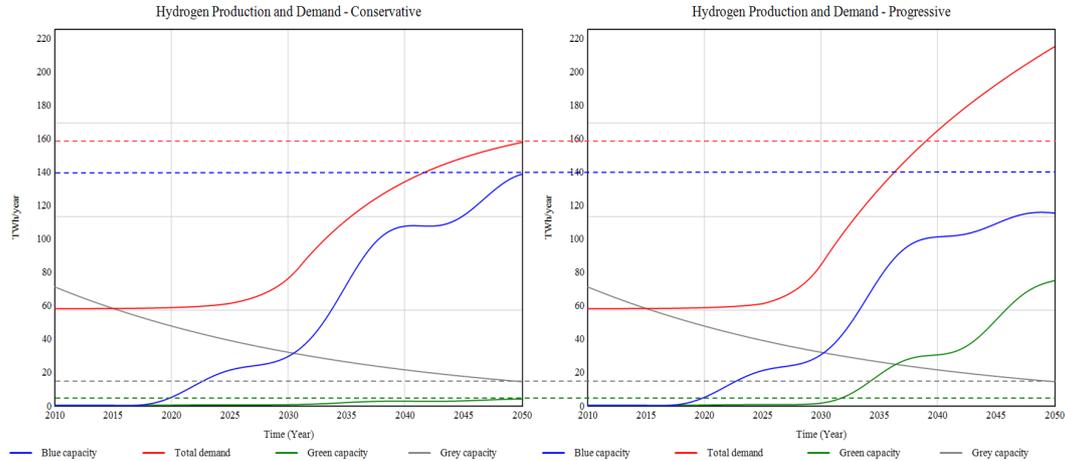


Figure 16: Hydrogen production capacity for each type of hydrogen and total demand in TWh, for the conservative (left) and progressive (right) scenario

The divergence of the energy and fossil prices for the two scenarios show significant impact on the KPI's . Figure 16 shows the comparison of the conservative and the progressive scenario in the left and right figure for the annual production and total demand. The dotted line marks the 2050 output for the conservative scenario to compare with the progressive output. Looking at the production of green hydrogen production from electrolysis, the progressive scenario demonstrates a significant difference in electrolysis capacity installation compared to the conservative case. The electrolyzer capacity in 2050 reaches roughly 5.3 GW in the progressive scenario compared to 190 MW in the conservative scenario, equal to an annual output difference of 72 TWh. Because the electricity prices are expected to decline rapidly between 2020 and 2030 in the progressive scenario, the cost gap between green and blue

hydrogen is converging. The levelized cost of green hydrogen rapidly decreases from a price around 7 \$/kg between 2010 and 2020 to roughly 4 \$/kg in 2030 due to the decreasing electricity costs. The decreasing electricity costs therefore cause an increase in investments in electrolysis. At the same time, the increasing investments amplify the price reduction of green hydrogen through the inducement of the learning-by-doing mechanism that reduces electrolyzer capital costs. To elucidate this process behind the growth of electrolysis capacity in the progressive case versus the low growth in the conservative case, figure 17 displays each important step in this causal loop. When considering the progressive case, depicted by the red line in each figure, the expected decrease of the electricity price (a), results in a closing cost gap between green and blue hydrogen with a cost parity achieved around 2032 (b). Due to the increasing cost-competitiveness of green hydrogen, investments in green hydrogen production grow through which the cumulative installed capacity of electrolyzers increases. This instigates learning-by-doing and lowers the capex of electrolyzers (c). The combination of decreasing electricity price and the amplifying effect of learning-by-doing lowers the levelized cost of green hydrogen in 2050 towards 2 \$/kg in the progressive scenario (d).

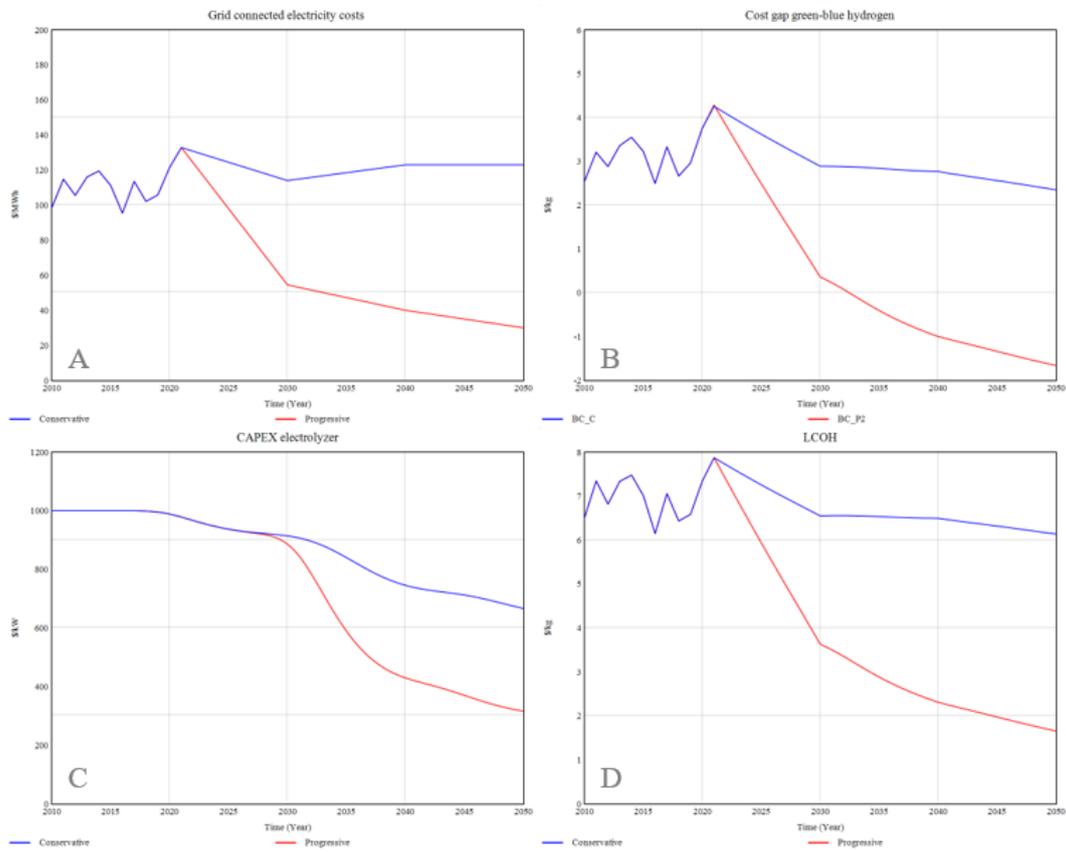


Figure 17: Causal process of the dynamics of green hydrogen costs in both scenarios. (a) Electricity price, (b) Cost gap between blue and green hydrogen, (c) Capital costs of alkaline electrolyzers, (d) Levelized cost of green hydrogen

The expected declining electricity costs and reinforcing mechanism of technological learning are the main drivers of the installation of electrolyzers in the progressive scenario. The share of green hydrogen of the total production for the two scenarios in 2050 range from 2% to 37%. Interestingly, the capacity of blue hydrogen does not differ substantially in both scenarios. As seen in figure 16, from 2040 a stagnation of installation of blue capacity is detected in the progressive scenario as a result of the achieved cost parity between green and blue hydrogen. Nevertheless, blue hydrogen production in both scenarios remains the dominant method of

production. Apparently the high capture rates for CCS, 90% for CG and 95% for SMR, prevent a price increase of blue hydrogen triggered by the strongly increasing carbon cost in the progressive scenario.

The final total demand in the scenarios range between 158 TWh and 216 TWh, but follows the same growth trajectory that initiates in the late half of the 2020's. When the demand growth is examined in more detail, it becomes apparent that the adoption of FCEV-trucks is nearly similar for both scenarios. The infrastructure installation which affects the purchasing of FCEV-trucks takes place in both scenarios, only slightly later in the conservative scenario. The pipeline capacity for unconstrained development of FCEV-transport is reached in 2031 and 2033, leading to a similar FCEV-truck adoption in both scenarios. In contrast to transport, the installation of HDRI-produced steel grows strongly in the progressive scenario leading to a demand of 67 TWh per year in 2050, relative to 15 TWh in 2050 for the conservative scenario. For comparison, the annual total energy consumption in the German steel making sector was 189 TWh in 2020 (IEA, 2021).

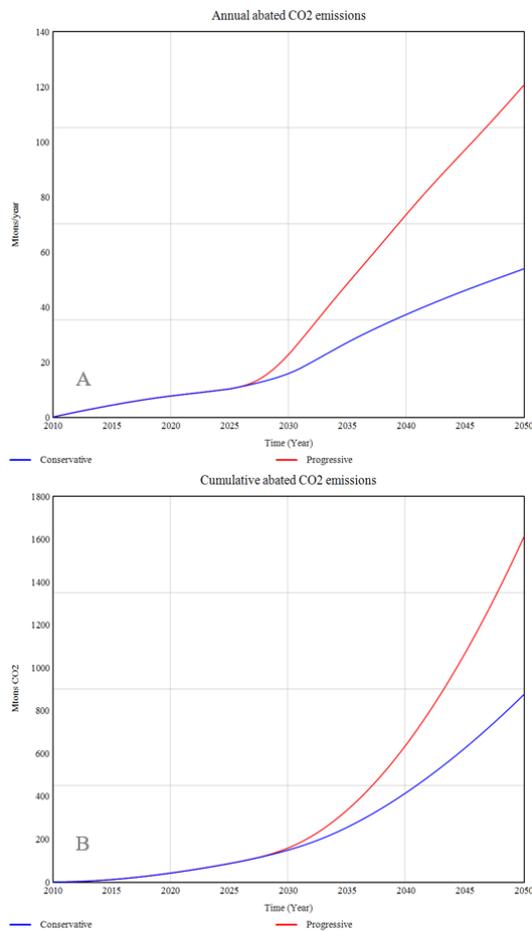


Figure 18: (a) Annual abated carbon emissions compared to 2010 in the conservative (blue) and the progressive scenario (red), (b) Cumulative emission reduction relative to 2010 emissions

The green-steel uptake can be clarified by the sensitivity of traditional steel manufacturing costs to the price of carbon. With a carbon price of 90 \$/tonCO<sub>2</sub> from the conservative scenario, carbon costs contribute for 32% to the total costs of steel. In the progressive scenario, the carbon price increases to 250 \$/tonCO<sub>2</sub> in 2050, resulting in a carbon cost share of 58%. The costs of BF-BOF steel in the progressive case increases, whereas HDRI-steel becomes more affordable, pushing steel manufacturers to invest in HDRI-steel making. Hydrogen consumption for blending into the grid remains similar in both scenarios, as natural gas remains relatively cost competitive with hydrogen in the progressive scenario. In figure 18, the annual abated carbon emissions compared to 2010 emissions (a) and the total cumulative abated carbon emissions compared to 2010 emissions (b) are displayed. The emission reduction in the conservative scenario is a result of the shift from polluting grey to blue hydrogen and slightly from the adoption of FCEV-trucks. In the progressive case, the annual abatement curve (a) shows a vast increase between 2025 and 2030. This large increase follows the transition in the steel sector, where the decarbonisation with green hydrogen results in large abatement of polluting coal emissions. The annual emission reductions reach maximums of 53 and 120 Mtons per year in 2050, resulting in cumulative CO<sub>2</sub> emission abatement in the conservative and progressive scenario of 870 and 1610 Mtons between 2010 and 2050 respectively.

### Insights from the scenario analysis

In the scenario analysis, the upper and lower ranges of possible future values of energy and carbon prices and the development of green hydrogen without policy measures have been

assessed. The organic or spontaneous expansion of green hydrogen can reach a maximum market size of 5.3 GW with a share of 37% of total hydrogen production under the most advantageous circumstances in 2050. However, the installed electrolysis capacities for 2030 and 2040 in the progressive scenario are 0.08 GW and 2.1 GW respectively. This rate of green hydrogen deployment is not even close to meeting Germany's green hydrogen production targets of 10 GW installed electrolyzer capacity in 2040. Even in the best scenario, the green hydrogen deployment initiates in 2030, which is too late to kick-start learning-by-doing and price reductions, resulting in a lag of green hydrogen that is not recovered in the first half of this century. Considering the barriers of diffusion as discussed in the basecase analysis, their presence is reflected similarly to some extent in the output of both scenarios.

Firstly, the cost gap between green and blue hydrogen is apparent in both cases. Blue and green hydrogen prices converge in the progressive scenario between 2020 and 2030, though this is too late for a serious market growth and naturally initiated price reduction. Second, demand is taking-off in each scenario regardless of policies. The increase of carbon costs is the largest incentive for end-users to adopt hydrogen technologies, however this occurs considerably late with a peak growth rate in late 2030's and predominantly in steel industry. FCEV adoption is taking off regardless of the external circumstances as a result of the decreasing costs for FCEV-trucks compared to Diesel trucks. An earlier demand uptake would prompt an accelerated increase of production capacity, although because of the lagging cost both scenarios this would imply an uptake of blue hydrogen. Third, an absent infrastructure is not severely resembled in the scenarios. The construction of infrastructure in the model anticipates considerably fast to an uptake in demand. This makes infrastructure only a constraining factor for transport for a limited period. Nevertheless, this implies that a faster demand uptake is self-reinforcing through an acceleration of infrastructure roll-out. Finally, in both scenarios the required role of policies has become apparent. If the system is left intervened, green hydrogen deploys too late, and too little. Blue hydrogen shifts from a transition- to an incumbent technology and determines the future of hydrogen, even in the most advantageous exogenous circumstances for green hydrogen. It has furthermore become apparent from the scenario analysis that to prevent the lock-in of blue hydrogen, it is crucial that cost-competitiveness between green and blue hydrogen must be achieved before large-scale demand growth for hydrogen starts to take-off. To summarize the findings of the scenario analysis:

- The scenario uncertainty range without policies for green hydrogen production capacity lies between 190 - 5300 MW.
- The expected rise of carbon price in the progressive scenario has minor effect on the deployment of electrolysis, since CCS rates for blue hydrogen are high and blue hydrogen costs remain low.
- Capital costs of electrolyzers decreases too late in the conservative scenario to display a strong cost-reducing effect in time.
- Carbon price increase has only effect major effects in the steel sector, pushing hydrogen demand for HDRI.
- Low electricity prices prompt the uptake of green hydrogen from 2030 in the progressive scenario.
- Even in the progressive scenario, hydrogen targets are far out of reach without interventions and blue hydrogen becomes the dominant hydrogen production method.

### 6.2.2 Parametric uncertainty

Parametric uncertainty is defined as the range of uncertainty in the KPI's as a result of the combined uncertainty ranges of input parameters. The parameters included in this analysis are listed in appendix E. The parametric uncertainty is examined for both scenarios, resulting in the cumulative range of parametric and scenario uncertainty. The parametric uncertainty results for the 95% interval range for 2050 a number of model output amongst which the

KPI's is denoted in table 5. The upper and lower limit values show the possible range for the output parameters as a consequence of the uncertainty in the input parameters and the uncertainty in the exogenous variables combined. Further visualizations in addition to the numerical outcomes in table 5 are provided in appendix F.

Table 5: Upper and lower range of the uncertainty analysis outcome from the two scenarios

Model outputs	Unit	Lower limit 2050	Upper limit 2050	Uncertainty space
Electrolysis capacity	MW	55	5854	4799
Carbon intensity green hydrogen	kgCO2/kgH2	1.4	2.0	0.6
Share of green hydrogen	%	0.7	32.2	31.5
Total demand	TWh	134	243	109
Annual abated carbon emissions	Mtons/year	23	147	124
Cumulative abated carbon emissions	Mtons	296	2194	1898

### 6.2.3 Uncertainty of CAPEX of alkaline electrolyzers

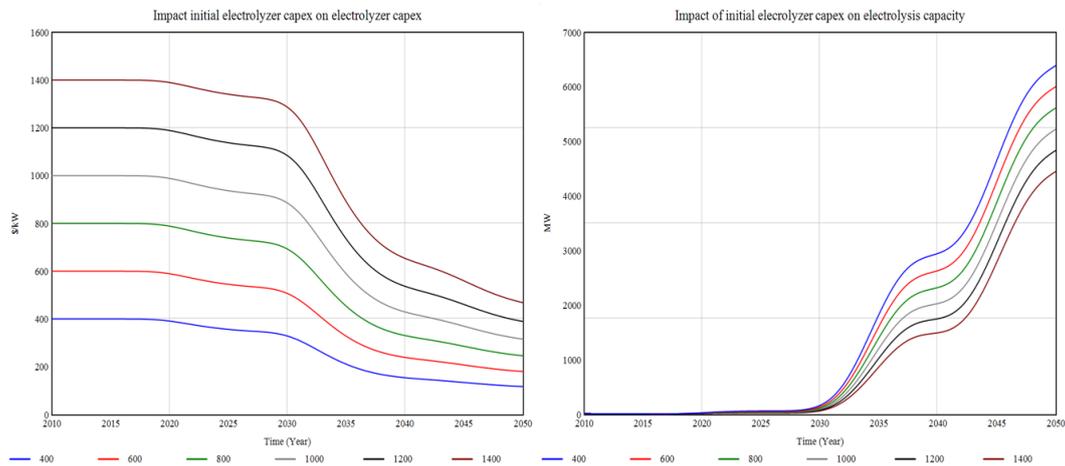


Figure 19: Effect of parametric uncertainty of the initial capital costs of electrolyzers on the variable capex and electrolysis capacity

The initial capital cost of alkaline electrolyzers is an important but uncertain parameter. The capital costs contribute for approximately 7 to 10% to the final levelized costs of green hydrogen, dependent on the electricity costs. This paragraph discusses the range of uncertainty and the impact of the capital cost uncertainty range on the model output. In literature, a diverse range of capital costs per unit of production for observed historical and current capital costs, as well as for expected future costs for 2030 and beyond can be found. In table 19 in appendix G, an overview of different capital cost estimations from literature is given. The publishing year is of relevance in this overview, since this reveals if a value is a calculated estimation, or if it is empirically defined. For the model, the capital costs of 2010 define the initial modeling costs and are of most relevance. Smolinka et al.(2015) define capex values for 2010 in a range of 900-3000\$/kW. More recent, Proost (2019) defines a more narrow range for 2010 of 500-1500\$/kW. For 2020, the observed values from literature issued in 2020 or later reaches from 900 - 1400 \$/kW, after which the estimation range for 2030 expands to approximately 115-1600 \$/kW and for 2050 80-800 \$/kW (115-1000 \$/kW and 80-511 \$/kW respectively without the high outliers of (Cihlar et al., 2020)). The divergence in capital costs of the empirical defined values is due to different assumptions about the system configuration (the inclusion of plant components such as solely the electrolyser stack

or the entire system) and differences in plant size, since a larger unit size reduces capital costs (Böhm et al., 2020; Cihlar et al., 2020).

The sensitivity of the model to the initial capital costs has already been included in the sensitivity analysis in chapter 5.4. Electrolysis capacity in the basecase showed a sensitivity range of approximately 320 to 380 MW for an initial capital cost input range of  $\pm 10\%$  around 1000 \$/kW. Because of the parametric uncertainty of the initial value, the impact of the capital costs is investigated in further detail. In figure 19 the input range of the initial capex in 2010 is varied from 400 to 1400\$/kW, applied to the progressive scenario. The learning-by-doing mechanism is clearly present in this scenario, starting after 2030. Interestingly, the diverse capital costs of the electrolyzer converge over time to reach a final cost range of 118-471 \$/kW in 2050. The convergence can be attributed to the non-linearity of the learning-by-doing function, which shows correlation between the severity of the price reduction and the height of the initial costs. When contemplating on this cost range for 2050 with regards to literature, it lies between the expected range for 2050 of 80-511 \$/kW from observed studies. The effects of the initial capex uncertainty on the electrolysis capacity are displayed in the right figure of 19. The input uncertainty of the capex leads to a range of 4.4 and 6.3 GW for 2050, which is a significant difference. Not only suggest these outcomes that due to parametric uncertainty the results of the model must be interpreted with caution, it also indicates the importance of choosing the correct input value for this specific parameter (In chapter 8, a further reflection on model limitations and uncertainty is given). As denoted earlier in the model formulation in chapter 5.2.2 the input value for the initial capex in the model is set at 1000\$/kW, which is within the limits for 2010 according to literature and is an acceptable value, also corroborating with literature, for the capital costs in 2020.

#### 6.2.4 Uncertainty of logit parameters

As described in the section model conceptualization (section 5.1), one of the major drivers in the model is the cost of hydrogen production. With the multinomial logit function,

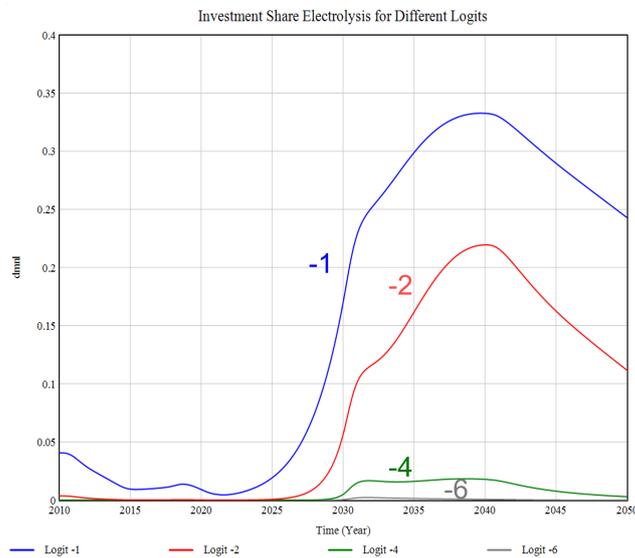


Figure 20: Effects of the value for the logit parameter on the investment share of water electrolysis. The reference value adopted in the model is -1.

For context, the cost gap between hydrogen from electrolysis and SMR-hydrogen at the bottom of the increasing slope of the investment share entails 98 percents in 2030, or a 29% price difference. For the lowest logit-values, -4 and -6, a minimal response is detected. The higher logit parameters -2 and -1 reveal more investment enthusiasm for green hydrogen, although the cost gap is existent.

introduced in section 5.2.3, the relative price differences of hydrogen are converted into investments in new hydrogen production capacity. As the sensitivity analysis demonstrated, the model shows significant numerical sensitivity to the value of the logit parameters. To zoom in on the impact of this parameter and discuss the chosen value for the model, the direct consequence of the logit parameter on the model behavior is tested. The effects of the logit parameter on the investment behavior are illustrated with the graph in figure 20. The graph shows the investment share in water electrolysis for a range between -6 and -1. The logit is examined for the progressive scenario. The figure reveals high discrepancy between the investment shares. For context, the cost gap between hydrogen from electrolysis and SMR-hydrogen at the bottom of the increasing slope of the investment share entails 98 percents in 2030, or a 29% price difference. For the lowest logit-values, -4 and -6, a minimal response is detected. The higher logit parameters -2 and -1 reveal more investment enthusiasm for green hydrogen, although the cost gap is existent.

The only decision criterion that the logit parameter represents is the relative cost or return of the investment, expressed in monetary value. The logit itself does not account for other drivers for decision investment, although there are countless. The modeler includes the weight of these alternative decision criteria such as sustainability, social acceptance and technological feasibility, into the multinomial logit function through the value of the logit parameter. A low logit resembles a very elastic market that adapts very quickly to price fluctuations and has high probability of choosing the lowest price. This results in a 'winner-takes all' market, where a minor cost margin or profit diminishes the competition fiercely. A slightly more moderate market in which a fraction of the investors are not solely cost-driven but include wider pallet of incentives to their investment decisions, results in more balanced investment shares. These investment oddities are reflected with higher logit parameters. According to van Vuuren (2007), who applies the multinomial logit function in energy systems modeling, the value of the logit can be determined by calibrating the formula against historically observed price fluctuations. Nevertheless, he states that its value remains somewhat arbitrary. Because of the absence of useful historical price data in the hydrogen sector the logit is arbitrary determined based on corroboration of model behavior with historical real-world behavior. The logit parameter value of -1 is depicted for three reasons. First, when looking at the historical investment pattern for electrolyzers since 2010 it is apparent that there have always been investments in electrolyzers, contributing to a minor share in hydrogen production. With a logit below -1, the investments in electrolysis are zero before 2025, what conflicts with the real-world behavior. Second, the hydrogen market in Germany is not a 'winner-takes all' market. Although the energy sector is profit driven and margins can be thin, the sector is at the same subject to the motion of sustainability. This implies that companies and investors increasingly incorporate sustainability in decision making, with or without external pressure from stakeholders or government regulations. Because this tendency is assumed to enhance up to 2050, a moderate logit parameter is depicted for the hydrogen sector. Third, the logit is a fixed constant in the model. Considering the previous argument of increasing sustainable awareness and broader value-driven investment decision making up to 2050, the logit of -1 might be a bit too optimistic in the early decades, but represents the tendency to adopt sustainable energy technologies in the later decades of the model timeline.

### 6.2.5 Oscillating investment behavior

As detected in the outcomes of the basecase and the scenario analysis, the diffusion curve of electrolysis demonstrates a rather irregular diffusion pathway instead of the expected smooth S-shaped curve. This results in intermittent growth with high growth rates around 2035 and 2045, but a stagnation of growth around 2040 and 2050 (as can be seen in clearly in the green line in the right graph of figure 16). This section reflects on the cause of this particular model behavior, possible solutions, and the implications for the model results.

The irregular diffusion behavior can be attributed to the model structure and can be considered a System Dynamics model artefact in the supply-submodel. The oscillating behavior of diffusion is typical in supply-chain modeling. According to Sterman (2000), supply chains are prone to oscillation because of time delays which cause production to chronically overshoot an undershoot the appropriate levels. The amplitude of the wavering supply or production is substantially larger than in demand, because of the time delay or phase lag between demand fluctuation and the reaction of production up- or downscaling. If this phenomena occurs in a supply chain with multiple links, the amplitude increases for each supplier in the chain because of inaccurate demand forecast and the phase lag in each supply chain link. Over time, this results in an increasingly distortion of the supply-demand balance along each step the supply chain. This phenomena is described by Forrester (1997) as the bullwhip-effect and is detected in various industries.

In the hydrogen supply chain model, this bullwhip effect is to a certain extend detected in the investment in new production capacity. The hydrogen supply in the model consists of two links, first investors respond to demand shortage, second plant constructors respond

to investors. As described in the model conceptualization in section 5.1, the investment in new capacity is triggered when the difference between hydrogen demand and supply is below zero. This supply-demand cost gaps indicates that new capacity is required to meet demand. When there is a shortage of supply in timestep  $t$  (length of approximately 11 days), there immediately follows an investment in new supply in timestep  $t+1$ . However, because of a delay time in construction for new hydrogen production plants, the supply-demand gap is not closed instantly. This has two consequences: first, the construction delay causes a shortage in supply as long as the new production plants are not finished. Second, as long as hydrogen demand grows without the finishing of new production capacity, new investments continue being activated. These two phenomena initially leads to a short scarcity in supply and eventually to an overshoot in supply installation. This shortage and overshoot mechanism repeats and leads to oscillating behavior of the supply-demand gap and consequently causes the irregularity in the deployment of electrolysis. After the periodical shortage, new capacity is sufficient to meet demand, but supply meets demand investments stop and the shortage starts to increase again. Because of the continuous characteristic of System Dynamics combined with the reinforcing feedback loop in this structure, the effects of oscillation on the system behavior are amplified over time. In appendix H, the behavior of the demand and supply curves further illustrated.

According to Sterman, the predominant cause of oscillation is the failure of managers or policymakers to understand the role of time delays and the impossibility of accurately predicting future demand, which he refers to as bounded rationality (Sterman, 2000). In System Dynamics modeling, there are several methods to respond to this phenomena. For exploration and insight in the implications of the oscillations on the model outcomes, three possible methods to counterbalance the irregular diffusion behavior were tested.

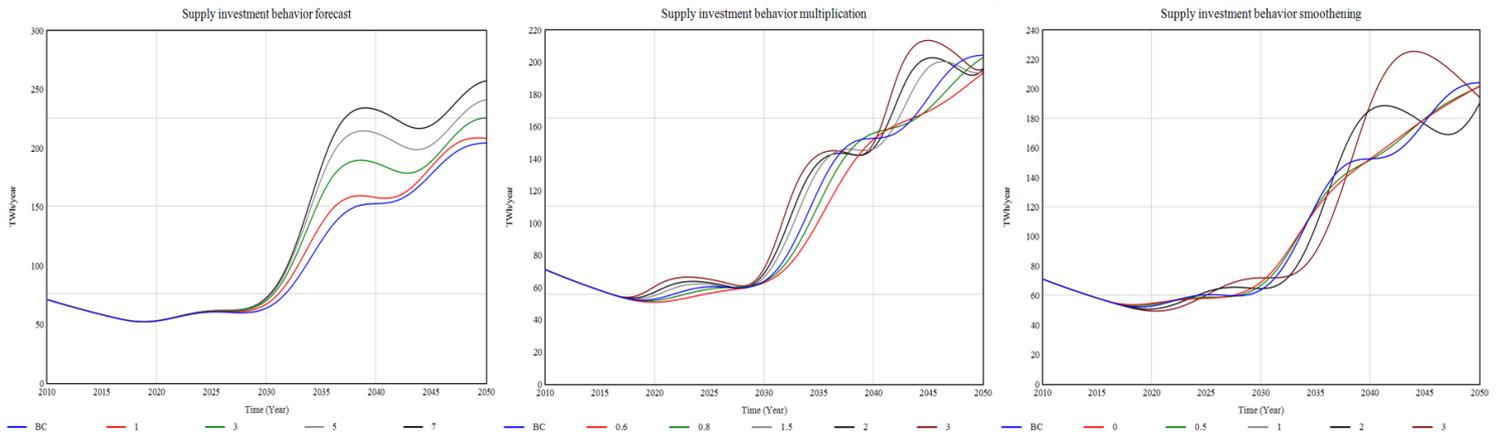


Figure 21: Three methods for counterbalancing the supply oscillation. (a) through forecasting demand. (b) through increasing investment quantity. (c) through adjusting investment delay.

First, a forecast function is introduced to incorporate future demand in the investment decisions. This option is suggested by Sterman in Business Dynamics(p.670) (Sterman, 2000). A forecast function represents the behavior of decision makers to extrapolate recent trends in demand in attempt to foresee supply shortages or demand increases and compensate for supply delays. In the model, this is incorporated with a forecast function between demand and the supply-demand gap. The demand is forecasted based on simple linear extrapolation with various forecast windows. This way, the supply demand gap is expected to increase before the actual demand increases, shifting investments in supply in advance of the demand growth. The delay time of construction for new production capacity is three years. In the left graph of figure 21, the diffusion behavior of electrolyzers for different demand forecast times is shown. It is apparent that increasing the time results in a larger overshoot of installation; compared to the basecase in the blue line, each variation is far

above. One reason for the amplified overshoot is the mechanism of the forecast function. Linear forecasting responds very poorly to sudden discrepancies in historical data. Because of this, the forecasts function response to the increasing growth rate of demand around 2030 is inaccurate and too heavy. For longer forecast windows (up to 7 years), this effect is magnified because of the continuous growth of demand. As a result of the unpredictable nature of demand growth, the forecast function is not an appropriate method to encounter the oscillating supply chain.

The second method that was tested is the adjustment of the installed quantity compared to the required demand. In the basecase, 1 unit of demand triggers the installation of 1 unit of supply. However, when alternating this equilibrium the amplitude of the oscillations might reduce. In the middle graph in figure 21, the effects of different investment quantities are displayed. The blue line indicates the basecase, where supply equals demand. When the investment is diminished with a factor 0.6 (red line), it is clear that the over- and undershoot reduces. Alternatively, when the installation is multiplied by a factor larger than 1 compared to required demand, the oscillations increase. Lowering the investment results in a more balanced behavior, but similarly in a consequent shortage of supply, that ultimately would end in an equilibrium with a large shortage of supply. Alternatively, the multiplication of investments leads to a consequent overshoot in supply, magnifying the bullwhip effect through increasing over-and undershoot without considering the phase lag. The visualization of the oscillation of the supply-demand gap is displayed in appendix 21. The outcomes of this test suggest that adjusting the supply-demand balance is in this case not a suitable method to counterbalance the oscillating behavior, since the basecase finds equilibrium between extreme oscillations and continuous shortage of supply.

As third method, the model the investment oscillations could be flattened with a third order delay. The basecase already incorporates a third order information delay of 1 year between the increase of demand and the investment response. By changing this delay, the phase lag between demand and supply is altered. In the right graph in figure 21, the outcomes of this experiment are displayed. It is apparent that reducing the delay time (red and green line), leads to a flattening of the oscillation, and vice versa, increasing the delay time significantly increases the overshoot. It can be concluded from this test that reducing or eliminating delay time results in a reduction of the supply chain fluctuation.

The findings of this short analysis provide insight in the effects and implications of the model structure on the final outcomes. The test outcomes in figure 21 confirm that artificially adjusting the behavior has its limitations. The first two methods result in amplified overshoots or continuous supply shortage. The third method reveals promising dampening effects, but one can argue that eliminating the delay time in the supply chain does not mirror the laws of real-world behavior and is therefore not suitable. Considering the implications of the model oscillation on the model outcomes can be done twofold. On the one hand, from a System Dynamics perspective, the oscillating behavior is interesting and useful because it strongly reveals the dynamics of the model and the effects of the model decisions on the model outcomes. It is an undeniable characteristic of supply-chain modeling. On the other hand, from an energy model perspective, the model-caused behavior increases uncertainty for interpretation. This oscillating model behavior might not correspond with the expected diffusion behavior, but at the same time cannot be artificially erased to smooth model outcomes considering the findings of Forrester (1997) and Sterman (2000) that oscillation, amplification and phase lag are three features that are pervasive in supply chains. Combining both perspectives, it can be suggested that the oscillating behavior is a feature of System Dynamics modeling, and that the behavior might not be uncommon for real-world supply chains, leaving room for interpretation of the modeling results regarding with this knowledge in mind.

### 6.3 Policy analysis

This section describes the effects of the policy interventions on the system for the conservative and the progressive scenario. First, the quantitative and behavioral influence of each policy on the system is explained. Second, the results for different policy configurations are presented for each key performance indicator. Third, more unconventional policies are tested. Finally, this section elaborates on the effects of combined policies and reflects on the policies with regards to the system drivers and barriers.

#### 6.3.1 Electricity tax discount

The tax exemption for electricity that is consumed for electrolysis is analysed for the two scenarios and four policy scenarios. The direct effects of this policy are best observed through the cost gap between green and blue hydrogen, since the policy dampens the production costs and increases cost-competitiveness of green hydrogen. This policy effect is shown for the progressive scenario in in the left graph of figure 22. In the *high fast* setting in the progressive scenario, cost parity will be achieved around 2026, compared to cost parity that is reached around 2033 in the progressive scenario without policies. In the conservative scenario, pushing this policy to its limits does not close the cost-gap, although a minimum price difference of 0.96 \$/kg is reached in 2032 in the *high-fast* setting (not visible in the graph). Interestingly, the temporary price reduction through the policy does not echo through the cost gap when the policy finishes after the ten-year period. For each scenario and each policy setting, the green hydrogen price recovers to its old cost pathway, revealing only slight deviation from the basecase costs. The minor after-effects in the price reveal a limited reinforcing effect of this policy over time, leading to only temporary benefits in cost reduction.

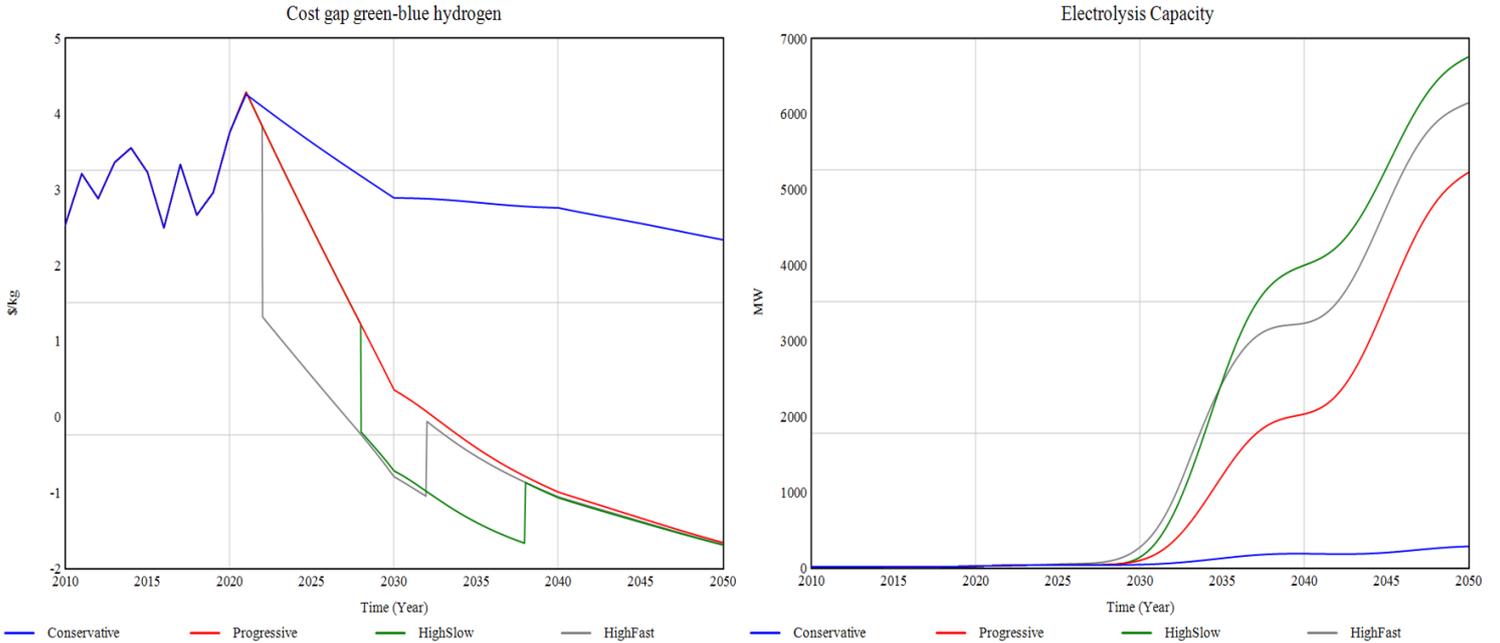


Figure 22: (a) Cost-gap between green and blue hydrogen temporarily decreases through the tax discount policy (green and grey line). (b) Electrolyzer capacity for the two scenarios under different timing of the tax discount policy

From the system point of view, the policy has most leverage on the supply side of the system, therefore the policy effect is assessed through looking at the electrolyzer capacity. The electrolyzer capacity under the *HighFast* and *HighSlow* policy settings for the progressive scenario is displayed in the right in figure 22. The green line, indicating the late policy start in 2028, lifts the electrolyzer capacity in 2050 to roughly 6.8 GW, which is an addition of 1.5 GW to the non-policy case. What strikes from the graph is the effect of the timing of the

policy implementation. Implementing the electricity tax discount from 2028-2038 (green line in both graphs of figure 22) surprisingly results in a higher final uptake than an earlier active policy period of 2022-2032 (grey line in both graphs) for both scenarios. This behavior can be clarified by looking at the cost gap of green and blue hydrogen again in figure 22. The relative costs of green hydrogen in both scenarios decreases rapidly between 2025 and 2030, after which cost parity is achieved and the price reduction rate starts to moderate. When the electricity tax discount is implemented in the early case, the policy has only a small period, approximately 2031-2033, in which green hydrogen is cheaper than blue hydrogen. By contrast, when the tax discount starts late, it magnifies the already growing cost gap even further compared to the early policy implementation, lowering the levelized cost of green hydrogen to 1.6 \$/kg in 2038. Consequently, the late policy amplifies the natural cost decline, what results in a burst in the green hydrogen investment share of green hydrogen between 2030 and 2040.

The electrolyzer tax discount has demonstrated to be a powerful lever on the supply side of the system. The effects on the demand side are negligible, with an uptake of 3 TWh in 2050 for the most supporting setting. The price reduction of green hydrogen finds very small (0.04% increase for FCEV-trucks) and temporary resonance in the market share of hydrogen technologies for the demand side. The limited effect on the demand of hydrogen also explains the negligible contribution to carbon emission-reduction of this policy. The share of green hydrogen in total hydrogen production increases, but the total hydrogen production remains almost constant because of minimal demand growth. Because the electrolyzers are grid connected, its carbon-footprint is close to blue hydrogen, what causes the emissions reduction in the end-use sectors and the emissions from hydrogen production to remain almost constant. Finally, the amplification of electrolyzer capacity comes at a cost. The costs for the most effective, slow policy in the progressive scenario reaches a maximum rate in 2038 to roughly 530 M \$/year, resulting in a cumulative cost of 2.2 B \$ after 10 years of the policy lifetime. The figures for demand, emission abatement and policy costs are displayed in appendix K.1.

### 6.3.2 Electrolyzer subsidy

The influence of the subsidy for electrolyzers is shown in figure 23. The output of the capex for the electrolyzer is displayed in the left graph for the *HighFast* and *HighSlow* policy settings in the progressive scenario in grey and green respectively. The output of the electrolyzer capacity for these policy settings is shown in the right graph with corresponding colors. The mechanism of this policy is similar to the electricity tax reduction, for the reason that they both suppress the levelized cost of green hydrogen in some way. The direct effects of the policy are depicted in the left graph of figure 23. When these results are observed, a comparable effect is detected as for the tax discount policy, however less strong in this case. Firstly, the fierce rebound of the capex after the subsidy ends also strikes out here, indicating limited resonance of the subsidy into the rest of the system. Apparently the cumulative electrolyzer installation during the subsidy period is not sufficient to significantly boost technological learning and show a cost reduction in the electrolyzer capex after the subsidy period ends. Secondly, the price temporarily drops, what results in an expected but limited uptake of electrolyzer capacity. In the best policy setting for the progressive scenario, the capacity grows from 3200 MW to 3620 MW. Furthermore likewise to the tax discount policy, the late implementation of the subsidy results in a stronger diffusion of electrolysis on the long term, caused by the similar price reducing phenomena as described in the previous section (6.3.1).

The growth of demand as an outcome of this subsidy is even smaller than for the previous policy, and thus negligible. Similarly, this policy does not contribute to carbon emission abatement. The policy costs for the highest subsidy setting in the progressive scenario peak around 300 M\$/year in 2034, but reveals steep curves for a limited durability. The cumulative policy costs in the most expensive and best case mirrors the character of this policy as a light-version of the electricity tax discount, with a total cumulative cost of 1.7 B\$ for the

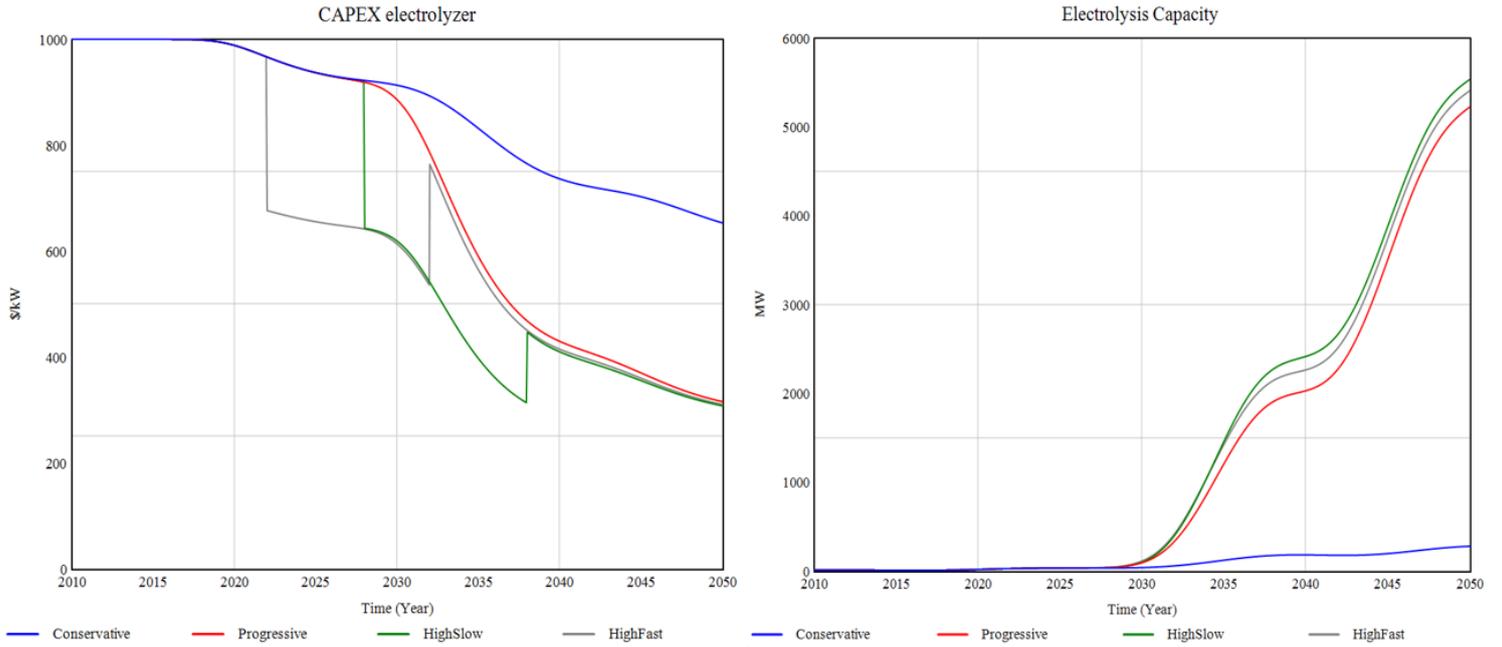


Figure 23: (a) Temporary price reduction of the electrolyzer capex through subsidy (green and grey line). (b) Electrolyzer capacity for the two scenarios under the 'high' subsidy but with different timing.

most effective late *HighSlow* policy implementation. In appendix K.2 additional graphs for the policy effects on demand, emission abatement and policy costs are displayed.

### 6.3.3 CCfD for steel manufacturing

Contrary to the previous examined policies, Carbon Contracts for Difference (CCfD) is a policy that is implemented on the demand side of the system. Therefore, to investigate the policy effects first the demand uptake is assessed, after which the effects on the electrolysis diffusion and cumulative carbon emissions are elaborated upon.

The effects of the CCfD are directly visible in the increasing demand for hydrogen in the steel sector. In figure 24, the annual hydrogen demand for the two scenarios is shown. Interesting is the development of HDRI in the progressive scenario. The *high fast* CCfD leads to an increase compared to the progressive basecase, but *high slow* and *low fast* reveal a slightly lower uptake, whereas *low slow* is lagging behind fiercely.

The complex nature of this policy explains this oddity in the outcome. The CCfD is a contract between the government and the steel manufacturer, in which a fixed strikeprice is defined. The strikeprice relative to the carbon price determines the financial support that the manufacturer obtains for making the transition to sustainable HDRI-steelmaking. This implies that when the carbon price increases, the abatement costs decline and the manufacturer therefore receives less financial support. Moreover, when the carbon price becomes higher than the pre-agreed fixed strikeprice, the steel-producing party profits of his abatement move and has to repay the government the difference between the strikeprice and the carbonprice. In the progressive scenario, the carbon price rapidly increases to a price that is higher than the strikeprice for the low and high policy settings, what results in an extra cost for HDRI-steel. Although it is in this case still more profitable than traditional steel making due to the high carbon costs, the share of investment in HDRI declines relative to the basecase. This is an unwanted reversed effect of the CCfD. The CCfD strikeprice must be increased in case when the carbon costs surges, or the CCfD must be cancelled to prevent low attractiveness for HDRI-investments.

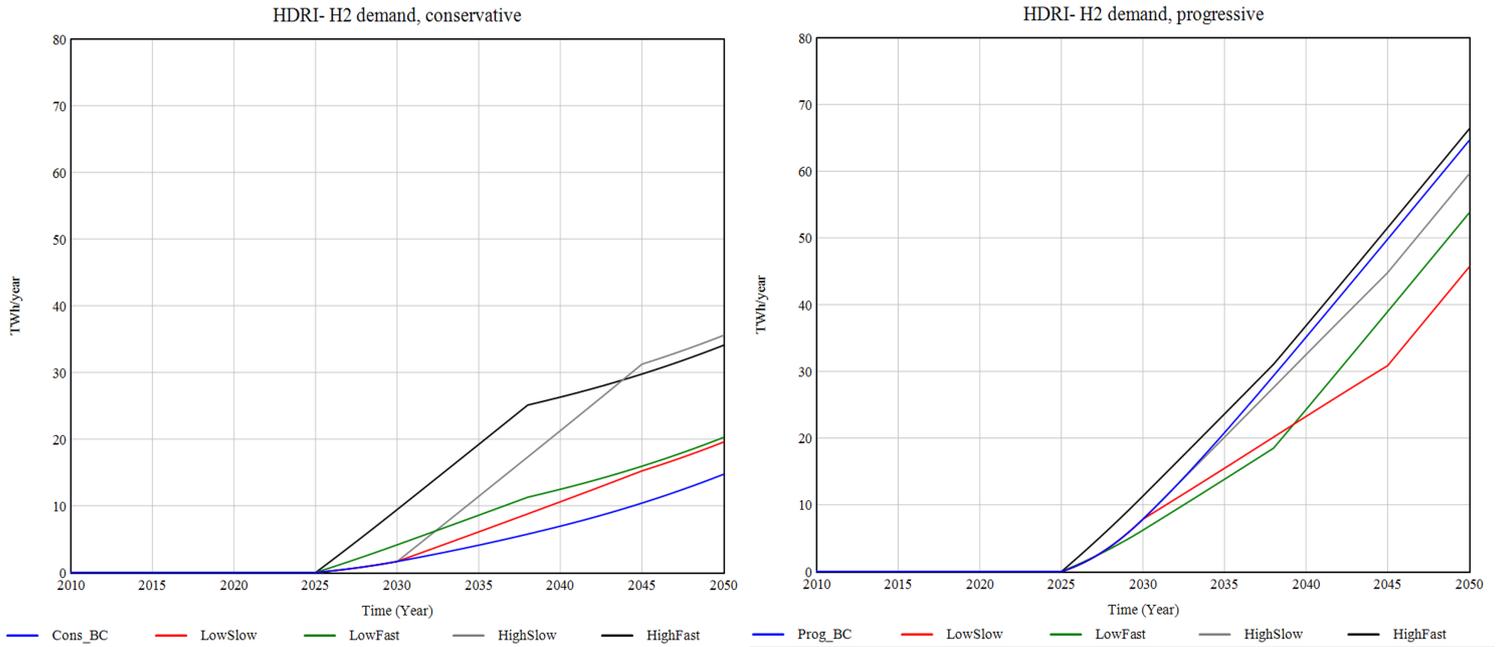


Figure 24: Hydrogen demand for HDRI-steelmaking for the four policy settings in the conservative (a) and progressive (b) scenario.

In the conservative scenario, the rise of HDRI-steelmaking reveals a more expected behavior, since the abatement costs per ton CO<sub>2</sub> remain larger than the carbon costs. A late initiation (from 2030) of CCfD shows however the largest rise in HDRI-steelmaking, with a surprising overtake from the slow policy of the early implemented policy, as seen in the left graph in figure 24. In the early case, the policy ends in 2038, leading to an early decay of the adoption, but in the slow case the policy ends in 2045 postponing the stagnation in investments. Apparently, the late implementation of this policy increments the growth rate of investments in HDRI since the competitiveness of HDRI-steel making is increasing as well over time due to increasing carbon prices. The higher HDRI-steelmaking share in the slow case is thus due to the fact that the investments expands with the increasing slope of the adoption curve as a result of increasing cost-competitiveness of HDRI-steelmaking, which results parallel in a steeper uptake of the late policy. Considering this observation, it seems that the increase of the carbon-price is almost as strong as the CCfD policy, since the force of this policy decreases when carbon prices rise. This would lead to a decreasing growth rate, which is not mirrored in the HDRI hydrogen demand growth.

When considering the effects of this policy on the entire hydrogen system, some minor policy leverage can be detected on the supply side. According to the model structure, the demand-side policy has a larger effect on the supply side, than vice versa. The hydrogen production is directly driven by the demand side, whereas the influence of the supply side on the demand side is only indirect through the cost of hydrogen via the of cost reduction of hydrogen production costs. The effects of the CCfD for electrolysis mirror the results of the HDRI-steelmaking growth slightly, considering that the expansion of electrolysis capacity shows parallel behavior for each policy as the demand growth. Turning now to the effects of the CCfD on carbon emission abatement and policy costs, there are large variations between the four different policy configurations. Because of the large footprint for BF-BOF-steelmaking, a transition to sustainable steelmaking results in rapid carbon abatement. In the conservative scenario without policies, an accumulative 874 Mtons are abated in 2050 relative to 2010. Looking at the best policy outcome for CCfD in the conservative scenario, a total of 1314 Mtons are abated in this time envelope. Hence, this policy on the demand side shows larger abatement potential than the supply side. Finally, the costs of the CCfD

policy are fluctuating heavily, due to the dynamic characteristic of this policy structure.

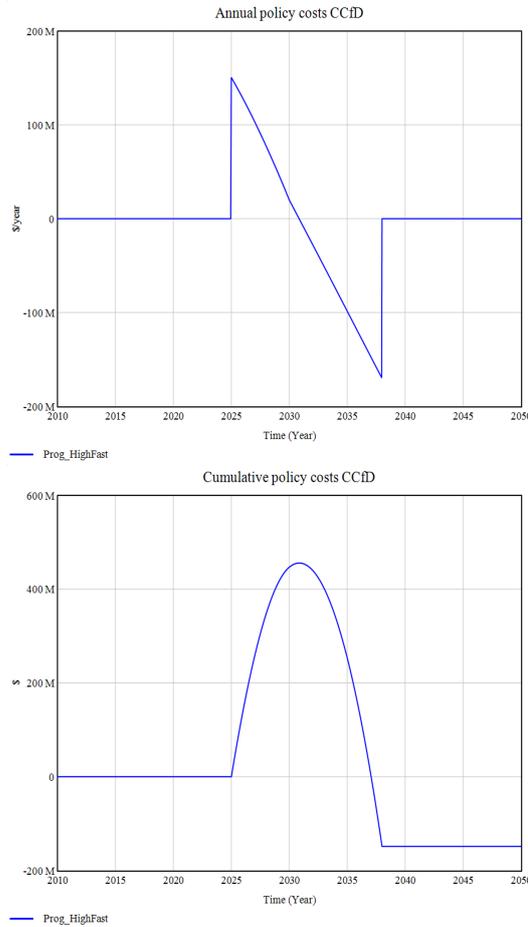


Figure 25: Policy costs for the *high fast* policy setting in the progressive scenario. (a) Annual costs indicating the cost parity of carbon price and abatement costs around 2031 (b) Cumulative policy costs, resulting in a profit for the government

stances depicted in figure 26 to an annual cost of approximately 19 M\$ and a total cumulative cost of 470 M\$ for the highest and fastest blending quota in the progressive scenario. Because of the limited impact of blending, the benefits for the cumulative abated emissions can be neglected, as well as the feedback effects to the supply side of the system and the deployment of green hydrogen.

### 6.3.5 Upfront infrastructure investments

This policy is affecting neither the demand nor the supply side of the system, but engages with the infrastructure side of the system and attempts to encounter the barrier of missing hydrogen infrastructure and the chicken-egg situation this has generated. Without policies, infrastructure expands as it responds to the increase in demand with a delay of approximately five years. This policy consists of centralized acceleration of the construction of hydrogen infrastructure, in which the government financially supports the construction of hydrogen pipelines before the growth of demand is visible yet. Because the infrastructure has

As explained, the government receives payment in case the carbon costs exceed the abatement costs, what happens in the progressive case. An example of this behavior for the *high fast* setting in the progressive case is shown in figure 25. The upper graph shows the annual policy costs, resulting in the cumulative costs. Because of the contract structure and the rapidly increasing carbon price, the government benefits in this case from this policy. Nevertheless, the hampering effects of this phenomena on for HDRI-steelmaking have also been shown. In appendix K.3, the cost graphs for the policy in the progressive scenario as well as the visualization of demand growth and emission reduction are displayed.

### 6.3.4 Blending quota

A quota is in theory a powerful instrument to artificially increase consumption for sustainable energy or technologies. The blending quota is implemented in 2025 in the fast case or 2030 in the slow case. Similar to the CCfD, this is a demand-side policy and affects the consumption of hydrogen directly. Contrary to the CCfD, the demand increase through the blending quota is very limited. In the earliest and highest quota in the progressive scenario, which incorporates a technologically maximum achievable blending volume share of 15% into the gas grid, with 20% of the grid used for blending, hydrogen demand for blending increases to only 6 TWh per year (see left graph in figure 26). This contributes barely to the total demand of hydrogen. The additional costs for hydrogen compared to natural gas per unit of energy increase as a result of the blending quota and lead under the circum-

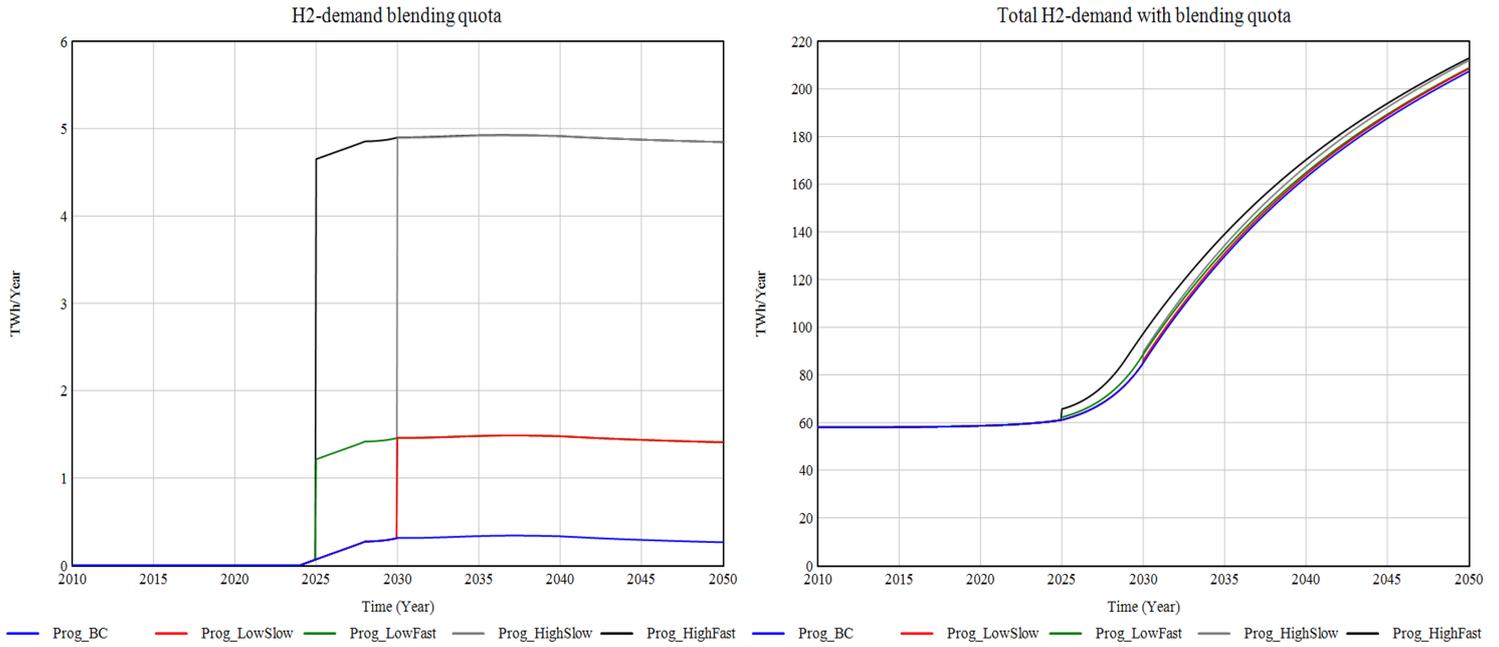


Figure 26: (a) Hydrogen demand uptake as mandated by the blending quota. (b) Contribution of the blending quota to the total hydrogen demand.

a feedback loop construction with the demand side, it should be a reinforcing lever for demand growth to construct infrastructure upfront. The upfront investment and construction shift the availability of infrastructure in the most severe investment package approximately 2.5 years forward in time compared to the basecase in both scenarios. This results in a saturation level of infrastructure that is achieved in 2028 already, instead of 2031. When the infrastructure investment policy is active, a similar time-shift can be detected in demand growth. FCEV-trucks deploy also roughly 2.5 years earlier when infrastructure is available earlier, reaching the fastest growth rate in 2028 instead of 2031. Although a slight acceleration in demand growth is observed, this quicker diffusion of infrastructure and FCEV-trucks does not induce demand growth on the long-term. This stagnating demand growth rate is a consequence of the saturation level of the infrastructure. When the saturation level of the grid is achieved, infrastructure is no longer a driving or obstructing factor for hydrogen demand growth. Because of the stagnating growth in FCEV -trucks observed around 2040, the total demand growth lessens as well resulting in minor long-term benefits. The total annual demand in 2050 for the progressive scenario without and with the most rapid and severe policy package differs only 5 TWh. On the supply side, a minor behavioral response of electrolysis capacity is detected when the investment policy is active. The acceleration of infrastructure impacts the entire supply chain and results in an acceleration of electrolysis capacity with one year. Furthermore, the final share of green hydrogen is lower when the acceleration investment policy is implemented. When the demand growth and consequently the investments in production capacity are artificially forwarded, the cost gap between green and blue hydrogen is slightly larger than one year later, leading to a larger investment preference in blue hydrogen compared to the non-accelerated case. This again implies the importance of timing of the policies, and the emphasis that must be given to combining the policies carefully at the right time. The effects of the upfront investment infrastructure do not mirror the severity of the absence of infrastructure as a roadblock to hydrogen development. Implementing infrastructure anticipatively in the model does not result in a breakthrough for green hydrogen diffusion, since infrastructure construction in the model already rather rapidly trails the demand uptake.

Visualization of the effects of the infrastructure acceleration policies on the hydrogen de-

mand, emissions and policy costs are shown in appendix K.5. The profits in carbon abatement from the upfront infrastructure investments are very slim and can be neglected for all policy settings in each scenario. In regard to the minor effects of the upfront infrastructure investments in both the demand and supply side, the costs per gained electrolyzer MW, TWh demand, or abated ton of CO<sub>2</sub>, are exorbitant. The model simulates solely the total costs of infrastructure construction that is pre-invested by the government, ignoring potential profits. This results in an annual expenditure of 420 M \$ and 1.7 B \$ in the low and high investment package respectively. Cumulative costs increase in these cases to 2.1 B\$ and 8.5 B\$, which are the highest cumulative costs of all policy types considered in this research and covers in the high policy case almost the entire hydrogen investment budget of the German Hydrogen Strategy.

### 6.3.6 Fossil-fuel tax and Coal phase-out

#### Fossil-fuel tax

The German Government has recently implemented two sustainable policies that are not focused on hydrogen in particular, but are expected to have influence on the diffusion of green hydrogen. The fossil fuel tax has been implemented in 2021 and is annually elevated up to 60\$/tonCO<sub>2</sub> in 2026. The inclusion of a carbon tax on fossil-fuel vehicles has implications for the total cost of ownership for Diesel trucks, what reduced the investment share in Diesel trucks relative to FCEV- and BEV-trucks as soon as the tax is implemented. Although the TCO of Diesel trucks fairly increases, this has surprisingly very little consequences for the deployment of FCEV-trucks. Because of the competitive price of BEV-trucks, the major transition induced by the tax on Diesel takes place from Diesel trucks to BEV-trucks, this is displayed by the increase of the red line (Diesel) and drop of the black line (BEV) in figure 27 (A). The FCEV-fleet grows only around 0.8% as a result of the tax on Diesel, leading to a share of around 26% of FCEV-trucks in the total truck fleet in 2025 in both scenarios. The carbon emission reduction from this demand side policy are very high due to the decline in the Diesel trucks, but the carbon abatement profits that are accounted for by the shift to FCEV-trucks are marginal. Although this is not a hydrogen-focused policy, the profits of the Diesel tax are roughly estimated at 1.8 B\$ at its peak in 2026, after which income starts to decline due to the transition to sustainable truck-types. The cumulative profits until 2050 sum up to 30 B \$ and 37.4B \$ in the conservative and progressive scenarios. In appendix K.6, the effects of the fossil-fuel tax on the hydrogen demand, carbon emissions and policy profits are shown.

#### Coal phase-out

The coal phase-out is already taking place and must be finished in 2038. Up until then, operating coal plants will be shut down in phases. More relevant for hydrogen is that the coal-phase out includes the ban on construction of new coal plants. For the production of hydrogen this implies that new coal gasification facilities are not built anymore from 2022 onward. The rejection of the installation of CG with CCS as hydrogen production methods transforms the investment landscape in hydrogen capacity drastically. On the one hand, a large share of the production investments shift to SMR capacity. Especially in the conservative scenario, the coal phase out results in a near monopolization of SMR in the hydrogen production sector leading to a growth of 33% SMR capacity between 2020-2050 with an investment share fluctuating between 95-98 % in this period. The progressive scenario displays a rapid peak in SMR capacity (black line in figure 27 (B)) when the phase-out is implemented, and shows more beneficial circumstances for electrolysis than the conservative scenario, therefore the electrolysis deployment in this scenario caused by the coal phase-out also receives a piece of the pie. Electrolyzer capacity displays an increase of 24% in the progressive scenario, from 3194 MW to 3985 MW in 2050. As can be seen by the green line in figure 27 (B), the peak of investment share in green production capacity is detected in 2038 reaching a share of 40%, what corresponds with the low price for green hydrogen at that moment as seen in figure 22 (A). More interesting is that the effect of this policy are visible in the entire system. A slight increase of hydrogen demand can be observed when coal is phased-out. The increased market share of SMR results in a small

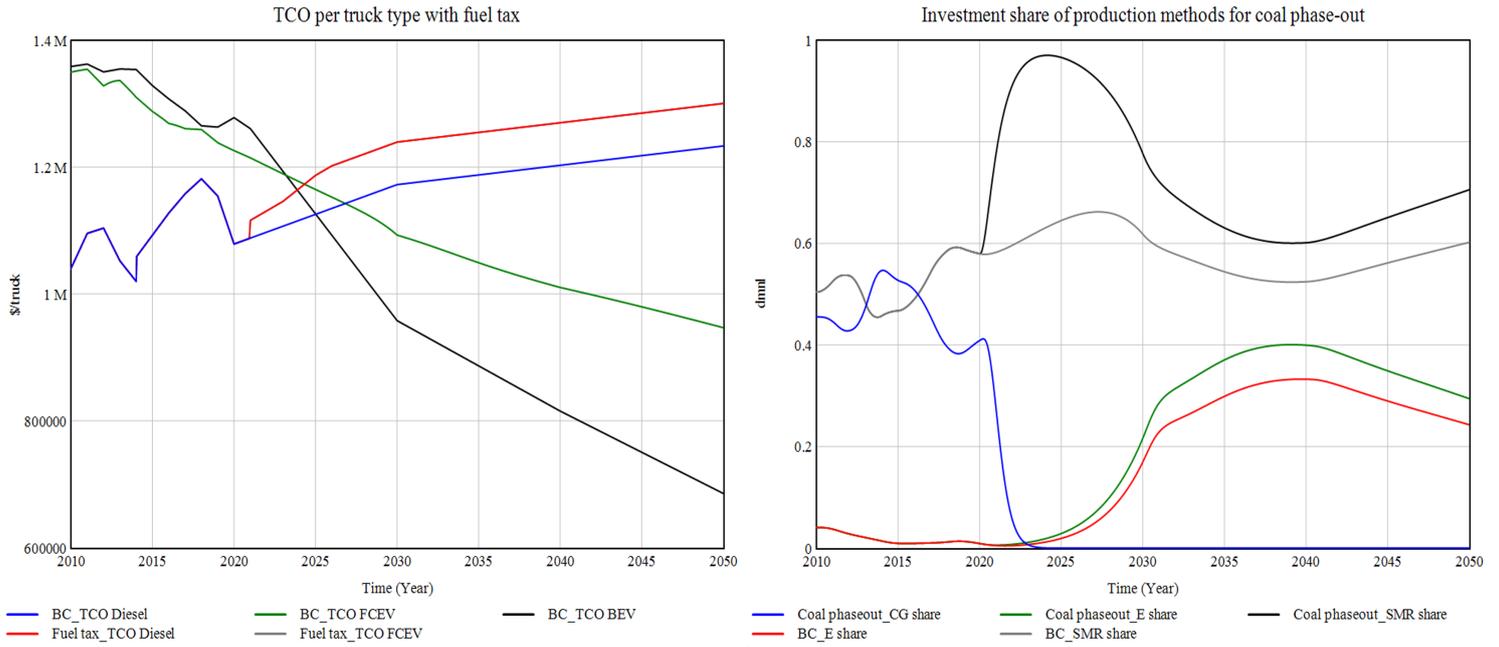


Figure 27: (a) Total cost of ownership per truck type in the progressive scenario where BEV-trucks become most cost competitive. (b) Investment share of hydrogen production methods for the progressive scenario (red, grey lines) and when the coal-phase out is active (blue black green).

price decline for hydrogen in the long term, compared to CG-produced hydrogen. The rising carbon prices lift the costs of CG, since an estimated 10% of emissions evades the carbon capture and storage and is subject to carbon costs. Another dynamic that emerges from this policy is a reinforced learning of electrolyzers in both scenarios. Because of the policy-induced diffusion of electrolysis, the learning initiates quickly after the initiation of the coal-phase out and results in an extra price reduction of 14.7% and 6.7% in the conservative and progressive scenarios.

#### 6.4 Policy effects on key performance indicators

Table 6: Impact of policy levers on electrolysis installed capacity for 2050

KPI	Electrolysis capacity (MW)							
	Conservative				Progressive			
Scenario	<i>LowSlow</i>	<i>LowFast</i>	<i>HighSlow</i>	<i>HighFast</i>	<i>LowSlow</i>	<i>LowFast</i>	<i>HighSlow</i>	<i>HighFast</i>
<i>Policy setting</i>								
No policies	187				5227			
Tax discount electricity	248	218	776	479	5556	5419	6756	6148
Investment support electrolysis	199	194	229	210	5537	5411	5537	5411
CCfD emission contract price	195	193	229	209	4384	4822	5098	5107
Policy switch blending quota	189	186	196	180	5247	5178	5247	5178
Infrastructure acceleration	187	184	188	172	5222	5099	5207	4819
Fossil fuel tax	192				5253			
Coal phase-out	341				5998			

The effects of the different policy settings in the two scenarios have been assessed on each KPI. For the KPI electrolysis capacity, the results are shown in table 6. The values denote the final installed capacity of electrolyzers in 2050 for each scenario and policy setting. In appendix J, similar output tables for the other three KPI's; demand, cumulative abated emissions and policy costs, are displayed. The tables summarize the outcomes of the policy analysis of the individual policies and show the effectiveness of the different policies and the importance of the timing. Additional visual representation of the policy table outcomes for both scenarios on each KPI can be found in the graphs in appendix J.1 and J.2. From the overview of the impact of each policy, this section reflects on the behavior of each KPI under the different policy settings.

### 1. Electrolyzer capacity

The tax discount for electricity is the most effective policy for the diffusion of electrolyzers. As discussed before, the timing is crucial, as the policy interferes with the electricity price and the effects of the policy are amplified when implemented at the right moment. This makes the *HighSlow* policy most effective. Surprisingly, demand side policies CCfD and blending quota have a minor or in some cases even negative influence on the electrolysis deployment. In each of the settings for the progressive scenario, the outcome in case of the active policy is less than the basecase. Similarly, a minimal effect is detected for acceleration of infrastructure policy. These policies accelerate demand, but when the market detects no cost-incentive to choose for green hydrogen because of a large cost gap between green and blue hydrogen, this acceleration will only induce blue hydrogen. Therefore, a minor expansion of electrolysis capacity is detected for these policies.

### 2. Hydrogen demand

Hydrogen demand is as expected most affected by the demand side policies. In the conservative scenario CCfD are most influencing the hydrogen demand growth in the *HighFast* policy setting. In the progressive scenario, blending and the coal phase-out induce demand growth most severely, and the combination of all policies in the *high fast* setting seems most promising. Similarly to electrolysis capacity, the policies separately and even combined show disappointing effects on the demand growth for hydrogen.

### 3. Total cumulative abated carbon emissions

In absolute terms, the CCfD is for both scenarios among the most effective policies to reduce carbon emissions. Due to the transformation of the polluting steel industry to HDRI-steelmaking, progress is made in abating carbon emissions. This policy is however also sensitive to the start time, as the model shows that the emissions reduction even stagnate in relation to the basecase, when the CCfD-policy is implemented too low and too early. Aside from CCfD, the coal phase-out shows large profits in carbon abatement for both scenarios.

### 4. Total cumulative policy costs

Finally, the costs are assessed for each policy. Firstly striking are the costs for electrolyzer capex subsidy, that are in most cases larger than costs for the electricity tax discount, but less effective for the KPI's. Furthermore, as reflected in the previous section, the costs for infrastructure are immoderately high, especially when considered in light of the effectiveness for the three KPI's described above. The policy costs of all policies combined are in line with the effectiveness of the policies on the other three KPI's. The costs for the *high slow* policy settings are the largest for both scenarios, in which the cost of electricity tax discount and infrastructure contribute mostly. Depending on the weight of each objective, the costs per unit of gain for each objective could be considered.

## 6.5 Policy combinations

The policies differ strongly in the effectiveness of accelerating green hydrogen production and pushing hydrogen demand. The distinction between demand- and supply side policies is also visible on the output of the system, where system inertia fades out the resonating effects of policies to the other side of the system. Since the policies have most effect on the side

Table 7: Outcomes of the KPI’s under combined set of policies for 2050

<b>Combined policies on all KPI’s</b>				
Scenario	Conservative		Progressive	
<i>Policy setting</i>	<i>No policies</i>	<i>All policies</i>	<i>No policies</i>	<i>All policies</i>
Electrolysis capacity (MW)	187	1629	5227	7244
Hydrogen demand (TWh)	158	191	215	236
Cum. abated CO2 (Mtons)	882	1336	1556	1810
Cum. policy costs (\$)	0	-12.5687 B	0	-19.8724 B

they are implemented but nonetheless show minor responses in other system components, the system communication offers opportunity to amplify the performance of policies. The policy settings have been tested individually and do, as described, not automatically reveal the best outcomes for the highest and fastest policy settings. With the importance of the policy timing in mind, an analysis of the combination of all policies similarly active is conducted for both scenarios. The best performing policy settings for the electrolysis capacity are included in this analysis. Noteworthy, this is an exploratory analysis, since the optimization of the policies based on multiple objectives is not included in this research. The outcome of the implementation of all policies simultaneously versus the outcomes without policies of the model KPI’s for 2050 is shown in table 7, and similarly for the KPI’s electrolysis capacity and demand, in figure 28. Additional graphs of outcomes of the combined policies can be found in appendix K.8. Reflecting on the outcomes of the combined policies in light of the single-implemented policies, several observations can be made.

First, the outcome of the combined policies is larger than sum of the outcomes of the the individual policies for the electrolysis capacity only: the gain of the combined policies result is approximately 1.5 GW and 2 GW for the two scenarios compared to basecase, while the gain of the individual policies separately push capacity is 0.8 GW and 1.6 GW. The sum of separate policies is not a valid quantification of the policy effectiveness, but it provides the understanding that the interaction of policies might have negative or beneficial effects. For hydrogen demand, it can be seen that the effect of the combined policies in the progressive case, 236 TWh, is even less than the effects of the fossil-fuel tax implemented independently (277 TWh). This can be clarified by the disappointing effects of the CCfD policy in the progressive case as described previously (section 6.3.3), offsetting the beneficial effects of other policies on demand when implemented simultaneously. Cumulative abated carbon emissions, show the best outcomes for the combined policy, but the sum of the effects of the individual policies remains larger than the effect of the combined policies in the progressive case. This KPI also indicates that the interaction between policy might dampen the effectiveness of the policies. The implementation of separate policies might therefore be in some cases more beneficial than the blind inclusion of all policies, as a result of the amplifying or damping effects policies have on each other. This leads to the second observation.

Secondly, the implementation of policies on the demand side must be accompanied by policies on the supply side to assure diffusion of green hydrogen over blue hydrogen. Most prominently, the causal link between the increase in hydrogen demand and installation of new capacity based on the levelized cost of hydrogen induces blue hydrogen to take-off at the expense of green hydrogen in some cases. The low adoption of green hydrogen restraints technological learning and cost reduction of electrolysis. The acceleration of demand through CCfD, blending quota and infrastructure acceleration shifts the take-off of demand forward in time. However, when green hydrogen is not yet competitive with blue hydrogen at the moment the demand increases, the production capacity shifts to blue hydrogen primarily. This is corroborated by the negative effects of the demand side policies on electrolysis capac-

ity shown in table 6. Vice versa, the implementation of supply-side policies has no negative causal effects on the demand side when demand side policies are absent, although the effects are very limited. This observation confirms the interconnection between the policies, and suggests that the implementation of solely demand-side policies has negative effects on the diffusion of green hydrogen.

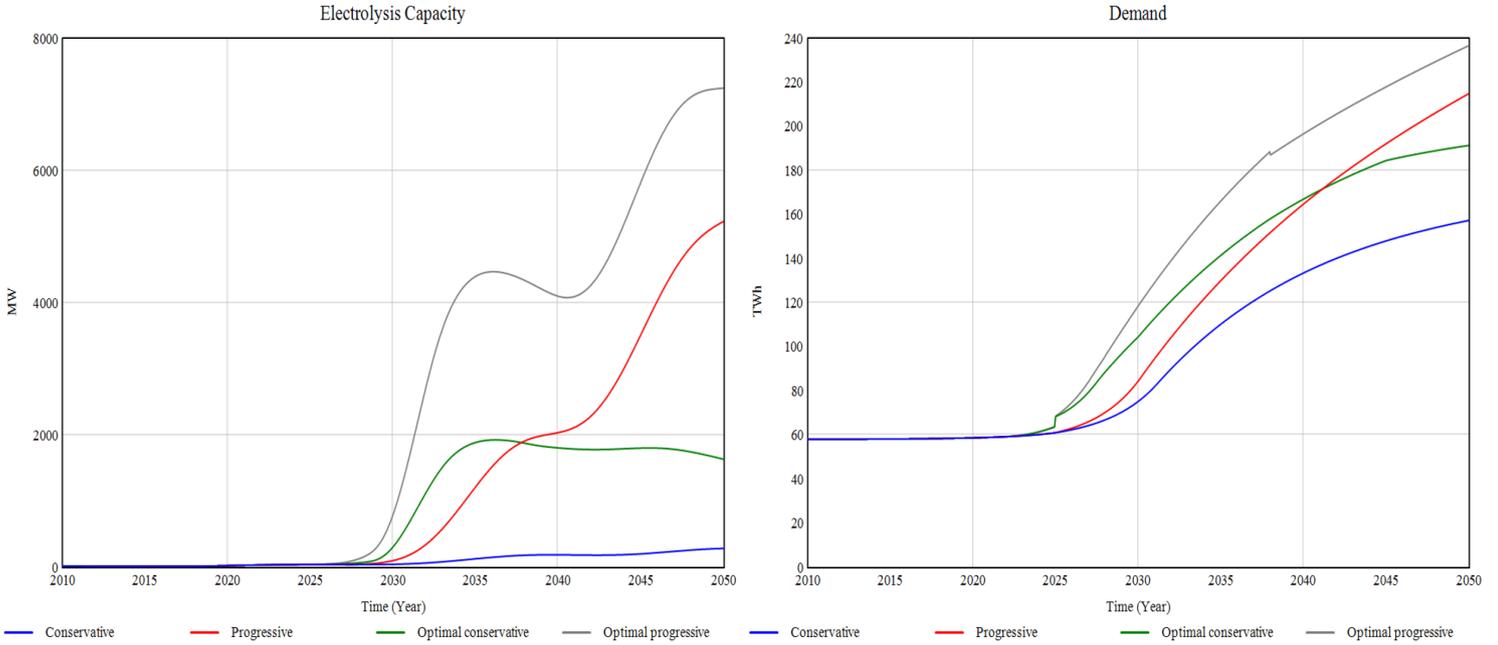


Figure 28: Effect of combined policies on electrolysis capacity (a) and hydrogen demand (b), displayed for the basecase of the two scenarios in blue and red, and for the combination of all best performing individual policies.

Third, some policies have very limited or negative effects on each of the objectives. Most prominently, the upfront infrastructure investments perform poorly in almost each configuration and even dwindles the development of electrolysis capacity for all cases. This is unexpected, as the absence of hydrogen infrastructure is specified as one of the largest obstacles to hydrogen diffusion. Moreover, this policy encompasses the highest expenditures of all policies, contributing to the poor performance of this policy. Another inadequate lever is the capex subsidy. Despite its contribution to the deployment of electrolyzers directly, its effectiveness for the other objectives is low. The policy analysis results demonstrate that this policy compared to the electricity tax discount shows inferior performance on all objectives, and results in higher cumulative policy costs. The poor performance indicate that the implementation of each policy at the same time is not the most effective approach. The coherence of these policies with others however requires further examination, since the amplifying effects of particular policy combinations might increase policy effectiveness.

Finally, as demonstrated, the effectiveness of the interventions corresponds with the timing of implementation leading to different optimal time envelopes for the policies to start. The timing of the combined policy configurations is equal for all active policies. This implies that some of the policies are not active in their optimal time-frame, diverging the policy results of the combined policies from their optimal outcomes. The rate and the timing of policies must carefully be addressed when seeking for optimal policy windows. The optimal configuration cannot be adopted straightforward from the individual policy analysis, because each policy combination creates different interactions and generates different policy outcomes.

Overall, these results indicate an inadequate effect on the growth of hydrogen. Intervening with all policies at the same time at the highest policy setting that is examined in this research does, even in the progressive scenario, not result in a rapid development of hydrogen

in general and green hydrogen in particular. It can be stated that the barriers to hydrogen that are active in 2020 are only partly dissolved in 2050 under the implementation of the individual or combined policies. Considering the policy outcomes for electrolysis capacity, the targets set by Germany in the National Hydrogen Strategy seem out of reach: the target for 2030 is 5 GW, and for 2040 a minimum of 10 GW. Under the best circumstances (progressive scenario) with the combined policy package in place, the capacity reaches 0.8 GW in 2030, 1.8 GW in 2040 and 7.2 GW in 2050 (see the left graph of figure 28).

## 6.6 Analysis of unconventional policies

The most effective policies have demonstrated to be electricity tax subsidy for the support of green hydrogen production, and carbon contracts for difference for the promotion of hydrogen demand in some cases. Nevertheless, the green hydrogen diffusion remains low and occurs late. The targets of the German Hydrogen Strategy remain out of sight even in the most progressive scenario. Although the effects of the tested policies are insufficient, the analyses have revealed insight in the leverage points of the hydrogen supply chain system. Namely, increasing demand on the one hand, and simultaneously lowering the costs of green hydrogen on the other hand. To achieve an accelerated diffusion of green hydrogen, stronger and alternative policies are required. This section discusses the effects of more unconventional policy levers that exceed the initially proposed policies in leveraging power. The aim of this analysis is exploratory and is to achieve preliminary insight in the system's behavior to the leveraging power of more unconventional policies.

### 6.6.1 Ban on carbon capture and storage

The debate on carbon capture and storage (CCS) is ongoing in Germany. With regards to hydrogen, the discussion is about benefits of blue hydrogen as a relatively affordable and easy-to-implement transition technology, whereas the downside of blue hydrogen consists of the possible lock-in of fossil fuels, residual emissions and postponing investments in green hydrogen (Dickel, 2020). In general, the reputation of CCS is not undisputed. In 2019, chancellor Merkel acknowledged that the storage of CO<sub>2</sub> is very controversial in Germany and other parts of the world, but also stated that CCS is required to achieve carbon net-zero targets. This statement opened the debate for policymaking and regulative directions about CCS in Germany. Following this statement, CCS is gaining support if it is not applied to existing coal- and gas fired plants to extend their lifetime. The acknowledgement resulted in policy support and the initiation of a CCS programme, funding pilot projects for carbon capture and storage for application in industry (Clean Energy Wire, 2020). Nevertheless, the public debate is still ongoing and the controversy is still present. Contrary to the previous coalition led by chancellor Merkel, the new coalition that was installed in early 2022 in Germany adopted an opposing vision on CCS for hydrogen. According to vice chancellor Habeck, blue hydrogen will be excluded from subsidy schemes and governmental support, since green hydrogen is the only long-term solution (EurActiv, 2022). Whenever money is put on the table, it must be for green hydrogen, his state secretary stated (Clean Energy Wire, 2022). In case CCS for blue hydrogen is not supported in any way through governmental means, this has consequences for the economic viability of blue hydrogen. Although concrete measures for policy measures are not yet announced, this statement provides an interesting point of departure for further policy exploration with the hydrogen supply chain model. This section explores the system's reaction and more specifically the diffusion of green hydrogen in case of a ban on carbon capture and storage.

To investigate the effect of the exclusion of blue hydrogen from future government support on the diffusion of green hydrogen, a ban on CCS is included in the model structure. Because it is a preliminary announcement and precise consequences on cost of blue hydrogen remain ambiguous, the model assumes an excessive high price of 20 \$/kg CO<sub>2</sub> for the carbon capture and storage of blue hydrogen emissions, opposing to the original costs of 0.045 \$/kg CO<sub>2</sub> for CCS. This exploratory assumption is examined for implementation of the exclusion on CCS in 2022 and 2030.

The results of the CCS-ban are displayed in figure 29. What is striking about the results is the vast increase of electrolysis capacity this policy enforces, as shown by the brown and black line in the left graph. The early ban on CCS implemented in 2022 results in 0.7 GW, 7.7 GW and 13 GW of installed capacity for 2030, 2040 and 2050 in the progressive scenario respectively. Similarly, a vast diffusion is detected in the conservative case with an installation of 5.3 GW in 2050 for the early ban. Turning now to the outcomes of the hydrogen demand under this policy, it can first be detected that in the progressive case the early CCS-ban is delaying the take-off of hydrogen demand for approximately 3 years

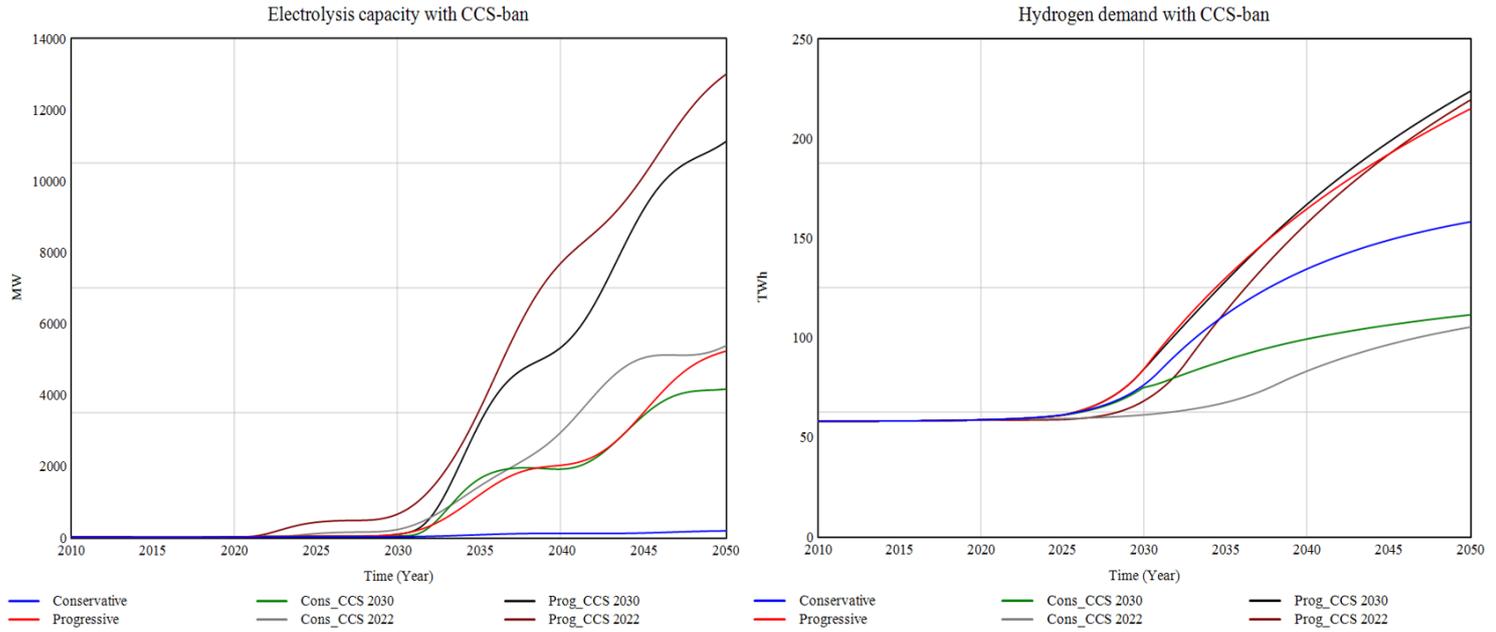


Figure 29: Electrolysis capacity (a) and hydrogen demand (b) with CCS-ban for both scenarios

as is indicated by the red line (basecase) versus the brown line. Nevertheless, the demand difference converges towards 2050, ending in a roughly similar demand. Second, the CCS-ban has impeding effects on the development of demand in the conservative case, leading to a fairly low demand of approximately 105 TWh in 2050, compared to 220 TWh for 2050 in the conservative basecase.

The powerful diffusion of electrolysis and the limited or even limiting effects on demand of the CCS-ban can further be explained through the graphs in figure 30. The left graph displays the effects of the rapid implementation of the CCS ban for the progressive scenario on the capacity of green, blue and grey hydrogen production and total demand. From 2022, the small amount of blue hydrogen capacity that was already present starts to deteriorate and is continuously replaced by green hydrogen production capacity. As soon as demand (red line) starts to ignite in 2030, blue hydrogen production is no longer viable because of the ban, promoting the installation of the large amount of green hydrogen capacity. Demand is in this case less than the basecase. Because of the low availability of blue hydrogen production capacity from 2022, hydrogen prices peak between 2022-2030, since green hydrogen is not cost-competitive or large-scale available yet. The absence of affordable blue hydrogen has significant influence on the increase of hydrogen demand as hydrogen becomes less cost-competitive with fossil fuels. This explains the postponed demand growth when blue hydrogen is absent. Now turning to the right graph of figure 30, the effects of the postponed exclusion of CCS are presented. Comparing the late implementation to the early implementation, it stands out that blue hydrogen installation starts to grow between 2020-2030, after which electrolysis starts to diffuse rapidly and blue hydrogen production depreciates. Furthermore, the demand for hydrogen starts to increase around 2025, which shows a similar timing as the basecase, and approximately 5 years earlier than in the case of an early CCS-ban. This observation corroborates the explanation for the postponed demand growth in other case, since the availability of affordable blue hydrogen increases competitiveness between hydrogen and conventional fossil-fuels in end-use sectors.

Although the analysis is exploratory and the policy is a somewhat ambiguous announcement, these findings suggest that the rapid exclusion of CCS from the future mix of hydrogen production methods might on the one hand, as expected, be beneficial for a large-scale

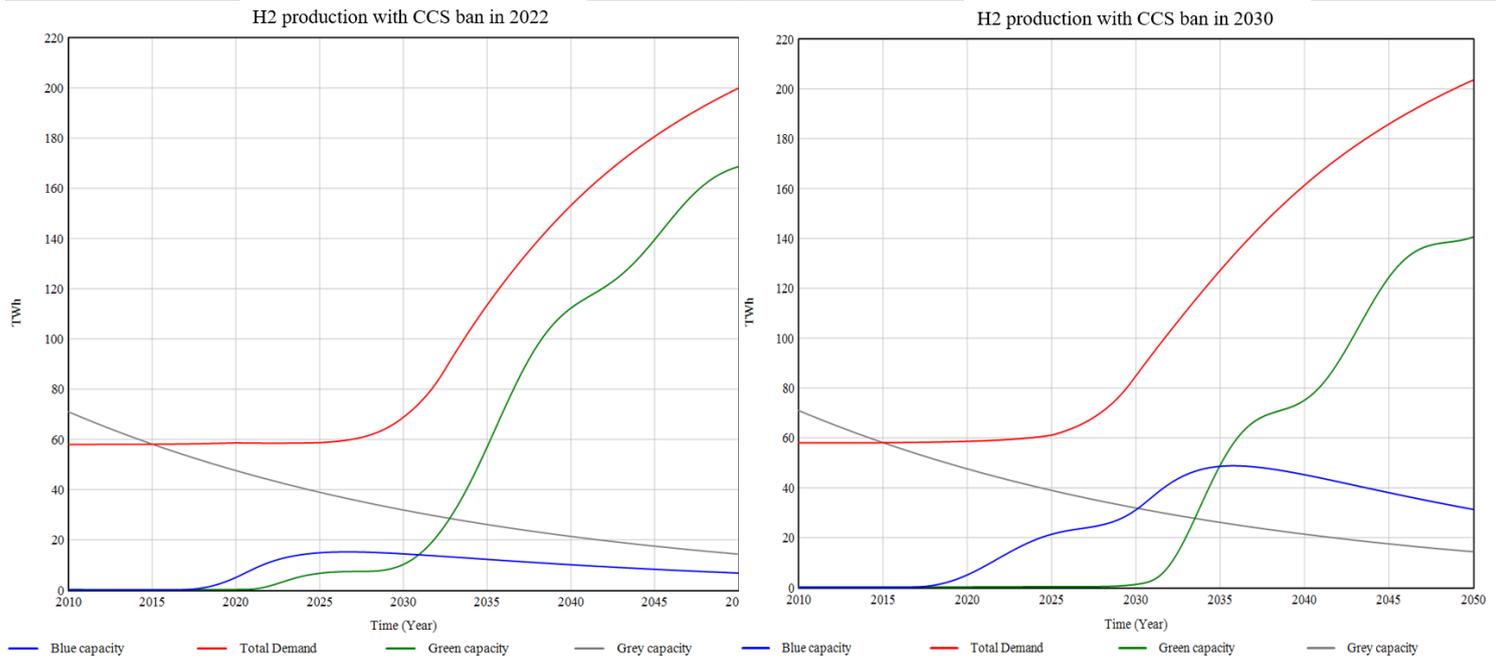


Figure 30: Electrolysis capacity (a) and hydrogen demand (b) with CCS-ban for both scenarios

diffusion of green hydrogen. On the other hand, the comparison of the timing of the policy suggest that the exclusion of affordable blue hydrogen on the short term might result in a delay of the growth of hydrogen demand. Considering the mechanism that green hydrogen diffusion only occurs when demand increases, a delay of demand growth is not beneficial for the acceleration of green hydrogen diffusion. These contrasting outcomes confirm both views of the discussion about the necessity of blue hydrogen as a transition technology, which are in short: blue hydrogen is required to increase hydrogen demand on the short-term and create a hydrogen market. In contrast: blue hydrogen is controversial and creates dependency on fossil-fuels. Whereas the aim of this research is to explore policies for the acceleration of green hydrogen diffusion, the most beneficial long-term effects are undeniably achieved with a rapid ban of blue hydrogen.

### 6.6.2 Combining conventional and unconventional policies

the rapid ban on blue hydrogen was explored. In figure 31, the outcomes of this analysis for electrolysis capacity and demand are shown. A rapid acceleration of green hydrogen production from 2030 is observed in both scenarios, complementing the accelerated demand growth take-off shows in the right graph. Although the targets for 2030 are still not achieved (1.7 and 2.5 GW for the conservative and progressive scenario), the goals for 2040 are realized in the progressive scenario with 10.9 GW respectively. In 2050, the electrolysis capacity accumulates to 8.3 GW and 14.7 GW for both scenarios. The oscillation of diffusion is in this case not only attributable to the model design, but also to the policy effect. In figure 32, the levelized costs of green hydrogen with the policies active are shown. The large contribution of the price decrease through electricity tax reduction and electrolyzer subsidies, the levelized costs plummet as long as these policies are active. However, when this financial support ends, the levelized costs in both scenarios recover rapidly towards their old level, which causes the sudden decline in demand in the conservative scenario (see green line in the right graph of figure 31 and the subsequent reduction of electrolysis capacity. The cumulative abated emissions that are achieved by this policy package are negligible, whereas the total cumulative costs of the policies towards 2050 are roughly 34 billion \$ and 24 billion \$ for the conservative and progressive scenarios, as displayed in

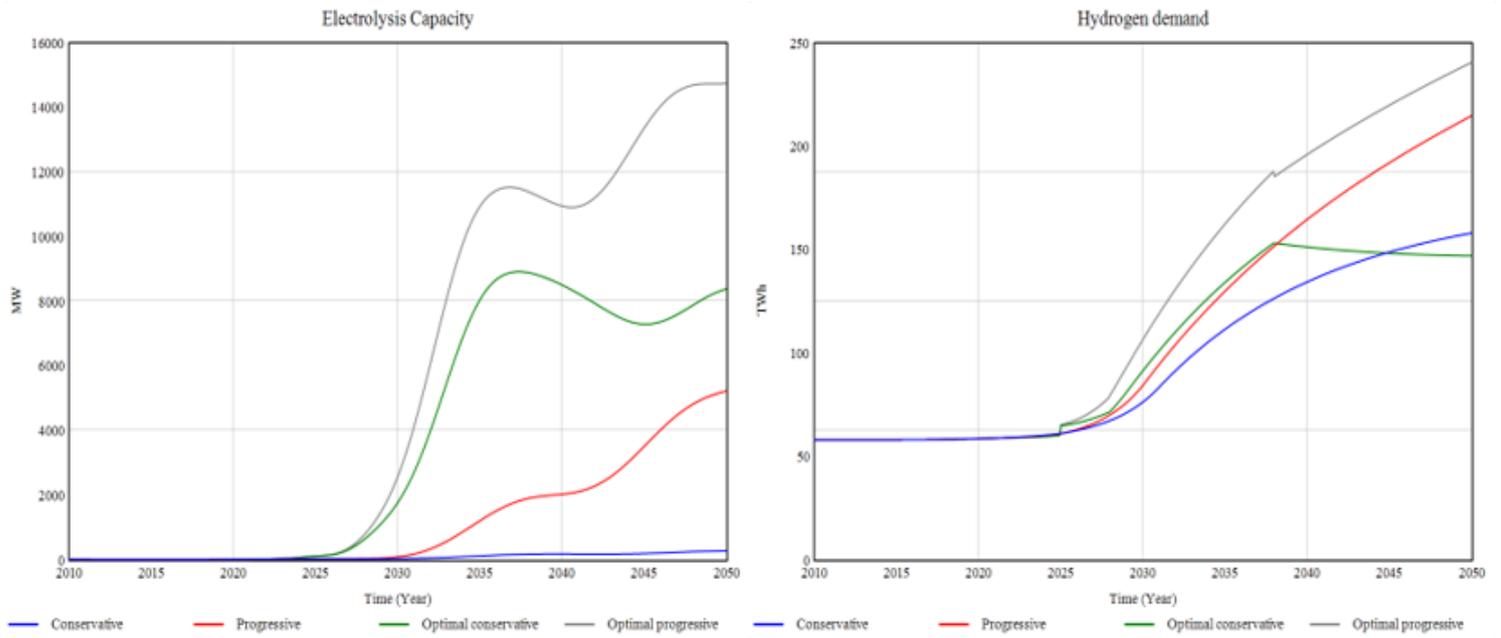


Figure 31: Electrolysis capacity (a) and hydrogen demand (b) with all conventional policies and CCS-ban in force for both scenarios

appendix K.10. Although the diffusion shows a setback around 2040, the outcomes of this analysis are promising. The ban on CCS supports the diffusion of green hydrogen, whereas the conventional policies compensate the delay in demand growth that was observed for the CCS-ban. The complementing policies provide an acceleration of demand growth and similarly a large-scale diffusion of green hydrogen, through which in the progressive scenario the long-term goals of the German hydrogen strategy are achieved.

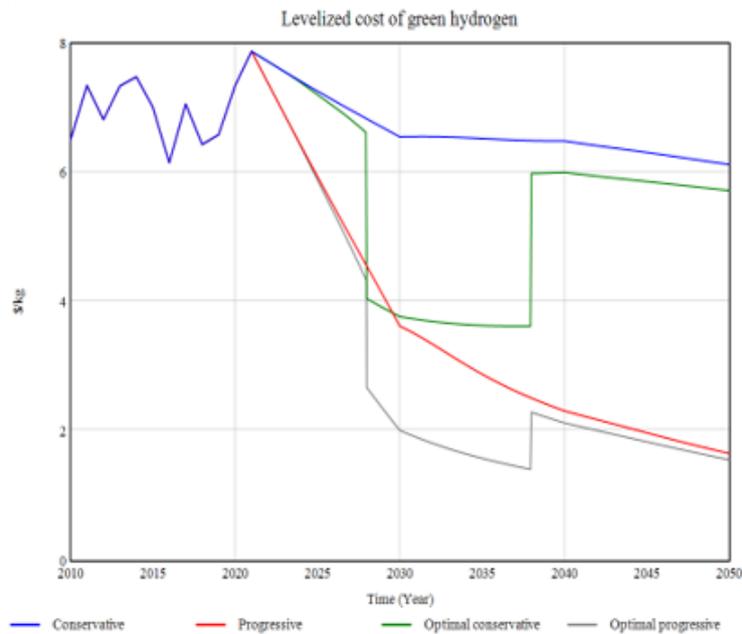


Figure 32: Levelized cost of green hydrogen with all conventional policies and CCS-ban in force

## 7 Conclusion

This chapter concludes on the findings from the model and policy analysis. The main conclusions will be explained and answer to the main research question will be provided. Moreover, this chapter reflects on the scientific and societal relevance of this research and provides a set of policy recommendations.

### 7.1 Main research findings

The purpose of this research was to gain quantitative insight in the dynamics of diffusion of green hydrogen and assess the leveraging impact of policies on the diffusion of green hydrogen. A system dynamics modeling approach was selected to simulate the hydrogen supply chain from a system perspective, which provided understanding of the structural dynamics and behavior of green hydrogen diffusion and the possibility to experiment with policies. The country-level scope of the model was chosen to allow for a technological aggregation that is suitable for SD modeling and as an appropriate scope for policy analysis. Through desk-research, the current technological and political context for hydrogen development in Germany was examined. The context of hydrogen in Germany was subsequently conceptualized from a system perspective with a subsystem diagram and a causal loop diagram. In the formulation phase, the conceptual model was quantified through mathematical equations and parameters. After model testing, the uncertainty analysis demonstrated the implications of model uncertainties, after which a number of scenarios and policies were analyzed to understand the system behavior and explore measures for the acceleration of diffusion.

The main research question of this research was:

*What is the impact of drivers and barriers on the diffusion of sustainable hydrogen and how can this diffusion be accelerated?*

The answer to twofold this question is consists of two parts. The first part of the model analysis examined the basecase and the system behavior without policy interventions. These outcomes confirm the obstructing impact of the barriers that were found in literature.

- The model outcomes clearly mirror the lack of demand for hydrogen. Even in the progressive scenario the hydrogen consumption initiates in the late half of this decade to increase its growth rate no sooner than 2030. This market growth leads to a moderate demand increase of 205 TWh (0.738 EJ) towards 2050. The late take-off of hydrogen demand is on the one hand due to the absence of infrastructure. The chicken-egg situation is apparent here and obstructs adoption of FCEV-trucks in the transport sector. This stalemate is disrupted around 2030 through the increase in hydrogen demand in the steel sector. The increasing cost of carbon stimulates the transition to hydrogen in the steel sector. Hydrogen demand thus slightly grows, albeit late, when the drivers infrastructure availability and carbon costs, are existent.
- The model results show the implications of the cost-gap between grey and blue hydrogen. Without policies, the electrolysis capacity demonstrates a growth toward 5.3 GW in 2050 in the most favorable scenario. This is only 27% of total production, the other share is provided by blue hydrogen. Because of high capital costs and electricity costs, the cost-gap between green and blue hydrogen in 2030 is roughly 4 \$/kg, what forces production investments towards blue hydrogen capacity. Hence, without increasing cost-competitiveness of green hydrogen, green hydrogen diffusion will lack in favor of blue hydrogen.
- The absence of infrastructure is only partially confirmed as a barrier of diffusion in this study. A lack of pipelines averts the deployment of FCEV-trucks, but total demand nevertheless increases due to the rising carbon costs that drive the transition in the steel industry. This pushes the construction of infrastructure to a country-covering level of 40.000 km occurs considerably fast in the simulation, even without supporting policies. The absence of infrastructure can therefore be considered as delaying, but

not completely obstructive.

- The lack of policies and regulations intensifies the hindering effects of the above described barriers to green hydrogen diffusion. The simulation without policies demonstrates a moderate demand growth and a thriving blue hydrogen industry at the expense of sustainable hydrogen production, and shows that policies are indispensable to impel green hydrogen diffusion.

It can be concluded from the basecase and scenario analysis without policies that the detected barriers of diffusion impede the development of green hydrogen. Without adequate policy interventions, future hydrogen demand will grow only moderately and green hydrogen will become a subordinate of blue hydrogen.

The second part of the research question is addressed with the policy experimentation. The exploration of policies demonstrates that a rapid activation of announced and conventional policies do not guarantee a fast-forwarded diffusion of green hydrogen. Furthermore, the timing of policy implementation has significant effects on the policy effectiveness, and the combination of supply-side and demand-side policies is essential. To achieve high levels of green hydrogen production on the long-term, unconventional measures must be considered.

- From the supply-side policies, the tax discount for power that is used for electrolysis has the largest effect on the increase of green hydrogen production capacity. Because of the large influence of the electricity price on the levelized cost of green hydrogen, an alleviation of costs leads to a cost-parity with blue hydrogen in 2028 in the best case. The second best supply-side policy, electrolyzer equipment subsidy, has significantly less impact on the cost of hydrogen, due to the smaller share of capital costs in the levelized cost of hydrogen. Nevertheless, it has a positive price reducing impact on the learning-by-doing mechanism. Combining the two supply-side policies is essential to close the cost gap between green and blue, but is not sufficient for large scale green hydrogen diffusion.
- The policy outcomes show moderate effects for the demand-side policies. These findings suggest that CCfD's are useful to support the transition in the steel sector, but only when the carbon price is moderately increasing. When the carbon cost is expanding rapidly and the strike price is not adequately high, this policy even shows an adverse effect on hydrogen demand growth. A blending quota demonstrates a limited increase in demand, but is more effective than CCfD's when the carbon costs are high such as in the progressive scenario. Generally, policies have only limited leveraging effects on the demand side as the naturally driven hydrogen demand growth by carbon costs is stronger.
- In line with the effects of infrastructure as a barrier as described above, the financial support for infrastructure has insignificant effects on the growth of the hydrogen sector. The demand and production for 2050 remain almost equal to the basecase, regardless of the infrastructure acceleration. Nevertheless, the subsidies for infrastructure do have an accelerating effect on the demand growth, causing FCEV-truck to deploy roughly 2 years earlier. This suggests that diffusion can to a certain extent be accelerated through rapid infrastructure construction.
- Contrary to expectations, a delayed implementation of some of the policies is more beneficial for green hydrogen diffusion in the long term than a rapid policy implementation. Activating the electricity tax reduction and electrolyzer subsidy in 2028 results in a larger diffusion rate than policy implementation in 2022. Because electricity costs are expected to decrease over time, a delayed artificial cost reduction lowers the levelized costs more than an early cost reduction of green hydrogen. It can be stated that this counter-intuitive outcome is found by virtue of the system dynamics approach, as it shows how the dynamics of a system can be unexpected and difficult to grasp without simulation. For the demand-side and infrastructure policies the impact

of postponing the policy is not applicable, given that early policy activation shows higher long-term demand.

- The analyses of the separate policies compared to the combined policies reveal two insights. First, the effect of all policies combined is less than the effect of the sum of all policies individually. This indicates that the simultaneous activation of policies is not reinforcing and that the negative effects of some policies nullify the leverage of other policies. Second, implementation of demand-side policies without a simultaneous activation of supply-side policies have no beneficial effect on the diffusion of green hydrogen. When hydrogen demand grows without simultaneous cost reduction of green hydrogen on the supply-side, green hydrogen will be overruled by blue hydrogen.
- The implementation of a ban on CCS leads to an exclusion of blue hydrogen production and a large-scale diffusion of electrolysis on the long term. An early implementation of the ban obstructs the growth of blue hydrogen and shows a growing electrolyzer capacity from 2025. On the contrary, an early ban on CCS leads to a delay in the take-off of hydrogen demand growth of roughly 5 years. Because blue hydrogen is cast aside, only expensive green hydrogen is available what makes it difficult to compete with fossil-fuels. The conclusion on this policy is twofold: an early ban is beneficial for green hydrogen diffusion on the long term, while a late ban is beneficial for hydrogen demand on the short term.
- Finally, the combination of all regular policies plus the preliminary announced ban on CCS displays a significant diffusion of electrolysis that initiates rapidly from 2028 onwards. The acceleration of diffusion for this policy case is still not sufficient to achieve targets for 2030. Because the demand for hydrogen is not significantly forwarded, an acceleration of green hydrogen diffusion does not occur. Nevertheless, this heavy policy package demonstrates that on the long-term the targets for green hydrogen can amply be achieved, with approximately 12 GW of installed capacity in 2040.

It can be concluded from the analysis of individual and combined policies for diverse time-frames that; for the diffusion of green hydrogen the cost reducing policies for electrolysis are most beneficial; the effect of timing of these policies is counter-intuitive and of significant impact; demand-side policies are only effective for green hydrogen diffusion when implemented together with supply-side policies; acceleration of diffusion can only be achieved through fast-forwarding the demand. Furthermore, because the best combination of regular policies might not be sufficient to achieve the German green hydrogen targets, alternative and stronger policy levers must be implemented on a short time to ramp up diffusion towards 2050.

## 7.2 Scientific relevance

In the literature gap in section 2, a number of limitations to existing hydrogen modeling studies were indicated. Current studies to the diffusion of hydrogen are on the one hand qualitative of nature resulting in in-concrete policy recommendations. On the other hand, existing quantitative models often adopt a scope that is too large for appropriate, country-level policy analysis, focus mainly on technological and economic aspects, and are sometimes a black-box. This research therefore attempted to construct a transparent, quantitative simulation model that includes a wider perspective than techno-economic factors solely, and has a suitable scope for policy exploration. System dynamics has been widely applied before to model the diffusion of innovations and energy technologies, and a number of studies have assessed the diffusion of hydrogen vehicles with SD. However, the application of SD for simulation of the diffusion of sustainable hydrogen has until now not been conducted.

This study contributes to the scientific field of diffusion modeling, and energy system modeling for several reasons. First, the model is quantitative. Although the model has an exploratory character, the phenomena of technology diffusion is translated into mathematical equations and generates concrete, quantitative insights in the diffusion process. Second, the country-level scope has proven to be useful for the exploration of policies. Because of

the scope, real-world policies have been tested and concrete, executable recommendations are defined. Third, as one of the key features of SD, the model structure is very transparent and can be replicated. Assumptions and input values are transparent in the SD model, and can easily adjusted for future alterations. The transparency of the model structure is highlighted by the conclusions about the dynamics of the system and relation between parameters that are drawn. This does not imply that the outcomes of this research are superior to the results of existing studies, nor that the outcomes are impeccable. The research offers an alternative approach to the problem, and has its limitations. Nevertheless, this research can thus be considered as a novel application of SD for quantitative modeling and policy exploration of sustainable hydrogen diffusion on country-level perspective. Besides the insights in the behavior of the system and the effects of different policies, it offers a tool for further exploration through possibilities for model expansion, improvement of assumptions and parameters, and application to a different case country.

### 7.3 Societal relevance

Hydrogen is considered as a promising energy carrier that, if produced through a sustainable method, can contribute to the sustainable future energy system. It can support decarbonisation in hard-to-abate sectors and alleviate the grid congestion and storage challenges for electricity. The energy transition can be considered a grand challenge, and this research attempted to resolve a tiny bit of that puzzle. Although the outcomes of the model are always uncertain and can never be adopted as a certainty, societal contribution of this research can be found in two aspects. The model that is constructed for this research contributes to the understanding of the dynamics in the hydrogen supply chain system. Although in a simulation environment, it has become apparent where levers can be implemented in the system to achieve certain objectives. Moreover, the modeling outcomes show that without policies, green hydrogen will remain absent and will never contribute to a sustainable energy system. The policy analysis provides a set of guidelines for policy makers on how to support green hydrogen. Despite the exploratory nature of the policy analysis, this research might therefore contribute to the sense of urgency that measures and leverage are needed today and provides preliminary insight in how to do so.

### 7.4 Policy recommendations

The findings of this study are of use for policy makers to develop interventions aimed at supporting green hydrogen diffusion. The following recommendations are made:

- Acceleration of the diffusion of green hydrogen can only be achieved if hydrogen demand growth is fast-forwarded. CCfD's have shown to be an effective policy for demand creation in the steel sector, on condition that the predetermined strike-price is high enough. To accelerate demand in transport for FCEV-trucks, infrastructure construction should be accelerated, but it can be argued that the effects are minimal compared to the large costs of this policy.
- Demand-side policies must never be implemented without simultaneous activation of green hydrogen cost-reducing policies on the supply-side. If deployment of hydrogen takes-off in end-use sectors without accurate cost-reducing policies in place for electrolysis, affordable blue hydrogen will be the production method of choice getting the upper hand over green hydrogen in the long term.
- Cost-reducing measures for green hydrogen on the supply-side of the hydrogen supply chain are the most effective levers to promote green hydrogen production over blue hydrogen production and therefore inevitable. Electricity costs must be alleviated through tax exemptions and capital costs of electrolyzers reduced through subsidy.
- Timing of policies must be taken into account, and might be counter-intuitive. The cost-reducing policies on the supply side are more effective when their activation is postponed. The expected decreasing electricity costs amplify the effects of the policies,

resulting in a larger green diffusion on the long-term. Nevertheless, extending the duration of the policy would even be more beneficial.

- To achieve large-scale adoption of hydrogen, the combination of conventional measures and unconventional measures must be considered. A ban on CCS additional to conventional policy measures offers a pathway to proceed sustainable hydrogen production over fossil-dependent production and achieve green hydrogen targets. Policy makers must think of groundbreaking and innovative policies to provide incentives for consumption of hydrogen and at the same time lower the cost of green hydrogen.

## 8 Discussion

This section reflects on the methodology and discusses the limitations of the model and the policy analysis, and the implications of these limitations. Finally, this section provides suggestions for further research.

### 8.1 Reflection on the methodology

System dynamics has demonstrated to be an appropriate method for modeling the diffusion of hydrogen for several reasons. SD allowed for making the complex non-linear behavior and feedback loops of the system visible and understandable in a transparent, and quantitative manner. Because SD not only delivers quantitative model outputs, but provides insight in the entire system mechanism, SD fitted to the exploratory and strategic characteristic of this research. Furthermore, the problem contained a number of mechanisms for which SD has previously proven to be a suitable modeling method, such as learning-by-doing, and adoption of technology. Finally, the application of SD has appeared to be very appropriate for the aggregation level and the scope of research, since the examination of diffusion as continuous flows provided adequate outcomes for this level of perspective and at the same time allowed for country-level policy testing.

The limitations of system dynamics for this research are on the one hand in the inability to incorporate discrete events in the model. Although the research adopted an aggregated scope, the construction of hydrogen production facilities or transformation of steel plants can be considered discrete events. Discrete Event Simulation could be applied to a more detailed assessment of the hydrogen diffusion. Furthermore, because of the continuous SD-approach, the perspectives and objectives of individual actors such as investors and consumers in the hydrogen sector are not included in detail. This might offer alternative insights as the diffusion is now modeled based on cost-drivers predominantly. Agent-based modeling could be a suitable tool to investigate this. Another limitation of SD is the lack of possibility to include geographical aspects, which could in the future be approached with GIS-modeling. The infrastructure submodel could have been more accurate if geographical features could have been included, as this section is now established on several simplifying parameters.

### 8.2 Limitations of the model

#### 1. Simplification of the hydrogen supply chain structure

Several components of the real world hydrogen supply chain have been excluded from this research. Firstly, the potential for green hydrogen in the power sector is not assessed in this research. Some hydrogen outlooks and scenarios expect that this sector will have a major share (ranging from 10-200 TWh per year for examined literature) in the future total demand of green hydrogen (Böhm et al., 2020; Hydrogen Europe, 2020; Gasforclimate, 2021). Including the power sector could result in a rapid expansion in electrolysis capacity, since the essence of hydrogen in this sector lies in power-to-gas: converting renewable energy to a molecular energy carrier. Secondly, in line with the exclusion of the power sector, storage is not incorporated in this research. Storage might offer possibilities to store large quantities of renewable electricity in the form of hydrogen. The inclusion of storage possibilities will lower the price of renewable hydrogen, since the relation between production and demand becomes time independent through the decoupling hydrogen demand from the irregularity of green hydrogen production with sustainable electricity. Following this, the third simplification is the connection of electrolyzers to grid electricity in the model. Future electrolyzer capacity might be connected to dedicated renewable electricity plants, lowering costs and the footprint of green hydrogen. On the production side, upcoming technologies such as biomass gasification and photolytic hydrogen production have not been assessed. These technologies currently are immature, but it is uncertain how these will develop technologically and economically towards the future. Finally, the potential for import and export of hydrogen is ignored. A possible future scenario for hydrogen in Germany would comprise a large share of imported hydrogen. Germany is already targeting contacts around the globe that

could potentially produce cheap green hydrogen for long-distance transmission to Germany (Pflugmann & De Blasio, 2020; BMWi, 2020; Gasforclimate, 2021).

## 2. Learning-by-doing is assumed on a national level

Learning of technology is incorporated in the model with a learning rate that was adopted from literature (Schmidt et al., 2017). A note of caution is due here since the learning of technologies does not occur on a national level, rather on a global level. The learning rate was found by Schmidt et al. (2017) based on the cumulative experience on a global level (24GW in 2015), but is applied in the model for a national level. This implies that the learning rate in the model shows a too conservative effect on the price, since learning on a global scale is simultaneously in process.

## 3. Exclusion of unit size growth

In line with the limitation in the learning rate, unit scaling as an effect of cumulative adoption not regarded in the model. The electrolyzer capacity in the model is normalized, and therefore the unit size is not a factor in the model. Unit growth, or up-scaling is the expansion of size or performance of a technology, which can lead to unit cost reductions through economies of scale (Luiten & Blok, 2003; Wilson, 2012).

## 4. Imaginary model parameters

There are a few model parameters that have no tangible real-world counterpart that make a limitation of the model. First, already extensively discussed throughout the research are the multinomial logit functions. The parameters for these function have major influence on the outcomes, although their value remains ambiguous and uncertain (van Vuuren, 2007). Altering the logit values could have resulted in a different diffusion of green hydrogen, but this is hard to predict since its effects are interconnected with the other components of the model. Second, the abstraction of the infrastructure component shows limitations through the assumed required infrastructure per unit of demand. Although this value is estimated from literature (Baufumé et al., 2013; Reuß et al., 2017), it remains a rough estimation. It is derived based on scenarios that adopt alternative assumptions than the current study. This makes validation a difficult process and might explain the surprisingly low model sensitivity to the infrastructure submodel, and the unexpected limited effects of the infrastructure policies.

## 5. Inadequate investment response

The oscillating investment behavior that is detected in the pathway of green and blue production capacity is a result of the model decision on investment in new capacity. The mechanism behind this behavior is extensively discussed in section 6.2.5. As demonstrated, altering the investment behavior structure would affect the diffusion pathway of green hydrogen to a more smooth incline. However, artificially polishing model behavior is not preferred, consequently the widespread elaboration about this issue throughout the research. When considering the implications of this limitation on the model outcomes, the model artefact leads to an oscillation with a period of approximately 12 years. It can otherwise be discussed that this model behavior resembles real world market oscillation as a consequence of the bullwhip-effect (Forrester, 1997), indicating delays and inadequate response to shortages in a supply chain. Alternatively, it could be attributed to the so-called ketchup bottle effect occurs in the hydrogen sector, where there will be a tipping point in hydrogen demand after which investments in green hydrogen production surge, causing the overshoot of production (Collins, 2021).

## 7. A note of caution on system dynamics modeling

It should be taken into account that the representation of the hydrogen supply chain remains an abstraction of the modelers vision on the real-world system. Although a bias in the model construction will always be present in system dynamics modeling (Sterman, 2000), this is limited as much as possible through careful construction of the model components and selection of data input. The input data is adopted from reliable sources, and if possible validated with alternative research. Similarly, the final model structure is a product of different knowledge sources from literature about the hydrogen supply chain system and

the fundamentals of technology diffusion combined. Furthermore, the model is tested with the conventional methods for system dynamics validation. Nevertheless, a general note of caution is due here. First, the model is not validated by an expert's eye. The opinion of an expert in the field could have shed new light on the model structure or the assumptions that have been made. Second, more generally on system dynamics, the objective of system dynamics modeling is to provide insight in the dynamics of a system and moreover the dynamics of a problem (Sterman, 2000). From that thought, the interpretation of the results of this study must be done with care. The model is tested and its outcomes provide insight in the system's behaviour, but with the model limitations described above in mind, the quantitative results of this study must be interpreted with care.

### 8.3 Limitations and implications of the model analysis

#### 1. Inclusion of other drivers for diffusion

The model only adopts technological, economic, and regulatory drivers for the diffusion of green hydrogen, which are abstracted with techno-economic input parameters, exogenous price variables and policy levers. Other drivers for diffusion that are not included in the model but which are present apparent from the drivers obtained from in the literature study are societal and environmental drivers. For example, McDowall et al. (2006) states that the carbon emission reduction targets are an important driver for green hydrogen. In the same way Ruijven et al. (2008) include air pollution as a driver for the transition to sustainable energy technologies and hydrogen. This model restrains in the exclusion of these type of drivers, who's inclusion would on the one hand have increased uncertainty of the model outcomes, but on the other hand have provided a more holistic view on the diffusion of green hydrogen.

#### 2. Limited scenario testing opportunities

The use of System Dynamics is very useful for exploring the behavior of a system in an exploratory matter and offers the opportunity to test model sensitivity and policy sensitivity. However, the use of System Dynamics is constrained for policy analysis through the limited options for further model exploration and policy analysis. It demands time-consuming manual input, what restricts the research to conduct only so much model analysis runs. This research therefore conducted an analysis for two exogenous scenarios and four policy scenarios in different combinations, resulting in a total of 54 tested combinations. Although this supplies information about the effects of the policy severity and timing for the outer boundaries considered legitimate for this system, its limitation lies in the search to more plausible scenarios and quantification of other scenarios in seek for the trigger for diffusion acceleration.

#### 3. Limited optimization possibilities

Similarly to the limited scenario testing possibilities in the Vensim-software package, the options for optimization of model outputs is limited as well. For complex models, the optimization tool is not appropriate to find best policy configurations. This leads to a shortage on insight in the true optimal policy package for diffusion acceleration. It has become apparent how the system responds to different policies and in what region of settings to seek for optimal outcomes, but a pathway of how and when the policies should be activated is not found and needs further investigation.

#### 4. Exclusion of constraints to growth

This study assumes only a number of constraints to the diffusion of hydrogen technologies based on infrastructure availability and relative costs. It would be interesting to assess the measured growth scenarios for their feasibility in other fields. There could potentially be unexpected limits to the diffusion rate of electrolysis, such as a limit in the manufacturing capacity of electrolyzers (Collins, 2021), resource constraints of scarce materials for fuel cells and electrolyzers (Kleijn & Van Der Voet, 2010; IRENA, 2022), societal constraints to the deployment of carbon capture and storage or renewable energy sources (Dickel, 2020), or a limitation in the availability of renewable electricity (FCH-JU, 2019). When assessing the

diffusion of green hydrogen, these amongst other real-world constraints should be kept in mind.

## 8.4 Recommendations for future work

There is first of all abundant room for progress in exploration of the policy options. Manual exploration could be extended through increasing the range of policy values and the time scope. The results of the current research require a prolongation in the form of testing even more policy combinations. It would be useful even to test the implementation of policies in the past to investigate a hypothetical diffusion rate. It is suggested that the implementations of even more unconventional policies can help in finding a more profound growth of green hydrogen, which might accentuate the necessity for fierce policy actions.

For further policy analysis, the use of automated model analysis tools is required. To investigate the effects of policies under deep uncertainty that accompanies the future energy system and test the policies for their robustness under uncertainty, further analysis of the system dynamics model should be conducted with the EMA-workbench (Kwakkel & Pruyt, 2013). This tool offers the possibility to examine the effects of policies over a myriad of possible scenarios. It also allows for robust optimization, to seek for the best policy configuration for model objectives.

As mentioned in the limitations, this research focuses on cost and technological drivers solely, and does not include the implications of other types of constraints. To develop a full picture of the hydrogen diffusion rate, other drivers besides cost and technological drivers should be considered in modeling and analysis. This would help policy makers to expand their view on the hydrogen supply chain to a more holistic perspective, and prevent for any constraints to growth from unexpected directions.

The outcomes of the policy analysis revealed the importance of the timing of the policies. Only preliminary conclusions about the timing of the policies are drawn in this research, but the implications for policy making are important. Further research should investigate the influence of timing on the policies in more detail. This might deliver fruitful insights for the more detailed design of green hydrogen policies, but might also result in a more profound understanding of the relation between policies and the system, and long-term policy making in the field of hydrogen diffusion.

The model utilizes Germany as scope. In future studies, it might be of possible value to apply the model to other countries or regions. The current research is conducted with all input parameters and variables for Germany, but could be applied to alternative countries with relatively little effort. It would on the one hand provide knowledge about the impact of the initial environment and existent hydrogen supply chain configuration on the outcome of policy levers. On the other hand it could be insightful to compare different case studies and adopt the lessons-learned from each case study into policy making.

Although a model is never finished, it is suggested that the model is improved on a few aspects for further research. First, it should be assessed what the value of the missing model components in each link of the supply chain would be and if these should be added to the model. In case it is deemed of added value, these components (power sector, biomass gasification hydrogen production) should be added to the model structure. Furthermore, the model should be validated with the eyes of an expert in the field, to discover model flaws that are currently possibly present in the model due to the single view of the modeler of this study.

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## A Barriers to green hydrogen diffusion described in literature

The following table summarizes briefly the most predominant barriers to diffusion of green hydrogen from recent literature. The articles are displayed in a descending chronological order.

Table 8: Summarizing overview of barriers described in literature

Reference	Pub. Year	Identified barriers to the diffusion of hydrogen
(Ren et al., 2020)	2020	<ul style="list-style-type: none"> <li>Low maturity of technology and lack of equipment</li> <li>Incomplete standards and regulations for reliability and sustainability</li> <li>High costs of hydrogen and incompleteness of infrastructure</li> <li>Unclear public acceptance and safety concerns</li> <li>Lack of policies</li> </ul>
(IRENA, 2020)	2020	<ul style="list-style-type: none"> <li>High production costs of green hydrogen</li> <li>Lack of dedicated infrastructure</li> <li>Energy losses at each stage of the value chain</li> <li>Lack of value recognition and absence of hydrogen market</li> <li>Lack of renewable electricity</li> </ul>
(Maggio et al., 2019)	2019	<ul style="list-style-type: none"> <li>High costs of fuel cells and electrolyzers</li> <li>Absence of hydrogen infrastructure for consumer purposes</li> <li>Lack of hydrogen demand</li> <li>High costs of electricity for powering electrolyzers</li> <li>Little governmental financial support</li> </ul>
(Detz et al., 2019)	2019	<ul style="list-style-type: none"> <li>Low carbon emission</li> <li>High costs and low availability of sustainable hydrogen production methods</li> <li>Slow improvements in costs reduction of electrolysis technologies</li> </ul>
(Hanley et al., 2018)	2018	<ul style="list-style-type: none"> <li>Absence of sustainable policies for hydrogen</li> <li>Small role for hydrogen in decarbonization targets</li> <li>Absence of hydrogen infrastructure</li> </ul>
(Astiaso Garcia, 2017)	2017	<ul style="list-style-type: none"> <li>Lack of government initiatives and support for infrastructure</li> <li>Lack of public knowledge about hydrogen as an option for sustainability</li> <li>Complex procedures among involved authorities</li> <li>Social acceptance of hydrogen deployment as safe technologies</li> </ul>
(McDowall, 2014)	2014	<ul style="list-style-type: none"> <li>Absence of refuelling infrastructure for FCEV</li> <li>Immaturity of hydrogen technologies</li> <li>High capital costs of electrolyzers and fuel cells</li> </ul>

## B Conceptual differences between simulation methods

The following tables summarizes the conceptual differences between system dynamics and the two other conventional simulation methods for policy analysis.

Table 9: Comparison of SD and ABM (Nieuwenhuijsen et al., 2018)

	<b>System Dynamics (SD)</b>	<b>Agent-Based Modeling (ABM)</b>
Approach	Continuous	Discontinuous
Level	Macroscopic	Microscopic
Perspective	Aggregated	Disaggregated
Central concept	Feedback loops, information flow, and accumulations	Objectives, rules, and communication
System components	Stocks and flows of material and information	Agents and their relations
Simulation engine	Integration of time steps using Euler or Runge-Kutta Method	Event-based or sequential scheduling
Mathematics	Differential equations	Objective functions
Behavior	Centralized system behavior	Decentralized individual behavior. Emerging phenomena as a result of many individuals

Table 10: Conceptual differences between SD and DES identified by Lane (2000) and Brailsford & Hilton (2000)

	<b>System dynamics (SD)</b>	<b>Discrete event Simulation (DES)</b>
Perspective	Holistic; emphasis on dynamic complexity	Analytic; emphasis on detail complexity
Resolutions of model	Homogenised entities, continuous policy pressures and emergent behaviour	Individual entities, attributes, decision and events
Data Sources	Broadly drawn	Primarily numerical with some judgemental elements
Problems studies	Strategic	Operational
Model elements	Physical, tangible, judgemental and information links	Physical, tangible and some informational
Human agents representation	Boundedly rational policy implementers	Decision makers
Clients find the model	Transparent/fuzzy glass box, nevertheless compelling	Opaque/dark grey box, nevertheless convincing
Model output	Understanding of structural source of behaviour modes, location of key performance indicators and effective policy levers	Point predictions and detailed performance measures across a range of parameters, decision rules and scenarios
Time perspective	State changes are continuous	State changes occur at discrete points of time
Stochasticity	Models are deterministic	Models are by definition stochastic in nature
Object behavior	Entities or objects are treated as a continuous quantity, rather like a fluid, flowing through reservoirs or tanks connected by pipes	Objects in a system are distinct individuals, each possessing characteristics that determine what happens to that individual

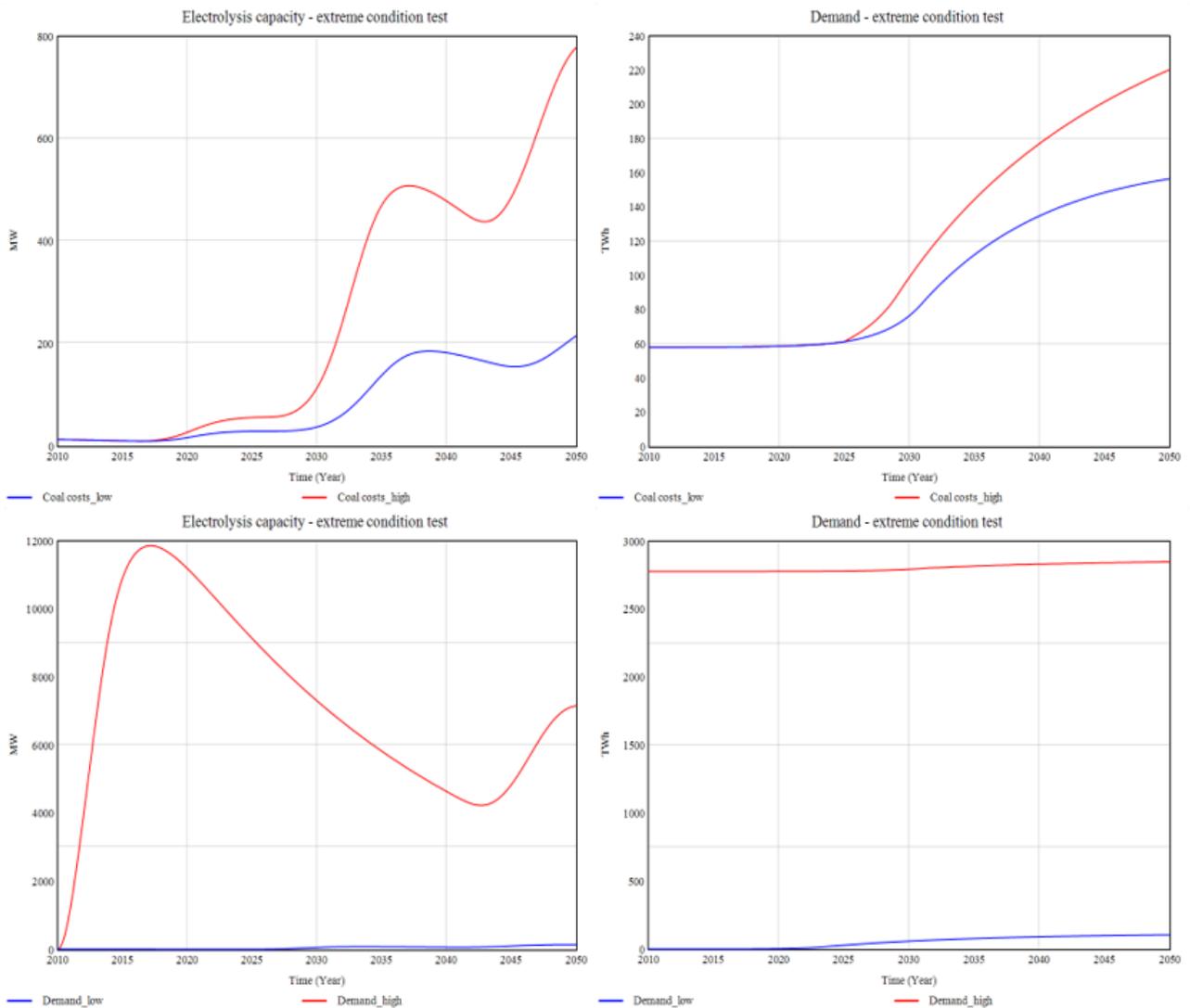
## C Verification and validation

### C.1 Extreme conditions test

The following graphs demonstrate the outcomes of the extreme condition test for electrolysis capacity and hydrogen demand. From top to bottom the following parameters are varied: Gas price, Existing Demand Chemical Industry, Initial CAPEX Electrolyzer, Electricity Price, Coal Price.

Tested Parameters	BC Value	Unit	Low extreme	High extreme
Gas Price	13	\$/MWh	0.0001	1000
Existing Demand Chemical Industry	58	TWh/year	0	1.00E+07
Initial CAPEX Electrolyzer	1000	\$/kW	0.0001	1.00E+07
Electricity Price	95	\$/MWh	0.0001	1000
Coal Price	40	\$/MWh	0.0001	1000

Table 11: Model parameter settings for the extreme value tests



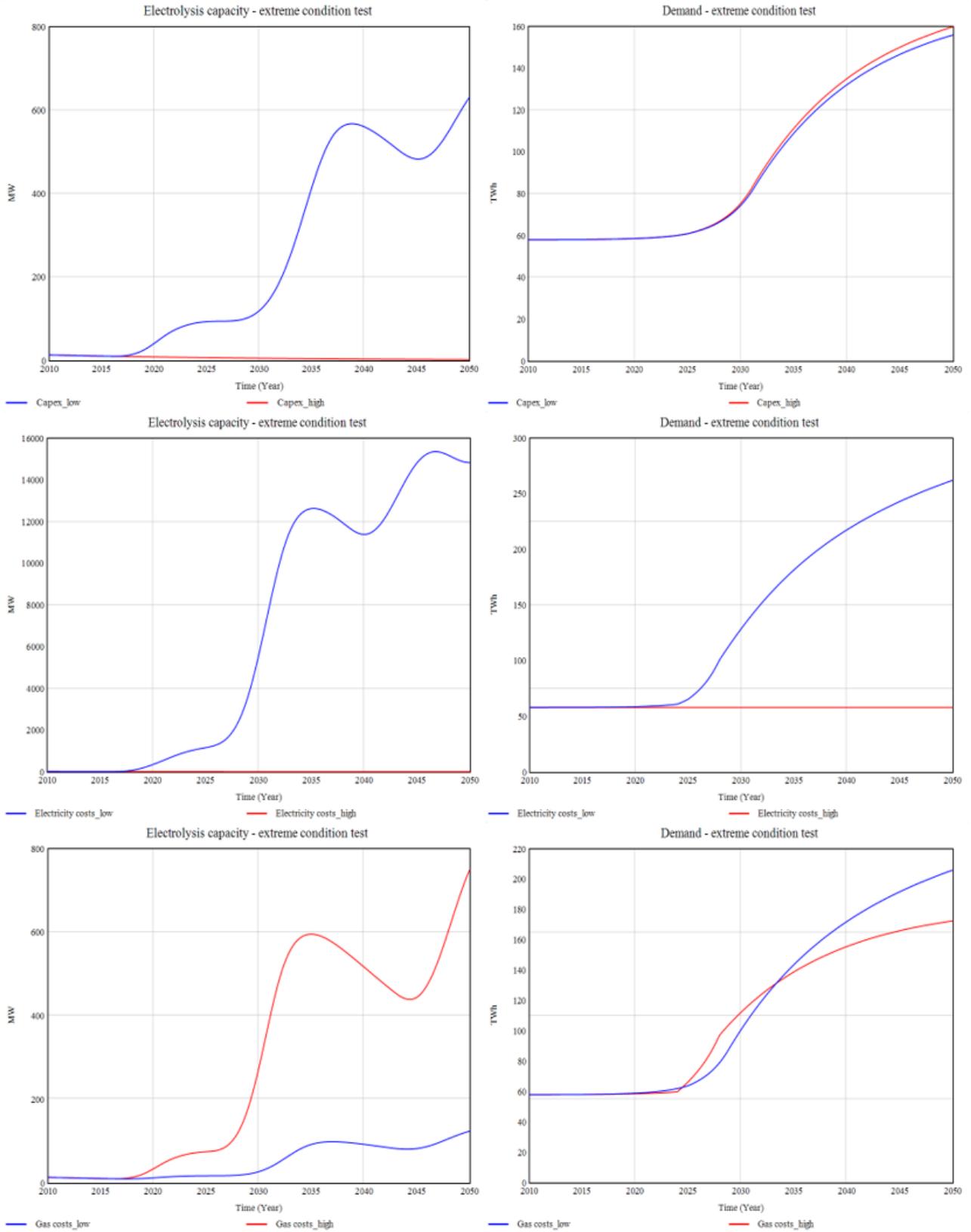


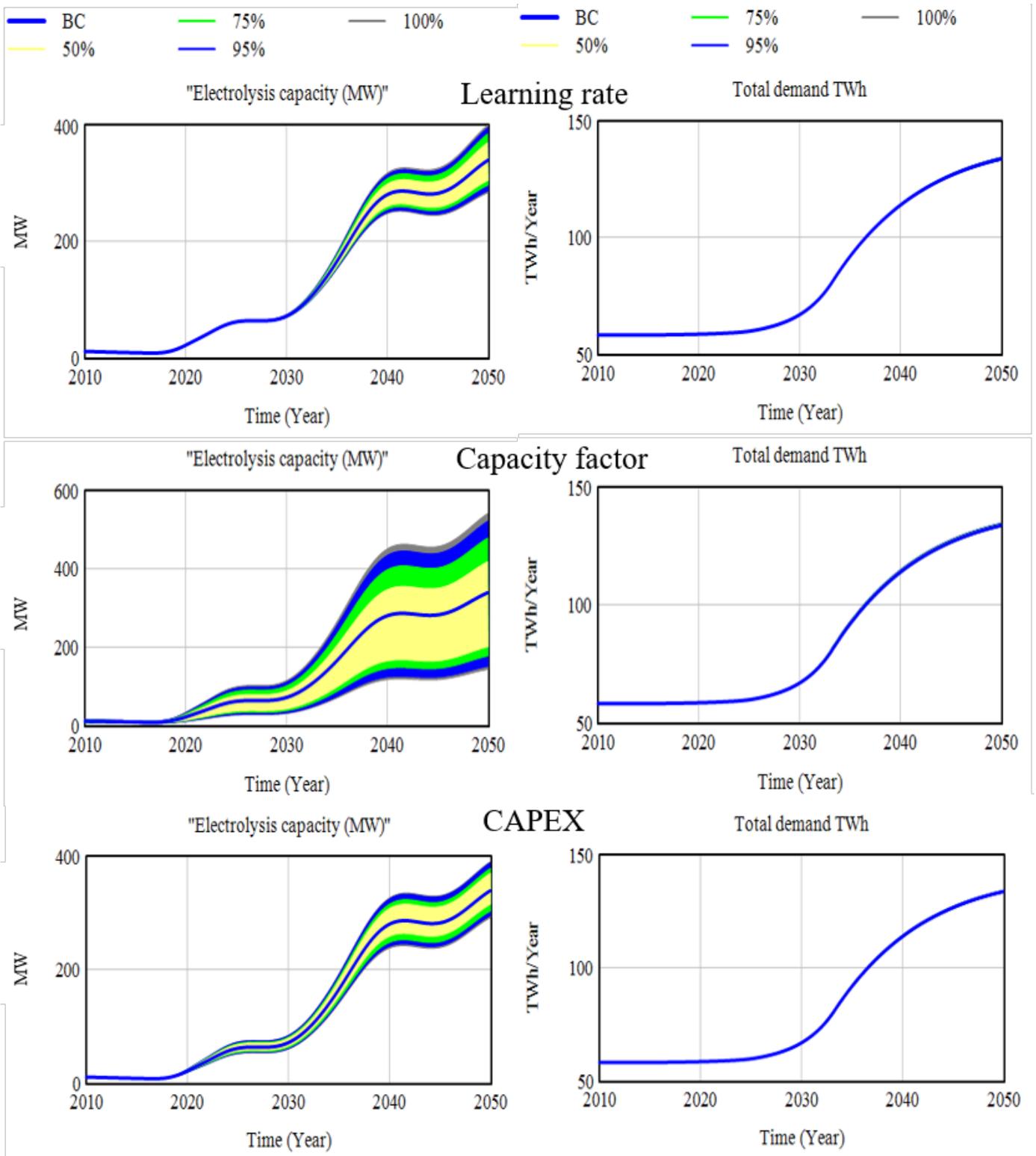
Figure 33: Results of the extreme condition test

## C.2 Sensitivity analysis

The following figures display the results of the sensitivity analyses. The varied parameters are denoted on top of the graphs and are varied for a  $\pm 10\%$  range. The logit parameters are varied extending the  $\pm 10\%$  range. The multivariate sensitivity is provided in the bottom figure, from which the logit parameters are also excluded. Below, the table with the input values for the sensitivity analysis is displayed.

Table 12: Sensitivity analysis input variables, BC values and upper and lower tested limits

<b>Tested model parameters</b>	<b>BC value</b>	<b>Lower</b>	<b>Upper</b>
Initial CAPEX electrolyzer	1000	900	1100
Learning rate electrolyzer	0.18	0.16	0.2
Capacity factor electrolyzer	0.9	0.81	0.99
Pipeline required	0.071	0.0639	0.0781
Logit parameter investment	-0.5	-1.5	-0.25
Logit parameter steel	-1.5	-3	-0.5
Logit parameter HDT	-1.5	-3	-0.5
Logit parameter blending	-4	-6	-2



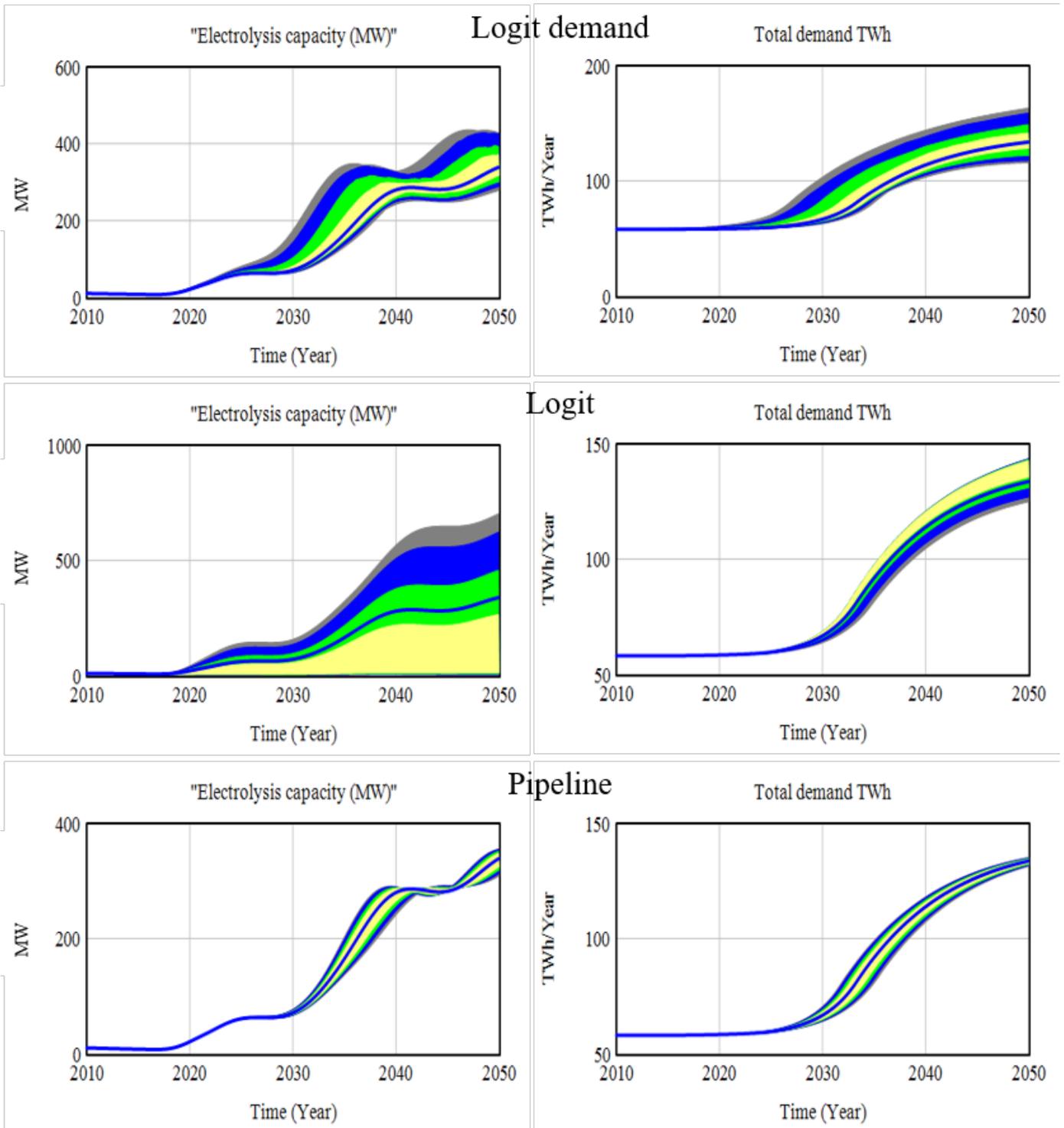


Figure 34: Results of the univariate sensitivity analysis

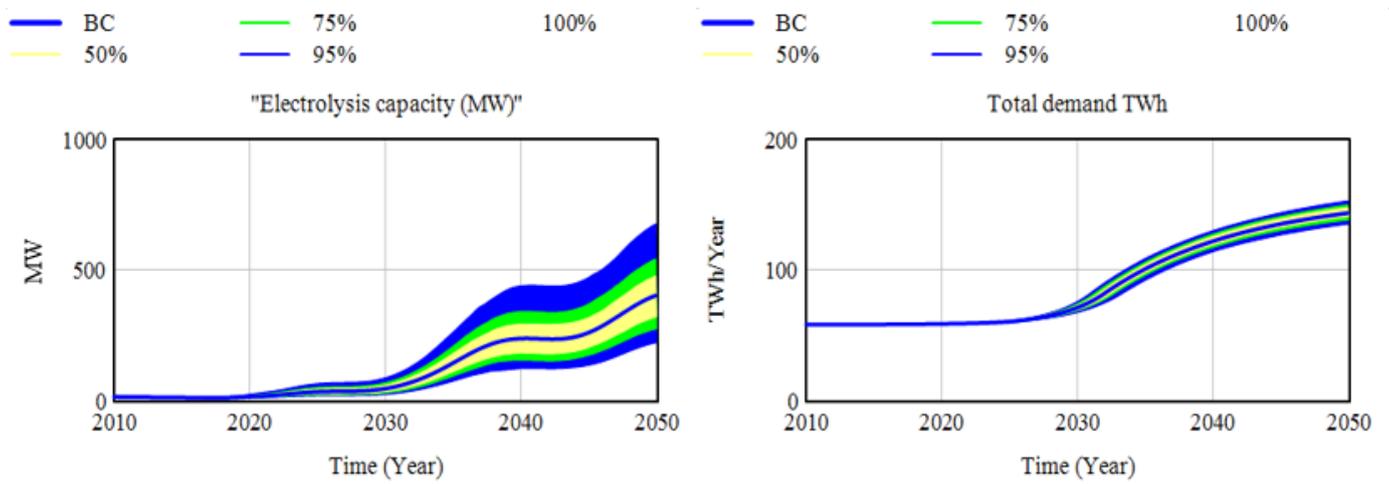


Figure 35: Outcome of the multivariate sensitivity analysis

## D Scenario Input

This appendix displays the conservative and progressive inputs for the energy and carbon prices for the two scenarios. The prices are based on the conservative, stated policy scenario STEPS, and the progressive, Net Zero Emissions scenario (NZE) (IEA, 2021). The costs are adopted without considering further assumptions of the IEA scenarios. In the graphs, the conservative costs are depicted in blue, the progressive costs in red.

Table 13: Cost input of the adopted exogenous variables for the two scenarios

Conservative scenario	Unit	2010	2020	2030	2040	2050
Electricity costs (grid)	\$/MWh	98,4	121,4	114,0	123,0	123,0
Natural gas costs	\$/MWh	39,9	28,9	29,2	30,4	31,5
Coal costs	\$/MWh	12,9	7,0	8,2	8,6	9,0
Carbon costs	\$/ton CO2	17,3	30,1	65,0	75,0	90,0
Progressive scenario	Unit	2010	2020	2030	2040	2050
Electricity costs (grid)	\$/MWh	98,4	121,4	54,5	40,0	30,0
Natural gas costs	\$/MWh	39,9	28,9	14,8	14,2	13,7
Coal costs	\$/MWh	12,9	7,0	7,5	6,9	6,3
Carbon costs	\$/ton CO2	17,3	30,1	130,0	205,0	250,0

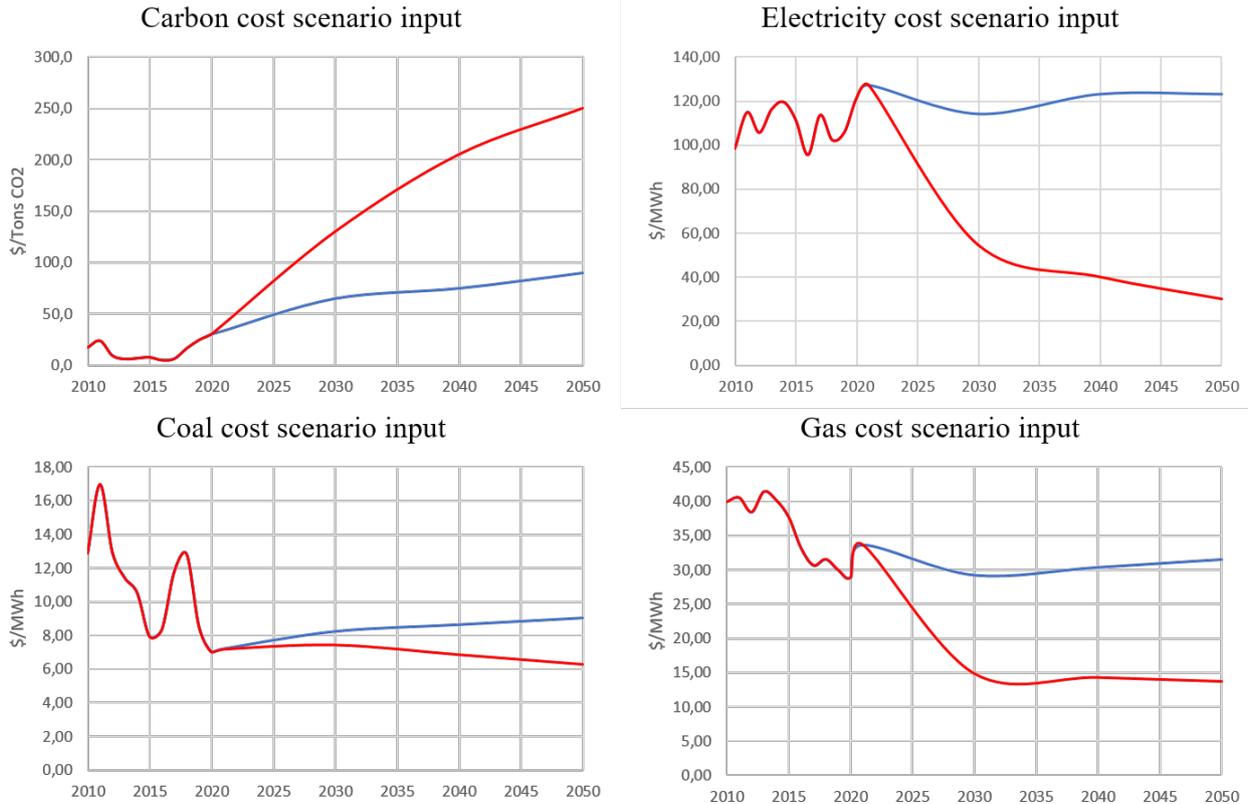


Figure 36: Cost curves of the adopted exogenous variables for the two scenarios

## E Parametric uncertainty analysis input

The following tables display the upper and lower uncertainty range of the parameters that are included in the parametric uncertainty analysis. The tables are categorized per submodel. The range is adopted from literature if stated, otherwise a range of  $\pm 10\%$ , or  $20\%$  is used as input, or else an assumed legitimate range based on model sensitivity.

Table 14: Parametric uncertainties in the production submodel

Parameters	Unit	BC value	Lower	Upper	Reference
LR of Alkaline electrolyzers	dmnl	0.18	0.12	0.24	Schmidt et al. 2017
Lifetime electrolyzer	dmnl	20	18	22	10%
Lifetime SMR	year	25	22	18	10%
Installation time ALK	year	2	1.8	2.2	10%
Lifetime CG	year	25	22	28	10%
Installation time CG	year	3	2.7	3.3	10%
Installation time SMR	year	3	2.7	3.3	10%
Capacity rate CG	%	0.95	0.9	1	Assumption
Capacity rate SMR	%	0.95	0.9	1	Assumption
CAPEX CG	\$/kW	2680	2144	3216	20%
CAPEX SMR	\$/kW	1680	1344	2016	20%
CCS costs CG	\$/kg CO2	0.0439	0.03951	0.04829	Parkinson et al.2019
"O&M fixed SMR"	% capex	0.047	0.0423	0.0517	10%
CCS costs SMR	\$/kg CO2	0.05	0.02	0.07	Gasforclimate, 2021
"O&M fixed CG"	% capex	0.03	0.027	0.033	10%
CG Carbon capture rate	%	0.9	0.85	0.95	Parkinson et al. 2019
SMR Carbon capture rate	%	0.95	0.86	1	10%
Electricity consumption CG	kWh/kg	1.5	1	2	CCS Institute, 2019
Electricity consumption SMR	kWh/kg	1.9	1.4	2.4	CCS Institute, 2020
Capacity rate electrolyzer	%	0.9	0.7	1	Assumption
Efficiency SMR	%	0.69	0.65	0.7	IRENA, 2018
Efficiency CG	%	0.58	0.522	0.638	10%
Emissions CG	kg CO2/kg H2	20.2	14.4	25.31	Parkinson et al. 2019
Emissions SMR	kg CO2/kg H2	8.9	8	10	Parkinson et al. 2019
Price reduction delay	year	2	1	3	Assumption

Table 15: Parametric uncertainties in the consumption submodel

Parameters	Unit	BC value	Lower	Upper	Reference
Max pipeline for full capacity	km	40000	36000	44000	10%
Distribution pipeline per TJ demand	km/TWh	0.071	0.04	0.16	Baufume et al 2013, Reuss et al. 2014
Transmission pipeline per TJ demand	km/TWh	0.021	0.015	0.06	Baufume et al 2013, Reuss et al. 2014
Share of retrofitting	%	0.69	0.13	0.69	Cerniauskas et al. 2020
Retrofit lifetime	year	40	36	44	IEA, 2020
Pipeline lifetime	year	40	36	44	IEA, 2020
Infrastructure investment response delay		5	3	7	Assumption
Investment smoothing time	year	1	0.5	1.5	Assumption

Table 16: Parametric uncertainties for the consumption submodel

Parameters	Unit	BC value	Lower	Upper	Reference
BF-BOF steel cost excl. var. costs	\$/tons	338	270.4	405.6	20%
HDRI steel cost excl. var. costs	\$/tons	408	326.4	489.6	20%
BF-BOF-H2 steel cost excl. var. costs	\$/tons	354	283.2	424.8	20%
CAPEX blending	\$/GJ	0.1	0.07	0.15	Assumption
"TCO Diesel excl. fuel"	\$/truck	604000	483200	724800	Roland Berger, 2020
"TCO FCEV excl. fuel"	\$/truck	919000	735200	1102800	Roland Berger, 2021
"TCO BEV excl. fuel"	\$/truck	1.20E+06	963200	1444800	Roland Berger, 2022
Blending rate volume	mass %	0.15	0.07	0.15	NREL, 2017; FCJHU, 2020
Fuel consumption FCEV	MJ/km	0.08	0.072	0.088	10%
Fuel consumption diesel	MJ/km	11.45	10.305	12.595	10%
Fuel consumption BEV	MJ/km	4.7664	4.28976	5.24304	10%
BEV learning	dmnl	0.013372	0.0120348	0.0147092	10%
FCEV learning	dmnl	0.008333	0.0074997	0.0091663	10%
"Coal consumption BF-BOF"	Ton/tons	0.707	0.5656	0.8484	20%
Electricity consumption BF-BOF	MJ/tons	1055	949.5	1160.5	10%
Carbon emissions BF-BOF steel	kg/tons	2200	1760	2640	20%
"CCS required BF-H2"	kg/tons	600	480	720	20%
H2 consumption HDRI	kg/tons	52	46.8	57.2	10%
Electricity consumption HDRI	MJ/tons	2731	2457.9	3004.1	10%
"H2 consumption BF-H2"	kg/tons	27.5	24.75	30.25	10%
"Coal consumption BF-H2"	kg/tons	0.6	0.48	0.72	20%
Carbon emissions BF-H2 steel	kg/tons	400	320	480	20%
Lifetime Blast Furnace	year	17	13.6	20.4	20%

Table 17: Parametric uncertainties in the emissions submodel

<b>Parameters</b>	<b>Unit</b>	<b>BC value</b>	<b>Lower</b>	<b>Upper</b>	<b>Reference</b>
Renewable share 2050	%	1	0.8	1	Fraunhofer 2020

Table 18: Parametric uncertainties in the logit functions

<b>Parameters</b>	<b>Unit</b>	<b>BC value</b>	<b>Lower</b>	<b>Upper</b>	<b>Reference</b>
Logit parameter	dmnl	-1	-1.5	-0.5	Assumption
Logit parameter HDT	dmnl	-4	-6	-2	Assumption
Logit parameter steel	dmnl	-1.5	-2	-1	Assumption
Logit parameter blending	dmnl	-4	-6	-2	Assumption

## F Parametric uncertainty analysis results

The following figures display the uncertainty envelopes that result from the parametric uncertainty analysis. The three KPI's; electrolysis capacity, demand and cumulative abated emissions are displayed with an uncertainty interval of 95%. The left graphs show the conservative scenario, the right shows the progressive outcomes. The red line indicates the alternative scenario.

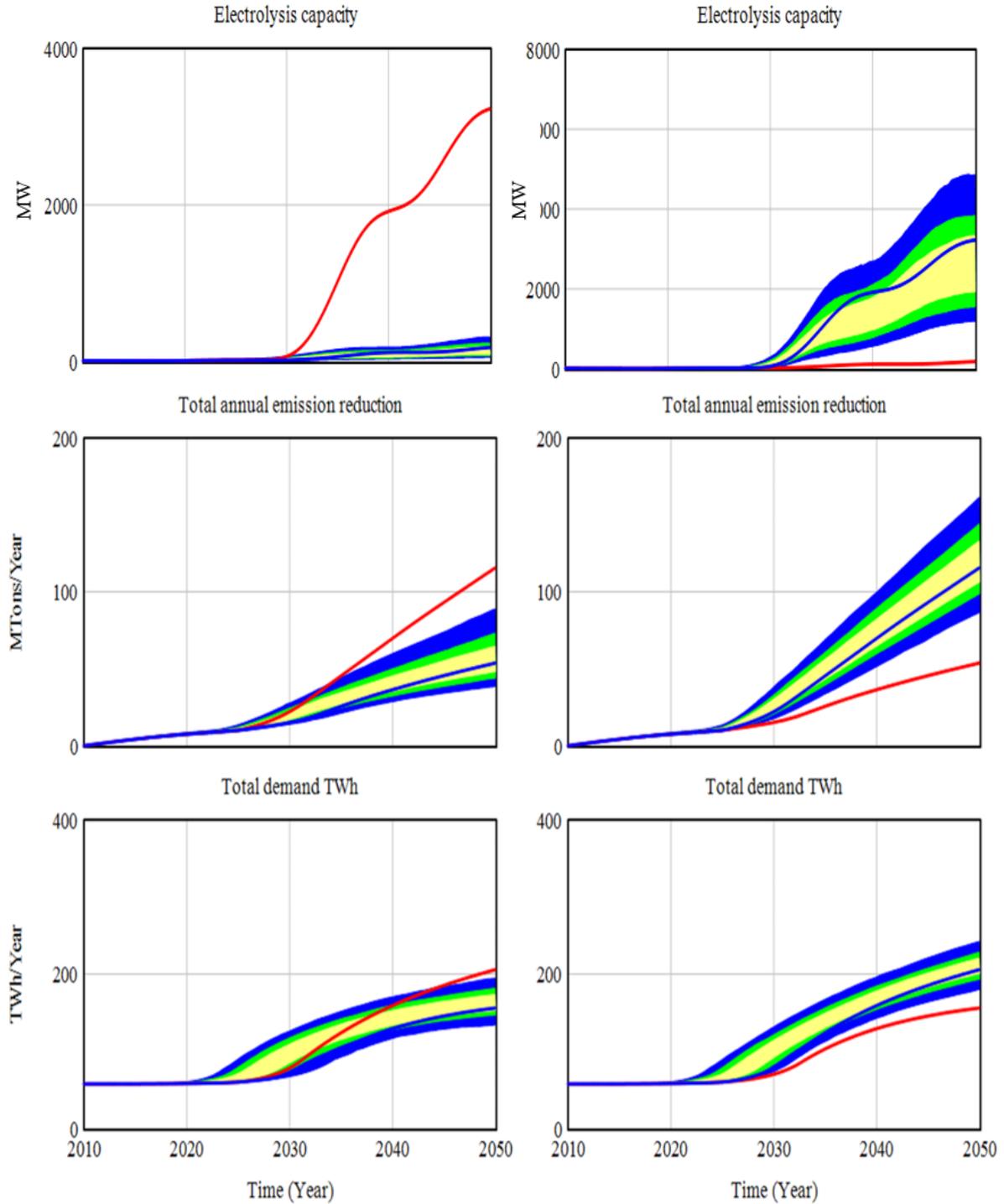


Figure 37: Outcomes of the parametric uncertainty analysis

## G Uncertainty in capital costs of alkaline electrolyzers

This table summarizes the values for the capital costs of alkaline electrolyzers from recent literature in a descending chronological order of publication year.

Table 19: Overview of the (expected) capital costs of alkaline electrolyzers from literature

Author	Title	Pub. year	Alk. electrolyzer costs [\$/kW]				Reference	Notes
			<2020	2020	2030	2050		
JRC TIMES	Blending hydrogen in the EU gas system	2022			426		(Kanellopoulos et al., 2022)	
Fraunhofer	Cost forecast for low-temperature electrolysis	2021		670-950	420-710		(Fraunhofer ISE, 201)	Cost range for 5 to 100 MW alkaline projects
IEA	Global hydrogen review 2021	2021		1000-1400	400-600		(IEA, 2021)	China electrolyzers around 1000 \$/kW. Average global costs for Alk. in 2020 is 1400 \$/kW
Hydrogen Council	Hydrogen insights 2021	2021		1120	250-300		(Hydrogen Council, 2021)	
Gas for Climate	European hydrogen backbone, analysing future demand, supply and transport of hydrogen	2021			270	133	(Gasforclimate, 2021)	System size: 100MW
IEA	The future of hydrogen	2020		900	700	450	(IEA, 2019)	
Bloomberg NEF	Hydrogen: The Economics of Production from Renewables	2019	2014: 2000	700-1200	115-135	80-100	(Bloomberg NEF, 2019)	
IRENA	Green hydrogen: A guide to policy making	2020		750-800			(IRENA, 2020)	
Böhm et al.	Projecting cost development for future large-scale power-to-gas implementations by scaling effects	2020	2017: 1100	1097	932	511	(Böhm et al., 2020)	System size: 5 MW, 800-1400\$/kW for 1-10MW systems in 2017.
Chilar et al.	Hydrogen generation in Europe: Overview of costs and key benefits	2020		600-2700	500-1600	200-800	(Cihlar et al., 2020)	Uncertainty about system configuration, resulting in large cost range.
Proost	State-of-the art CAPEX data for water electrolyzers, and their impact on renewable hydrogen price settings	2019		750	400		(Proost, 2019)	750 \$/kW for 5MW multi-stack electrolyzer, 400\$/kW requires upscaling to 100MW systems

IRENA	Hydrogen from renewable power: Technology outlook for the energy transition	2018		1090	695	(IRENA, 2018)	
Saba et al.	The investment costs of electrolysis	2018	1990's: 306 - 4748, 2014: 700		787- 906	(Saba et al., 2018)	Literature study to historical value of capex
Schmidt et al.	Future cost and performance of water electrolysis	2017		800- 1300	700- 1000	(Schmidt et al., 2017)	
Bertolucci et al.	Development of water electrolysis in the European Union	2014	2013: 1100	630	580	(Bertolucci et al., 2014)	
Smolinka et al.	Hydrogen production from renewable energies	2015	2010: 900- 3000			(Smolinka et al., 2015)	System size: 1.5 MW

## H Uncertainty in investment behavior

Additional graphs displaying the oscillation in the supply chain, as a result of phase lag between demand and supply. The first graph shows the supply and demand corresponding. The final three graphs show the oscillations of the supply-demand variable under different modeling methods.

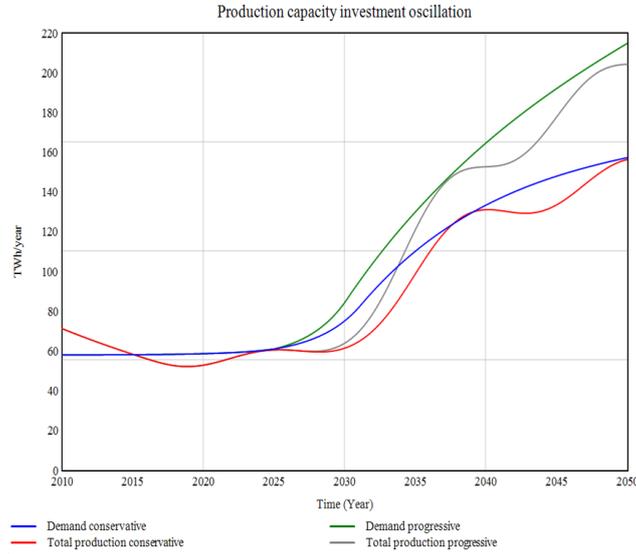


Figure 38: Demand and supply curves for both scenarios, showing the oscillating behavior of investments and periodical shortage of supply

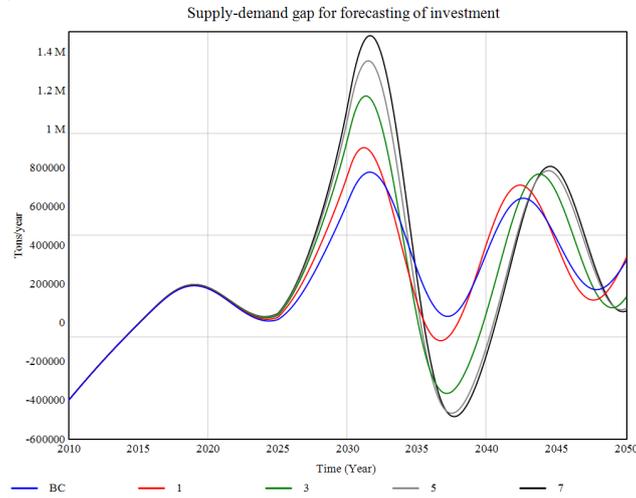


Figure 39: The gap between demand and supply in tons/year for different forecast windows of demand. The basecase (no multiplication) is denoted in blue. Longer forecast windows result in larger oscillations.

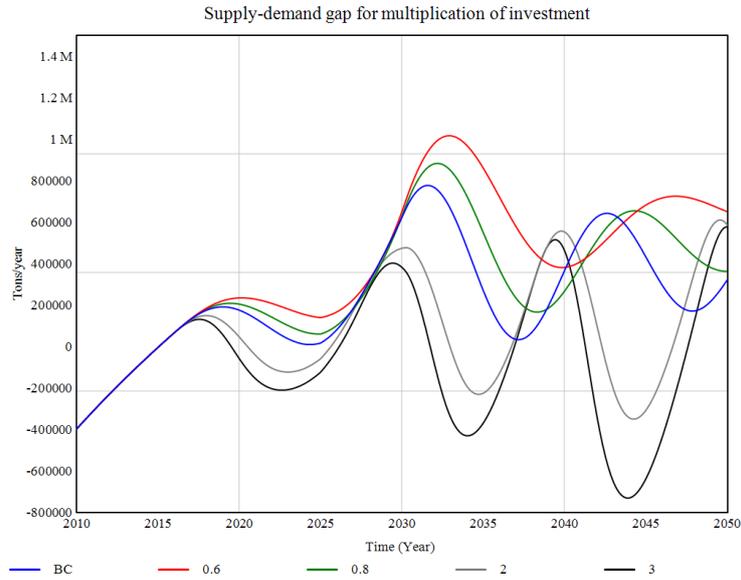


Figure 40: The gap between demand and supply in tons/year for different multiplications of investments in relation to demand shortage. The basecase (no multiplication) is denoted in blue. Multiplication by numbers below 1 has a damping effect on the oscillation. Multiplication larger than 1 increases oscillation.

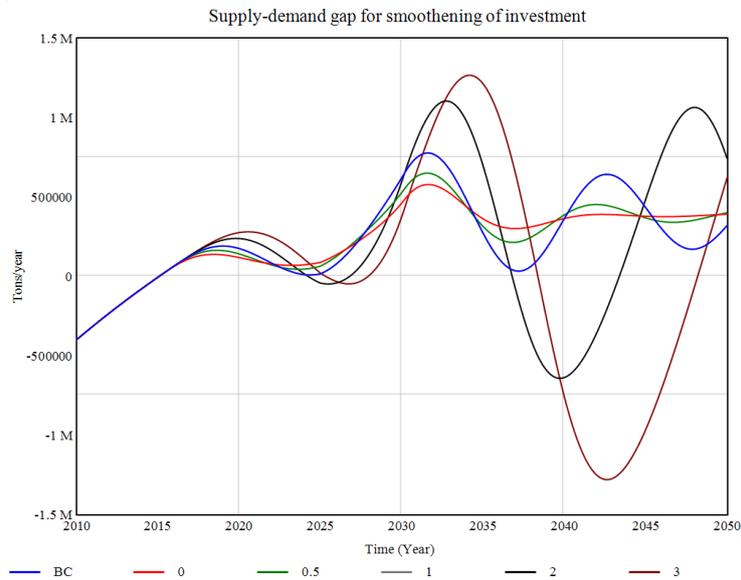


Figure 41: The gap between demand and supply in tons/year for different delay times between shortage and investments. The basecase (no multiplication) is denoted in blue. Reducing the delay time dampens the oscillation, and vice versa.

# I Policy settings for policy analysis

Table 20: Four different policy configurations diverging in strength and timing

<b>Low slow</b>	<b>Value</b>	<b>Unit</b>	<b>Start</b>	<b>End</b>
Electricity tax reduction	0.1	%	2028	2038
Electrolysis equipment subsidy	0.1	%	2028	2038
Carbon contracts for difference	200	\$	2030	2045
Grid blending quota	5	%	2030	
Infrastructure investment support	500	km	2028	2033
Coal phase-out	2030	-	2030	
Fossil-fuel tax	0.06	\$/kgCO <sub>2</sub>	2021	
<b>Low fast</b>	<b>Value</b>	<b>Unit</b>	<b>Start</b>	<b>End</b>
Electricity tax reduction	0.1	%	2022	2032
Electrolysis equipment subsidy	0.1	%	2022	2032
Carbon contracts for difference	200	\$	2023	2038
Grid blending quota	5	%	2025	
Infrastructure investment support	500	km	2022	2027
Coal phase-out	2030	-	2030	
Fossil-fuel tax	0.06	\$/kgCO <sub>2</sub>	2021	
<b>High slow</b>	<b>Value</b>	<b>Unit</b>	<b>Start</b>	<b>End</b>
Electricity tax reduction	0.4	%	2028	2038
Electrolysis equipment subsidy	0.3	%	2028	2038
Carbon contracts for difference	300	\$	2030	2045
Grid blending quota	20	%	2030	
Infrastructure investment support	2000	km	2028	2033
Coal phase-out	2030	-	2030	
Fossil-fuel tax	0.06	\$/kgCO <sub>2</sub>	2021	
<b>High fast</b>	<b>Value</b>	<b>Unit</b>	<b>Start</b>	<b>End</b>
Electricity tax reduction	0.4	%	2022	2032
Electrolysis equipment subsidy	0.3	%	2022	2032
Carbon contracts for difference	300	\$	2023	2038
Grid blending quota	20	%	2025	
Infrastructure investment support	2000	km	2022	2027
Coal phase-out	2030	-	2030	
Fossil-fuel tax	0.06	\$/kgCO <sub>2</sub>	2021	

## J Additional policy analysis result tables

This appendix shows the effects of the tested policies on the model key performance indicators. The tables indicate the effects of each separate policy on the KPI for 2050. Each policy is tested in two scenarios with four policy settings. The graphs below demonstrate the outcomes of the separate policies for the four KPI's in the two scenarios.

Table 21: Impact of policy levers on electrolysis installed capacity for 2050

KPI	Electrolysis capacity (MW)							
	Conservative				Progressive			
Scenario	<i>LowSlow</i>	<i>LowFast</i>	<i>HighSlow</i>	<i>HighFast</i>	<i>LowSlow</i>	<i>LowFast</i>	<i>HighSlow</i>	<i>HighFast</i>
No policies	187				5227			
Electricity tax reduction	248	218	776	479	5556	5419	6756	6148
Electrolysis equipment subsidy	199	194	229	210	5537	5411	5537	5411
Carbon Contracts for Difference	195	193	229	209	4384	4822	5098	5107
Grid blending quota	189	186	196	180	5247	5178	5247	5178
Infrastructure investment support	187	184	188	172	5222	5099	5207	4819
Fossil fuel tax	192				5253			
Coal phase-out	341				5998			

Table 22: Impact of policy levers on hydrogen demand for 2050

KPI	Hydrogen demand (TWh/year)							
	Conservative				Progressive			
Scenario	<i>LowSlow</i>	<i>LowFast</i>	<i>HighSlow</i>	<i>HighFast</i>	<i>LowSlow</i>	<i>LowFast</i>	<i>HighSlow</i>	<i>HighFast</i>
No policies	158				215			
Electricity tax reduction	158	158	157	157	215	215	218,73	217
Investment support electrolysis	158	158	158	158	215	215	215	215
Carbon Contracts for Difference	163	164	158	178	190	197	211	217
Grid blending quota	159	160	163	164	216	216	219	220
Infrastructure investment support	158	159	158	160	215	215	215	217
Fossil fuel tax	162				277			
Coal phase-out	165				219			

Table 23: Impact of policy levers on cumulative abated carbon emissions for 2050

KPI Scenario <i>Policy setting</i>	Cumulative abated CO2 (Mtons)							
	Conservative				Progressive			
	<i>LowSlow</i>	<i>LowFast</i>	<i>HighSlow</i>	<i>HighFast</i>	<i>LowSlow</i>	<i>LowFast</i>	<i>HighSlow</i>	<i>HighFast</i>
No policies	882				1566			
Electricity tax reduction	878	880	863	867	1566	1563	1578	1565
Investment support electrolysis	882	882	880	880	1566	1563	1566	1563
Carbon Contracts for Difference	960	1013	880	1324	1202	1206	1516	1642
Grid blending quota	885	892	893	915	1569	1575	1577	1597
Infrastructure investment support	883	897	886	923	1567	1578	1568	1604
Fossil fuel tax	900				1580			
Coal phase-out	979				1623			

Table 24: Impact of policy levers on cumulative policy costs for 2050

KPI Scenario <i>Policy setting</i>	Policy costs (\$)							
	Conservative				Progressive			
	<i>LowSlow</i>	<i>LowFast</i>	<i>HighSlow</i>	<i>HighFast</i>	<i>LowSlow</i>	<i>LowFast</i>	<i>HighSlow</i>	<i>HighFast</i>
No policies	0				0			
Electricity tax reduction	77 M	23 M	1,206 B	197 M	333 M	43 M	2,209 B	316 M
Investment support electrolysis	256 M	96 M	200 M	78 M	1,655 B	640 M	1,655 B	640 M
Carbon Contracts for Difference	311 M	384 M	200 M	2,319 B	-2,726 B	-1,160 B	-2,377 B	-169 M
Grid blending quota	117 M	141 M	400 M	492 M	120 M	143 M	340 M	432 M
Infrastructure investment support	2,122 B	2,122 B	8,489 B	8,489 B	2,122 B	2,122 B	8,489 B	8,489 B
Fossil fuel tax	-37,518 B				-29,960 B			
Coal phase-out	0				0			

## J.1 Policy overview, conservative case

This figure visualizes the data from the above described tables. The graphs show the effect of the five hydrogen-specific policies (fossil-fuel tax and coal phase-out excluded) at the most effective setting per policy, for each KPI in the conservative case.

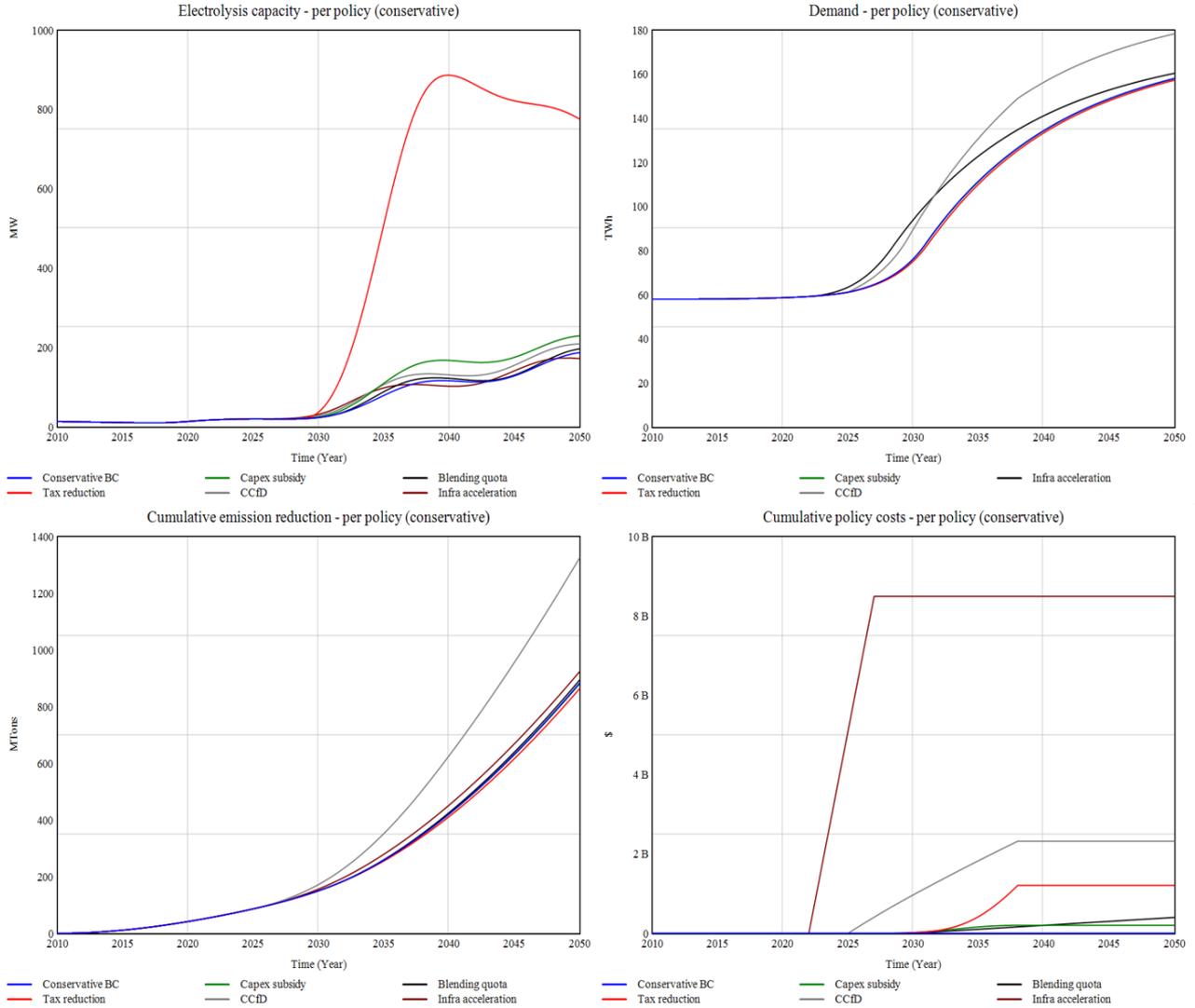


Figure 42: Overview of the separate policies in the *HighFast* setting on the four KPI's in the conservative case

## J.2 Policy overview, progressive case

This figure visualizes the data from the above described tables. The graphs show the effect of the five hydrogen-specific policies (fossil-fuel tax and coal phase-out excluded) at the most effective setting per policy, for each KPI in the progressive case.

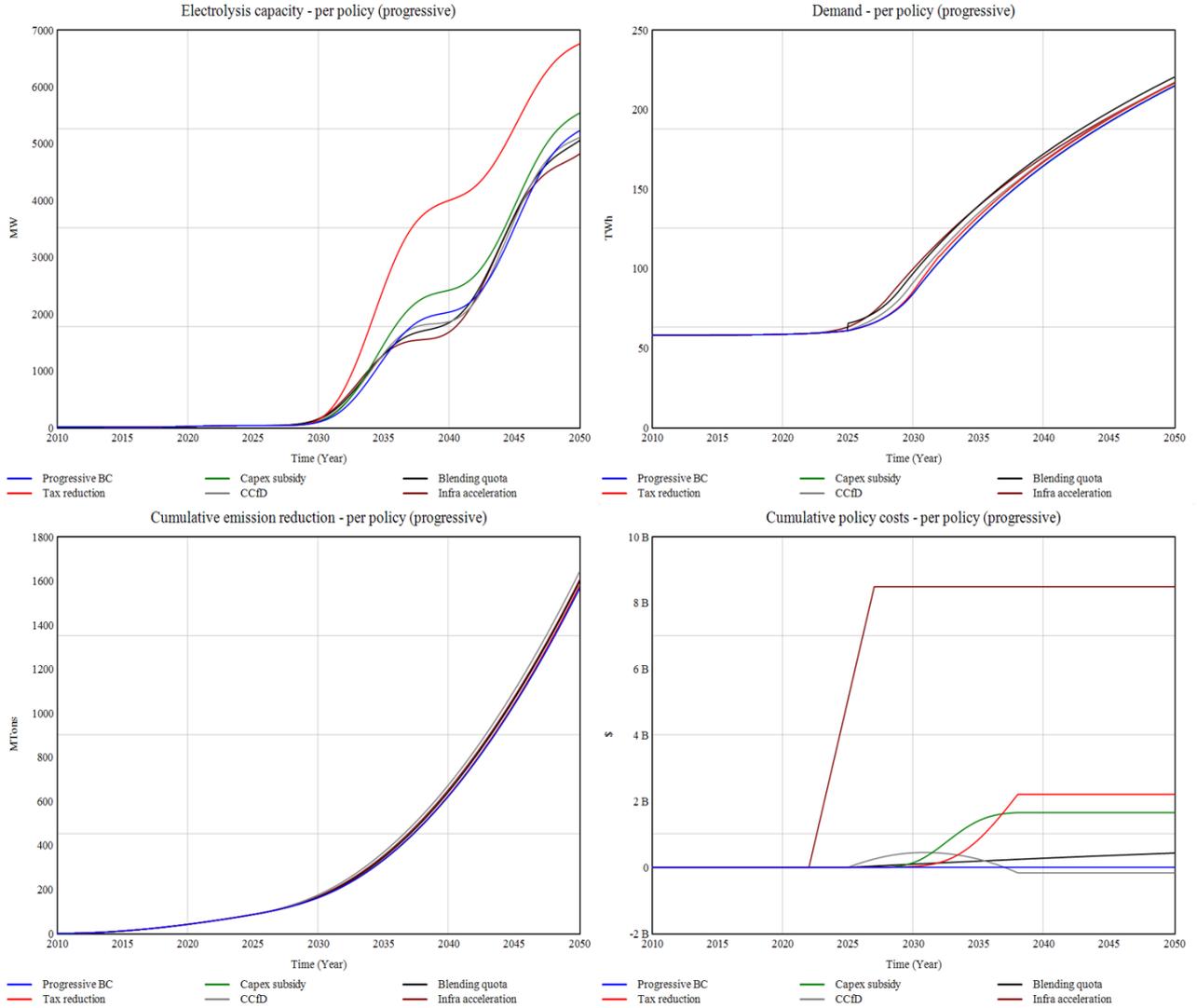


Figure 43: Overview of the separate policies in the *HighFast* setting on the four KPI's in the progressive case

### J.3 Policy outcomes for the combined policies

This table demonstrates the value of the four KPI's in 2050 for the combination of the best performing individual policies for the two scenarios.

Table 25: Outcomes of the KPI's under combined set of policies for 2050

Combined policies	Combined policies	
	Conservative	Progressive
Scenario		
<i>Policy setting</i>	<i>All best policies combined</i>	<i>All best policies combined</i>
<b>Electrolysis capacity (MW)</b>	1629	7244
<b>Hydrogen demand (TWh)</b>	191	236
<b>Cum. abated CO2 (Mtons)</b>	1336	1810
<b>Cum. policy costs (\$) <sup>2</sup></b>	-12.5687 B	-19.8724 B

## K Additional visualizations of the policy analysis outcomes

The following figures show the effects of each of the policies tested individually, on the following outputs: Demand, Levelized costs of green hydrogen, Annual emission reduction, Cumulative abated emissions, Annual policy costs, and Cumulative policy costs. The graphs show the baseruns for the conservative and progressive scenarios, and the two best performing policy settings for the progressive scenario (*HighSlow* and *HighFast*). The final set of graphs from appendix [K.8](#), indicate the outcomes of the combined policies, the CCS-ban, and the combination of the conventional policies and the CCS-ban.

## K.1 Electricity tax reduction

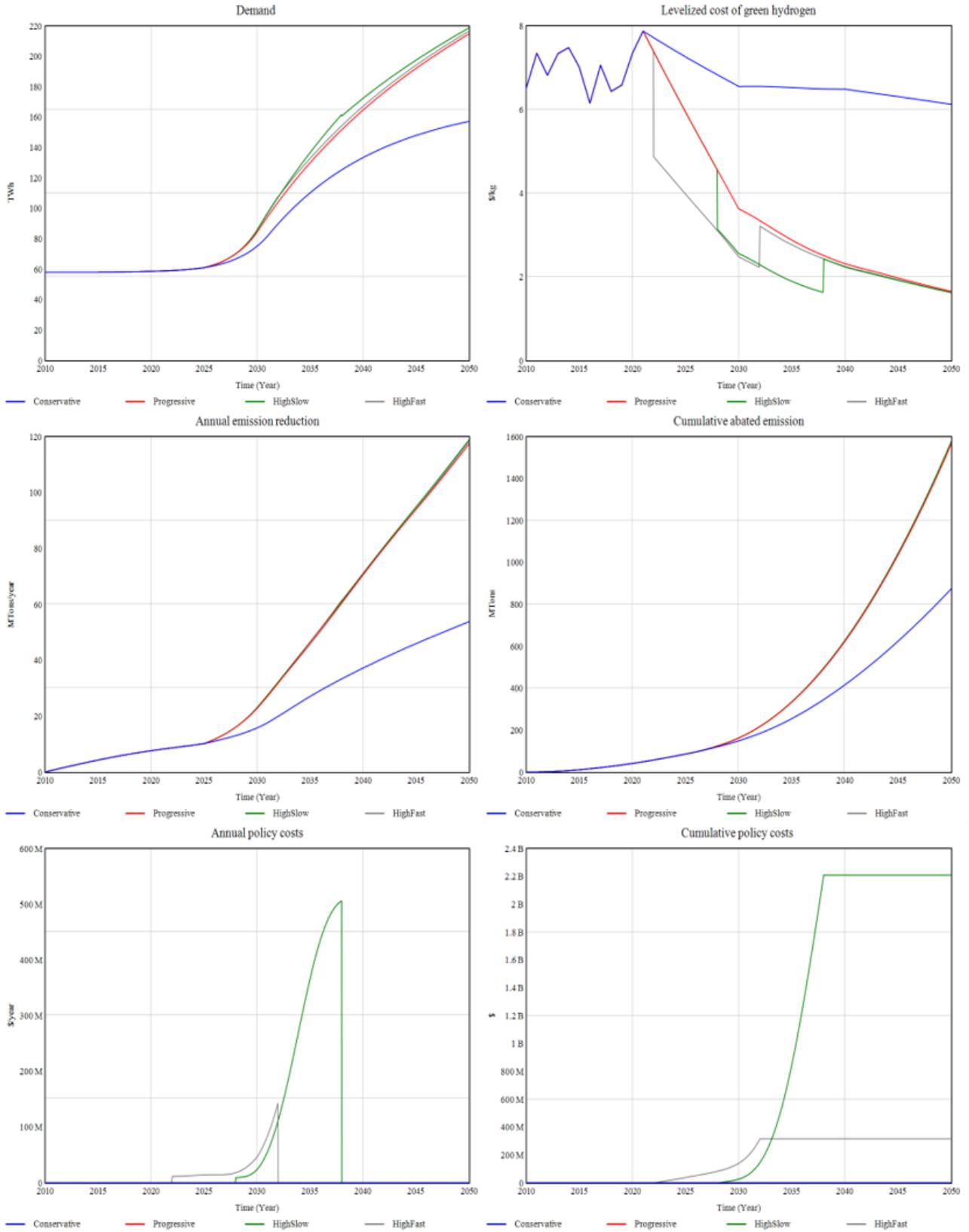


Figure 44: Additional results for electricity tax reduction policy

## K.2 Electrolyzer subsidy

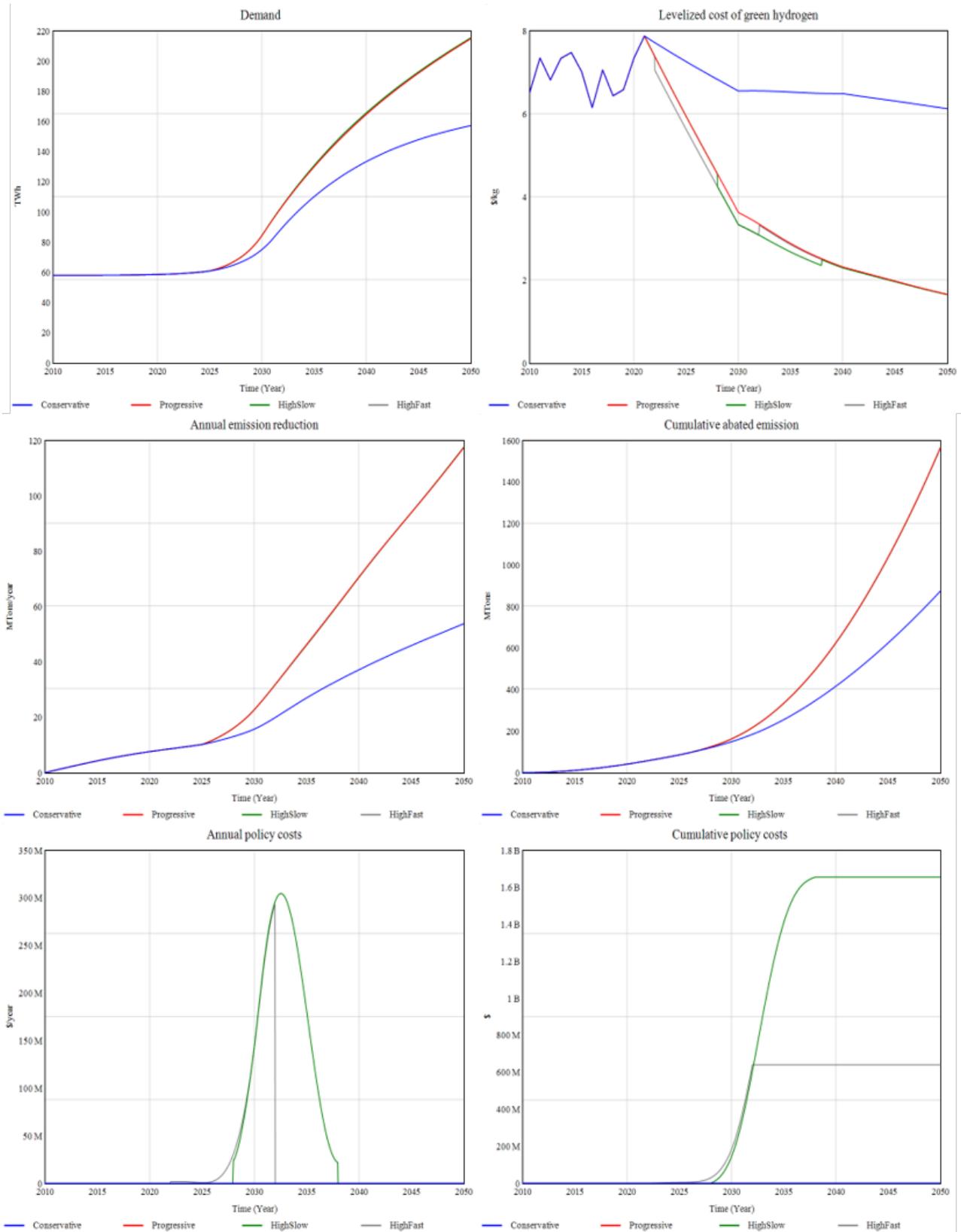


Figure 45: Additional results for electrolyzer subsidy policy

### K.3 Carbon Contracts for Difference

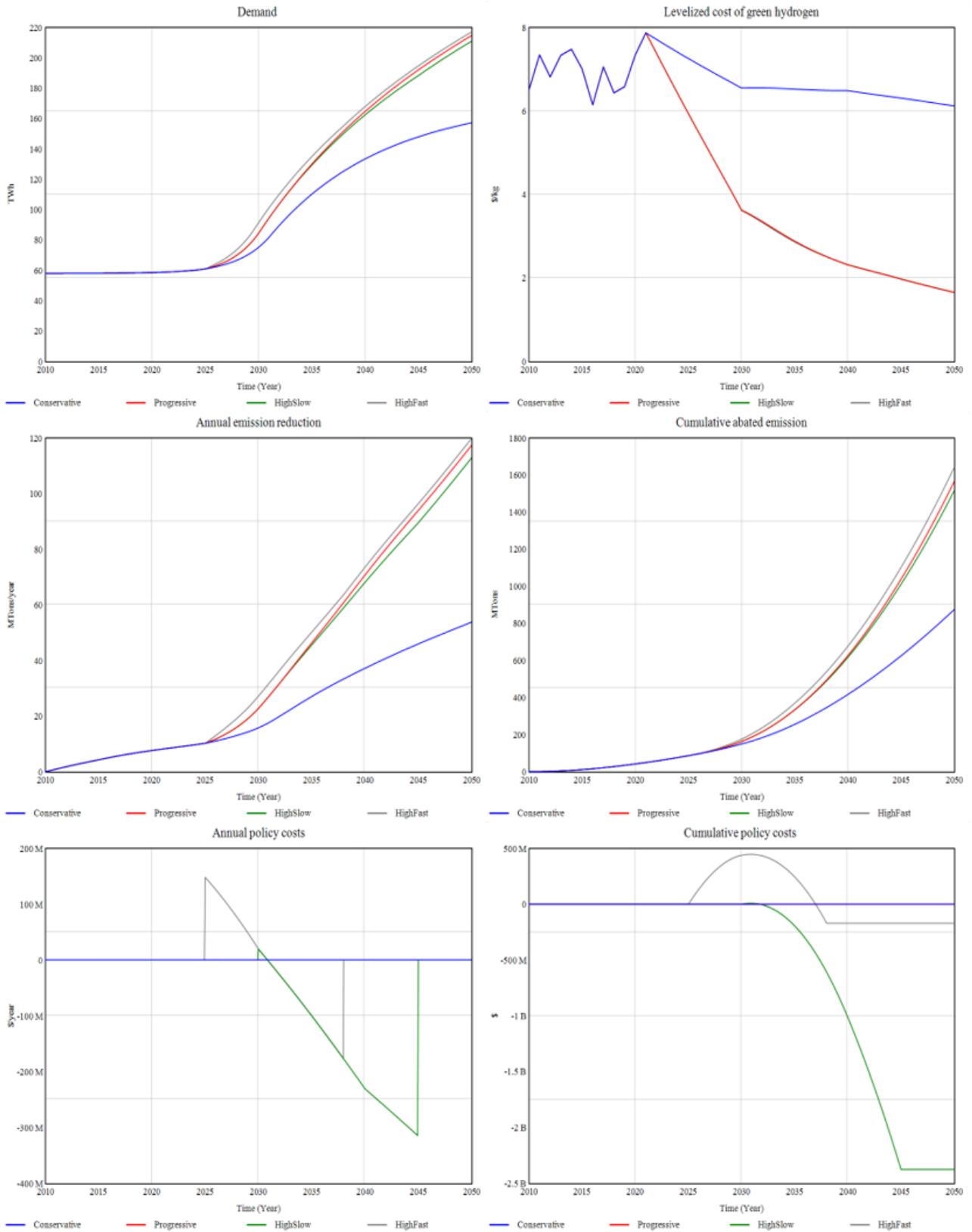


Figure 46: Additional results for Carbon Contracts for Difference policy

## K.4 Blending quota

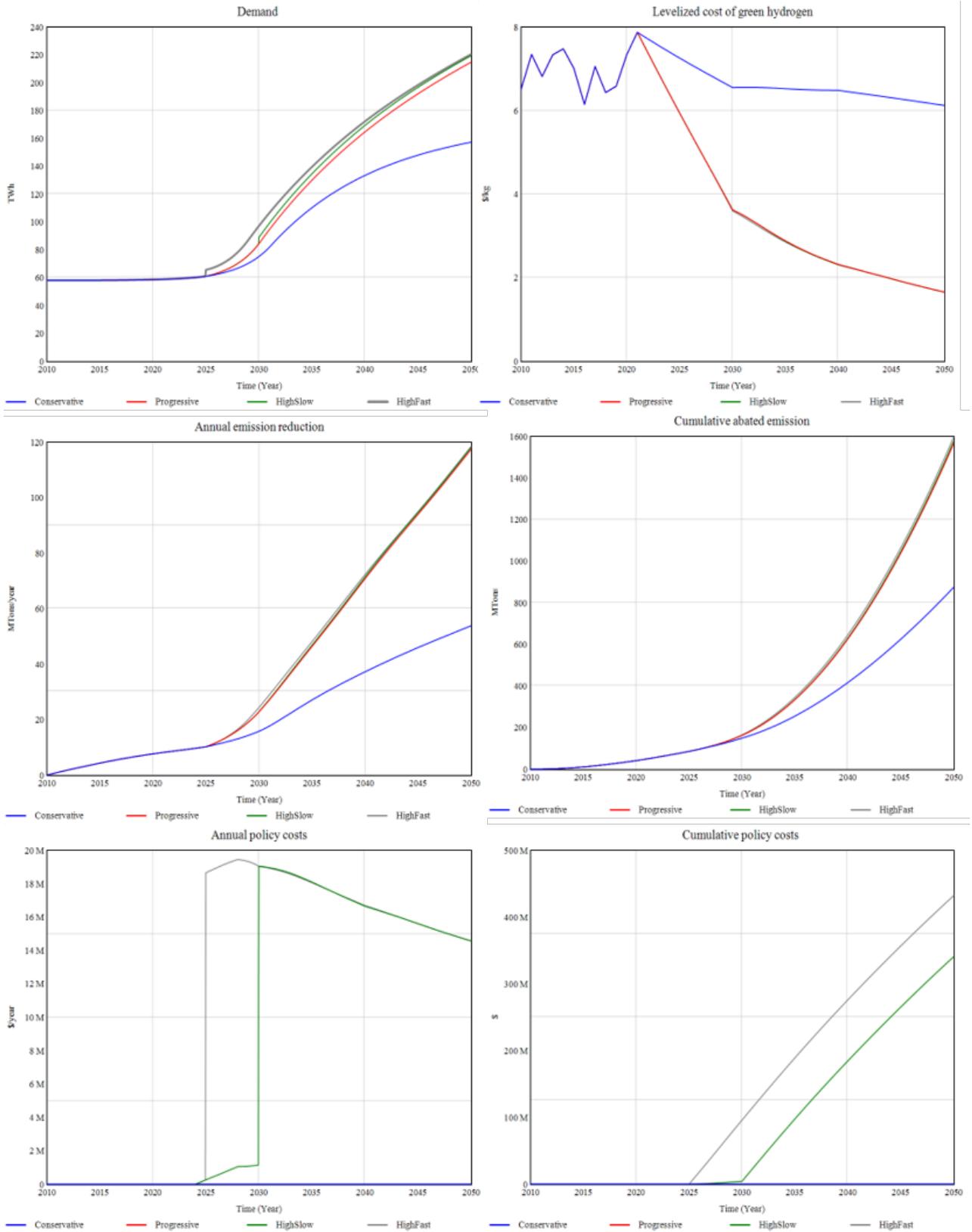


Figure 47: Additional results for Blending quota policy

## K.5 Infrastructure investment subsidy

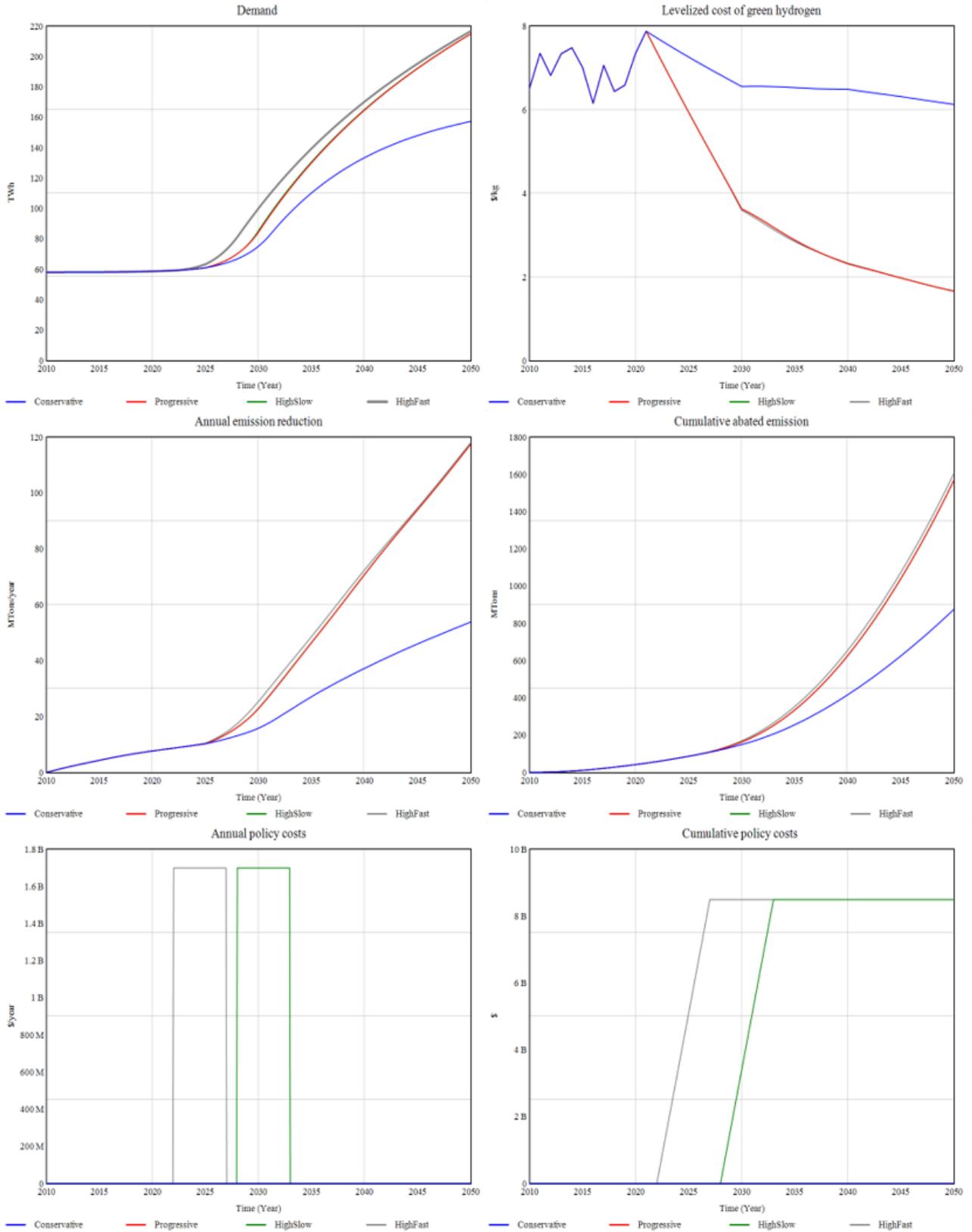


Figure 48: Additional results for Infrastructure investment subsidy policy

## K.6 Fossil fuel tax

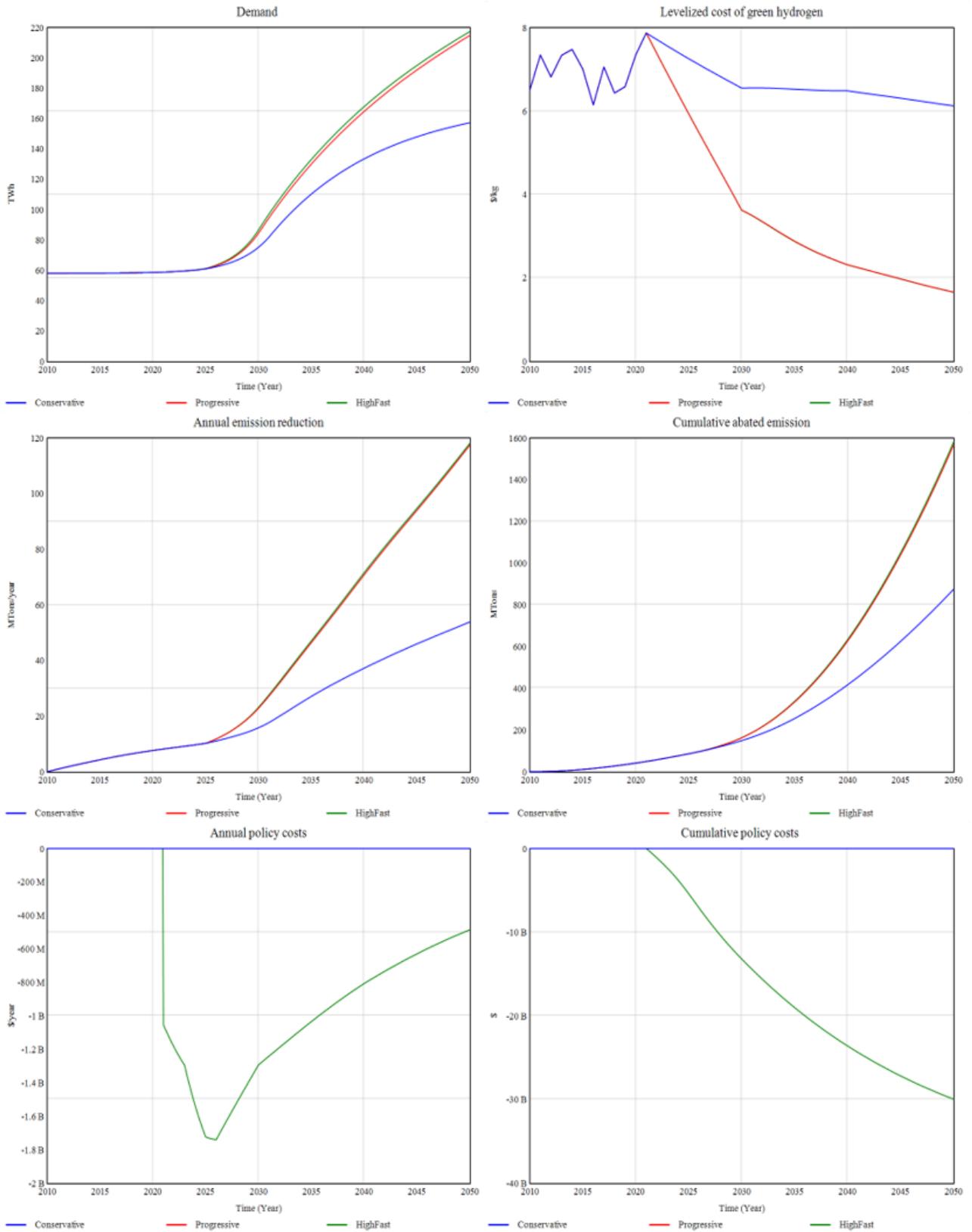


Figure 49: Additional results for Diesel tax policy

## K.7 Coal phase-out

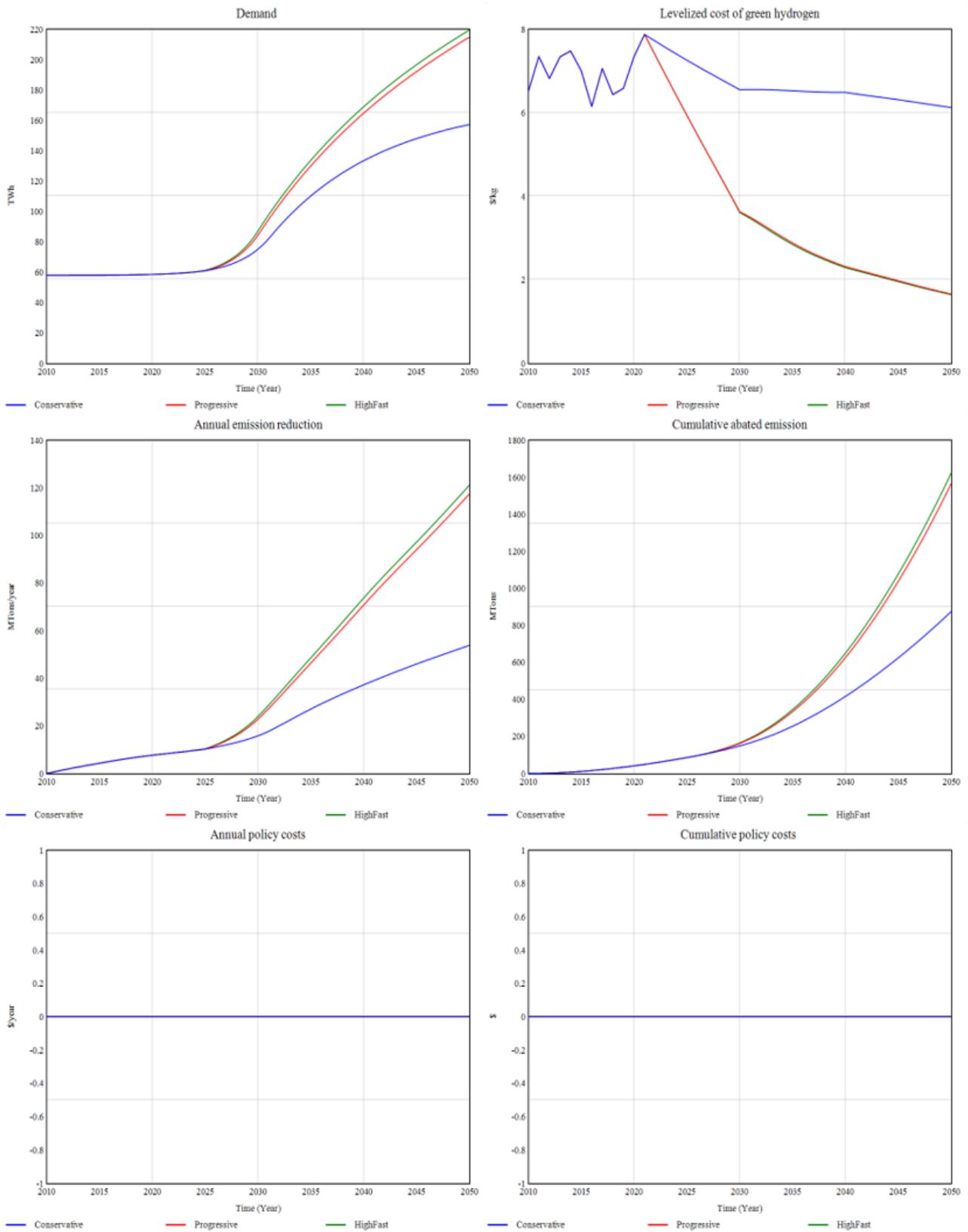


Figure 50: Additional results for Coal phase-out policy

## K.8 Combined policies

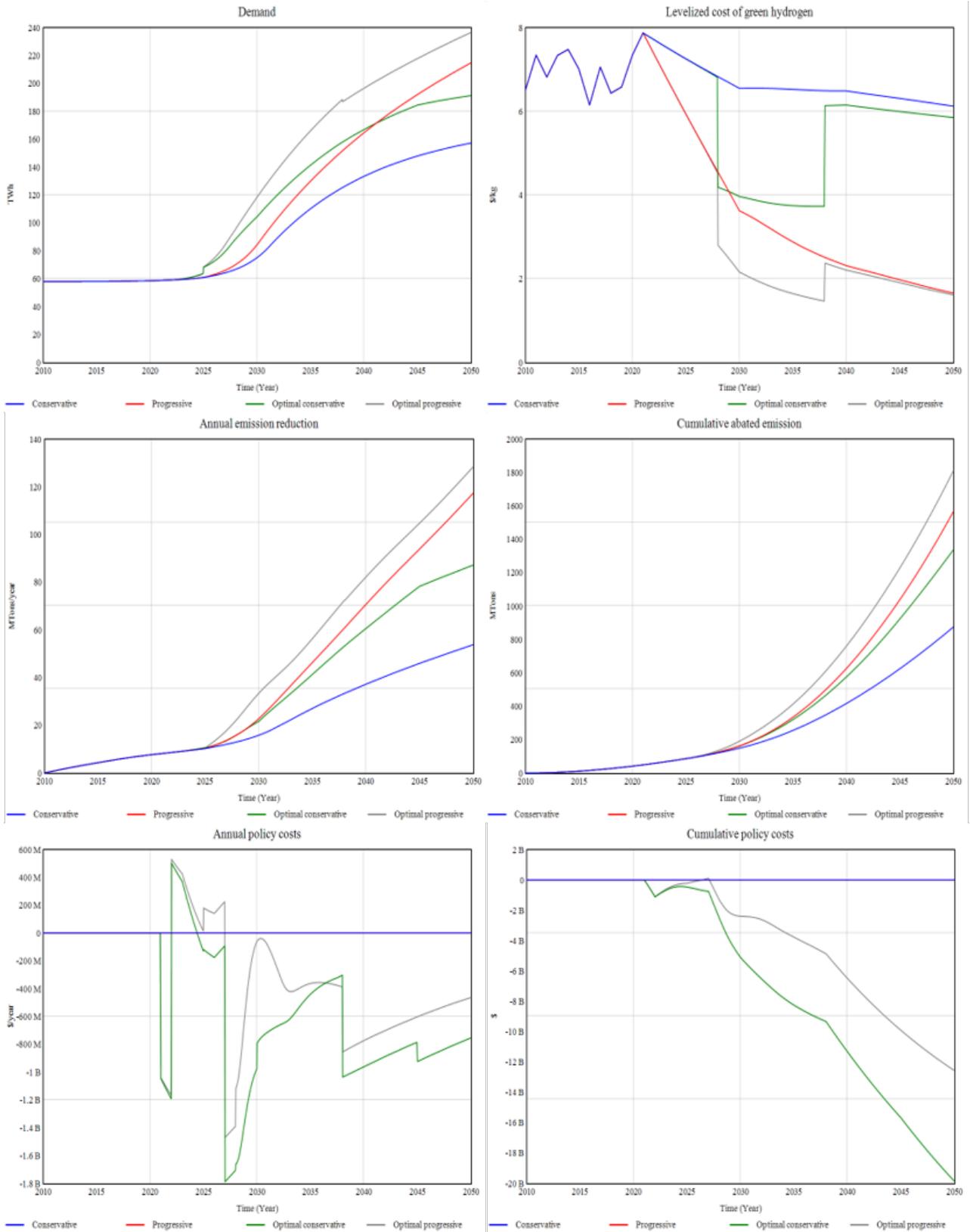


Figure 51: Additional results for the combination of the most effective individual policies

## K.9 CCS-ban

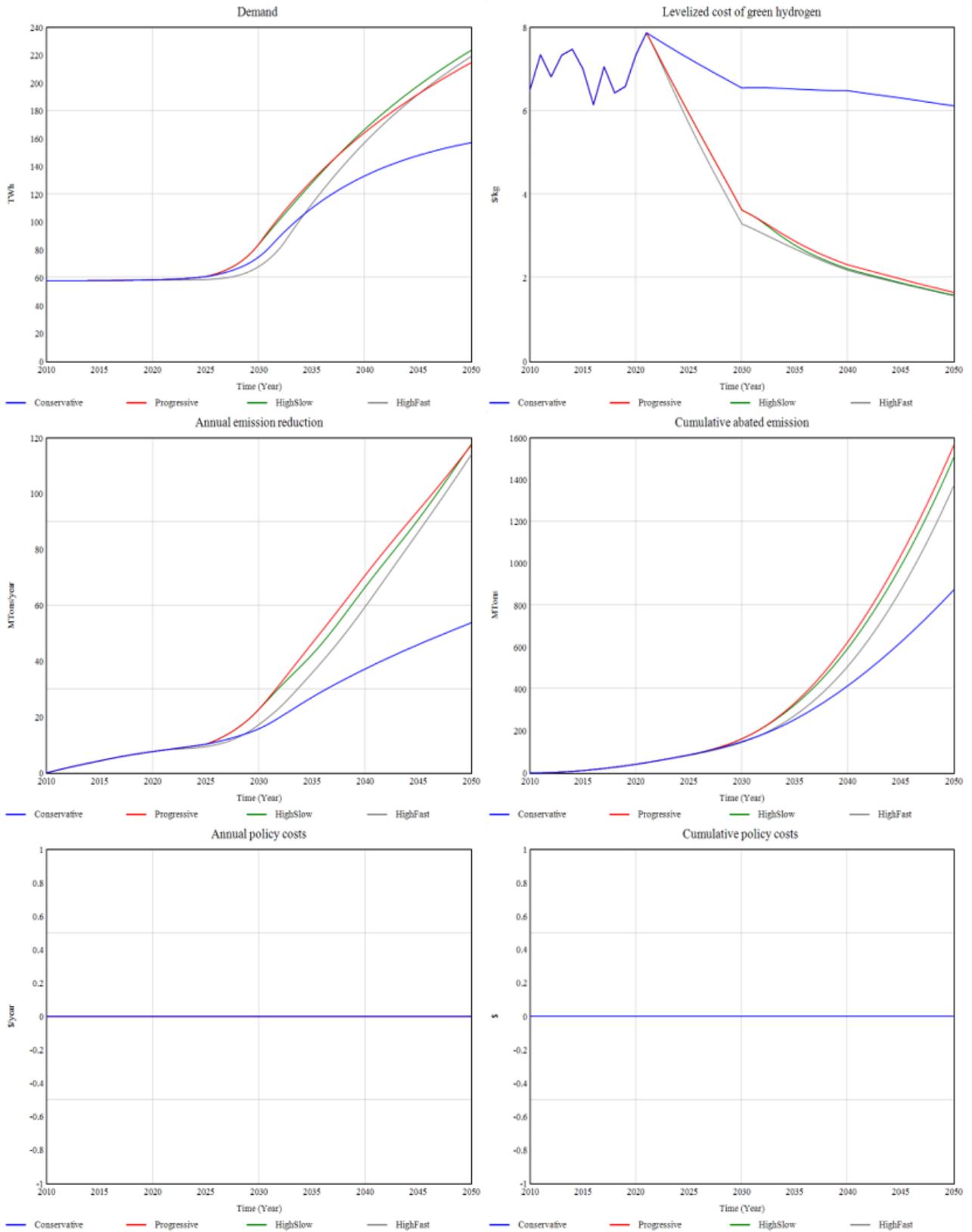


Figure 52: Additional results for CCS-ban policy

## K.10 CCS-ban and conventional policies combined

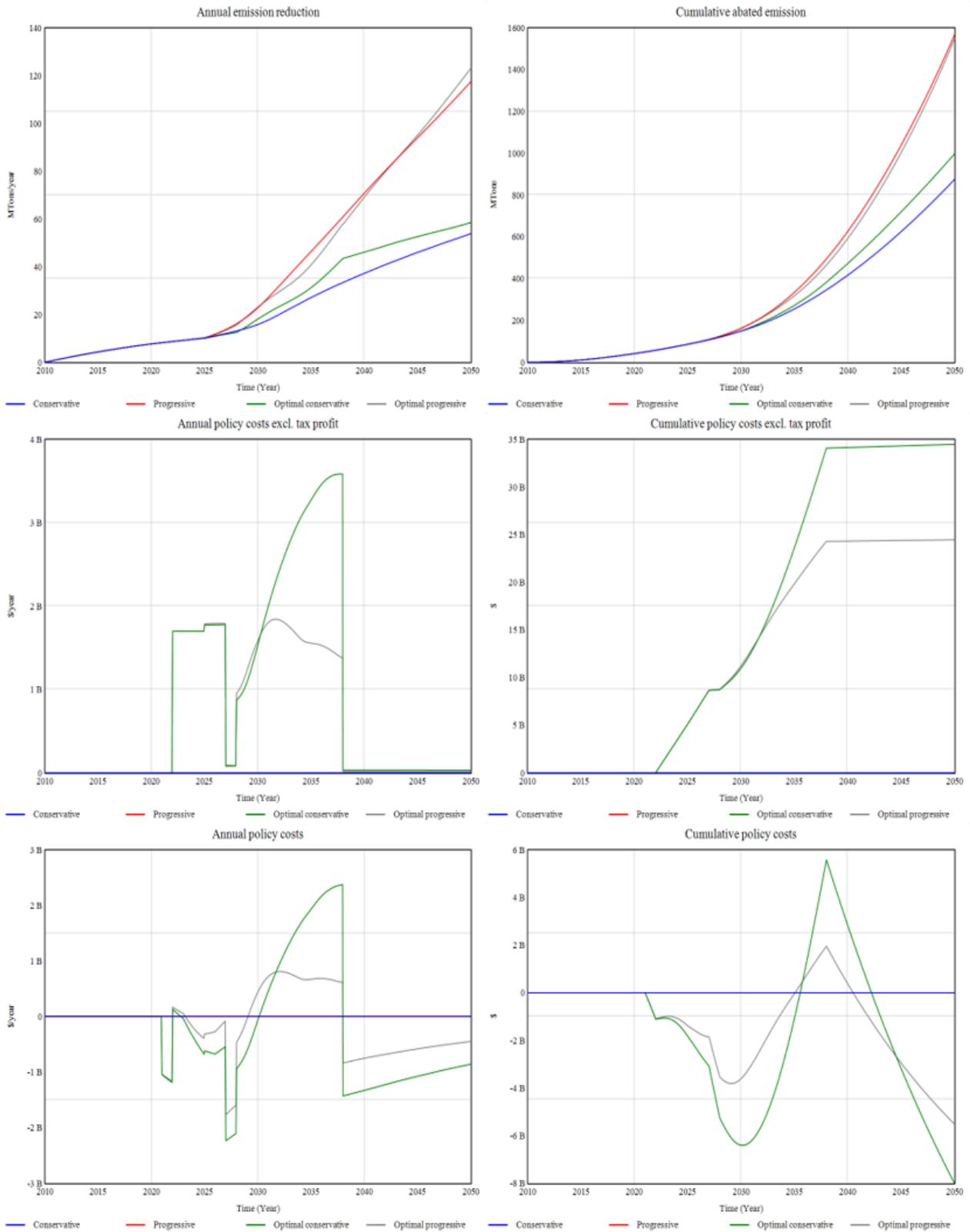


Figure 53: Results for the KPI's with CCS-ban and conventional policies active. The cost-graphs show the policy costs including and excluding the profits from the fossil-fuel taxation.

## L System Dynamics structures

The following figures show the principal structures of the system dynamics model in a simplified way. Variables in these figures that are written in *italic* or are enclosed with "<>" are variables that connect the submodel to other submodels. The exogenous variables for the LCOH-submodels are shown in red.

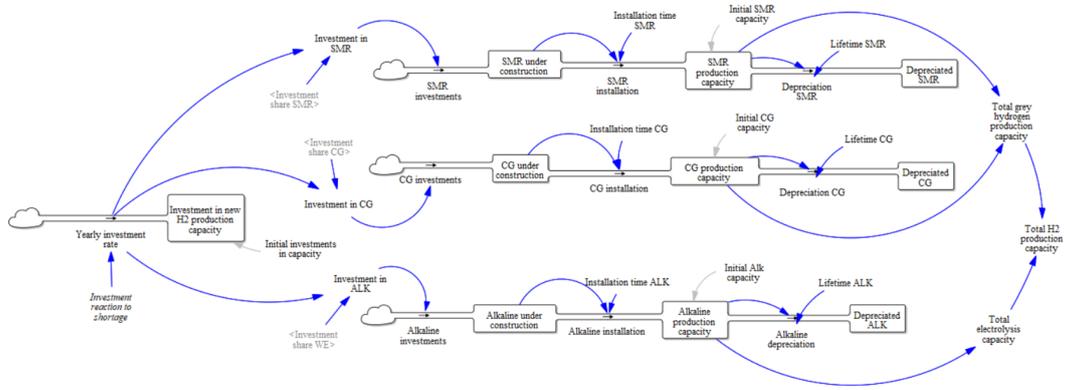


Figure 54: System dynamics structure of the production submodel

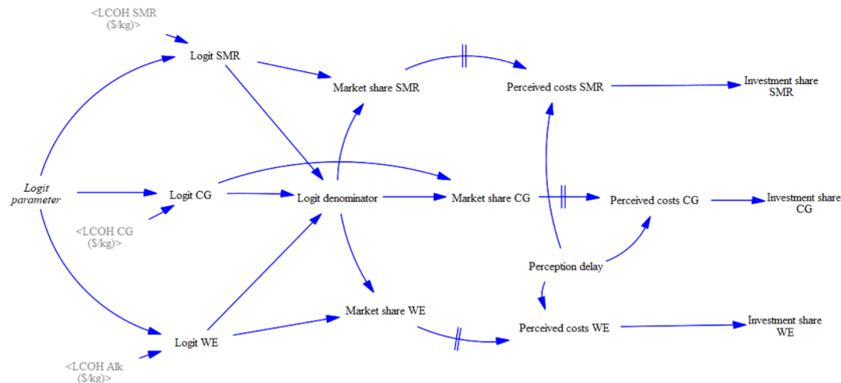


Figure 55: System dynamics structure of the investment submodel

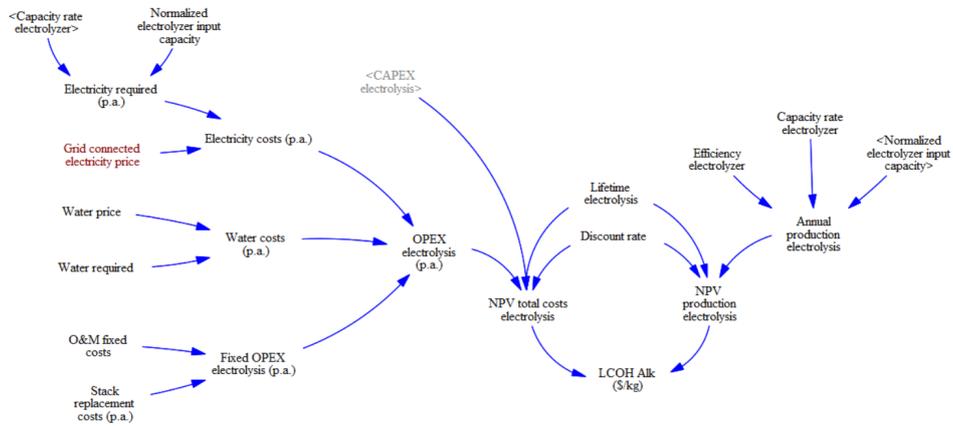


Figure 56: System dynamics structure of the levelized cost of green hydrogen, with CAPEX, OPEX and production

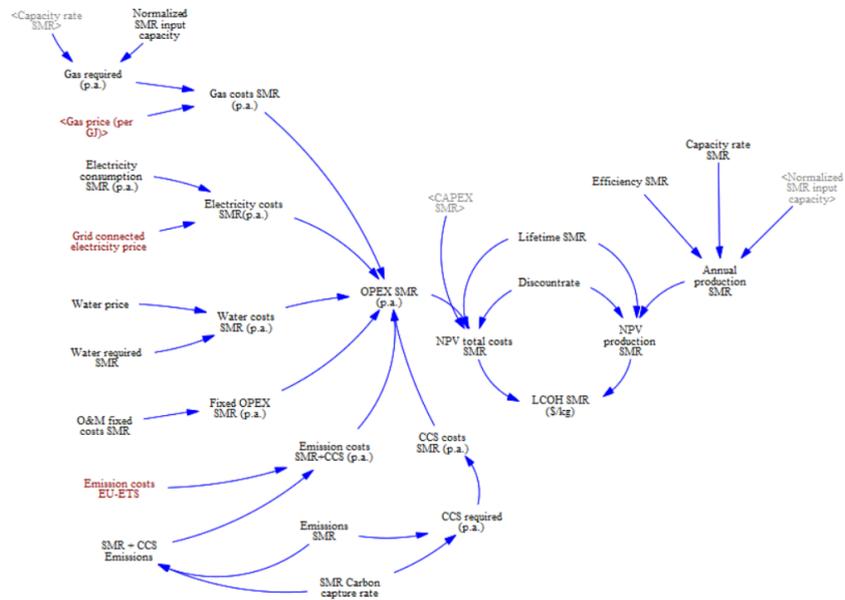


Figure 57: System dynamics structure of the levelized cost of SMR hydrogen, with CAPEX, OPEX and production

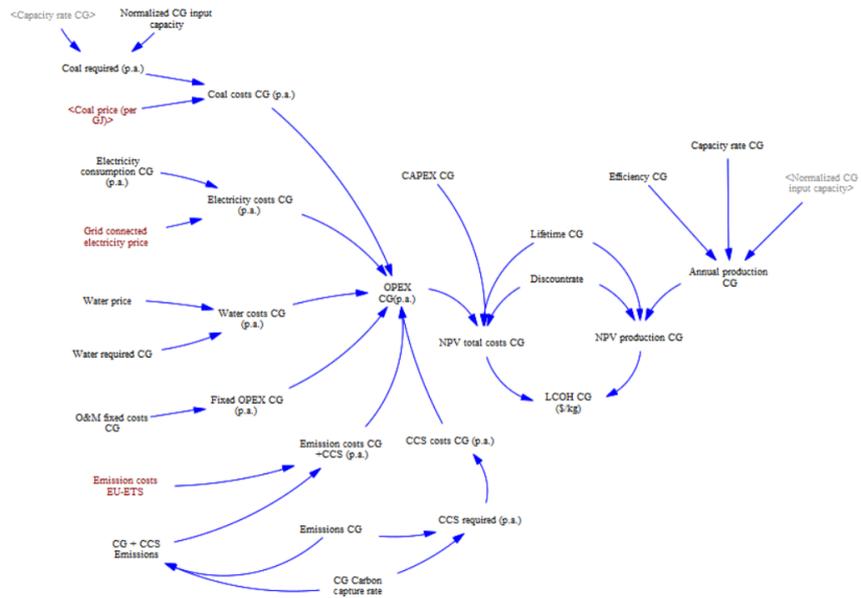


Figure 58: System dynamics structure of the levelized cost of CG hydrogen, with CAPEX, OPEX and production

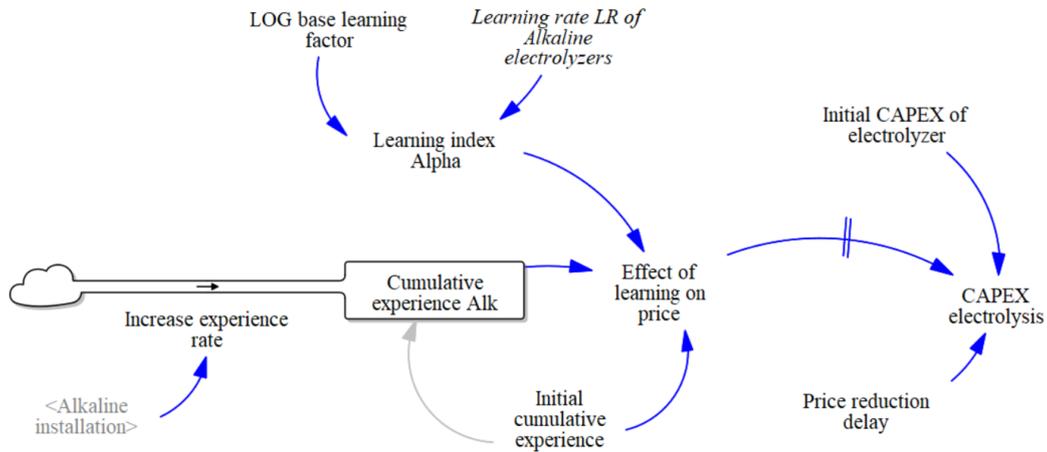


Figure 59: System dynamics structure of the learning-by-doing mechanism for capital costs of electrolyzers

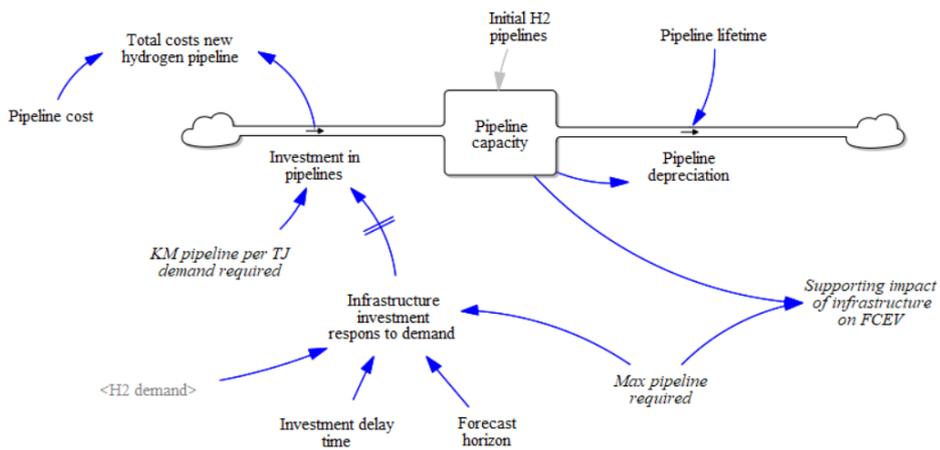


Figure 60: System dynamics structure of the construction of infrastructure

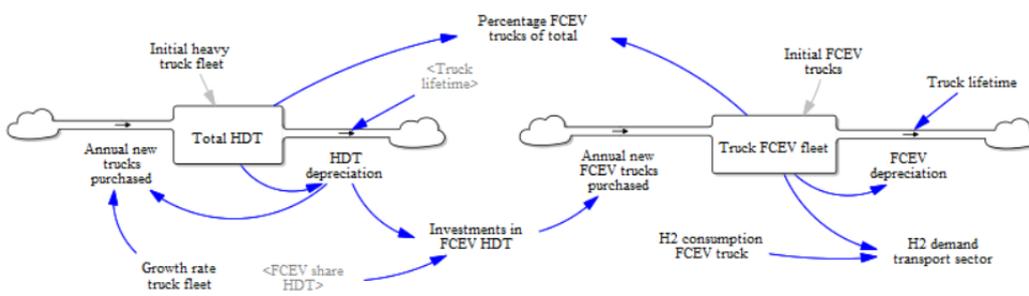


Figure 61: System dynamics structure of the adoption of FCEV-trucks, based on the FCEV share HDT

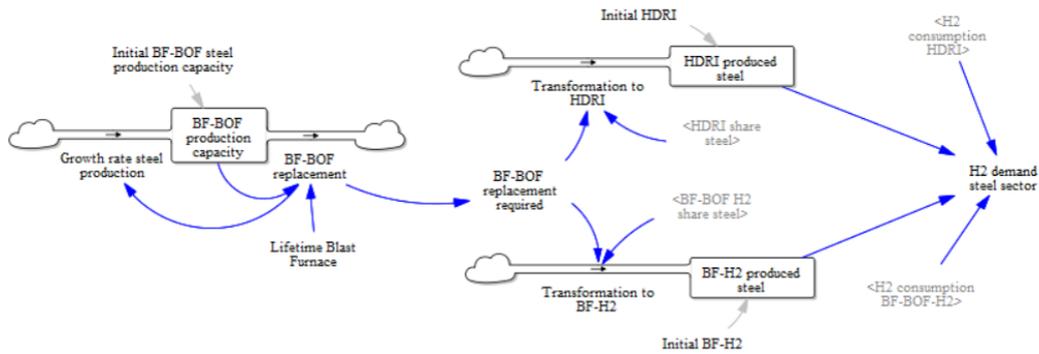


Figure 62: System dynamics structure of the deployment of two types of hydrogen-based steel making

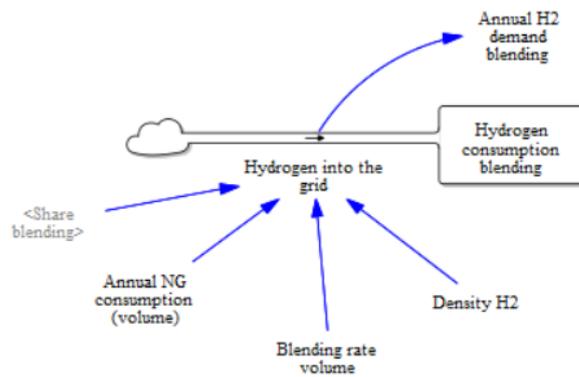


Figure 63: System dynamics structure of the demand for hydrogen for blending into the natural gas grid

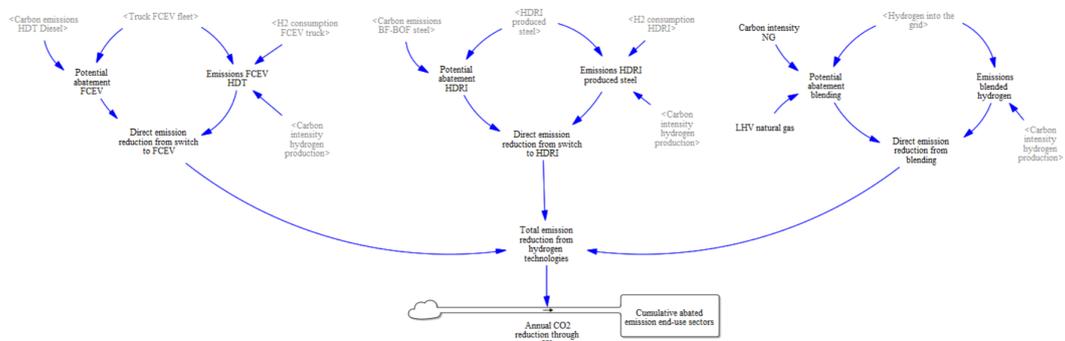


Figure 64: System dynamics structure for the calculation of the abated emissions in the end-use sectors through the adoption of hydrogen

## M System Dynamics model equations

This appendix lists all model equations from the Vensim Model in a random order.

1. Total production TWh = Production capacity grey TWh+Production capacity Alk TWh+Production capacity blue TWh
2. Investment reaction to shortage = MAX(DELAY3(-Net production capacity shortage per year, Investment smoothing time)
3. Net production capacity shortage per year = MIN(- Supply demand gap (Tons/year) / Day/year /Unit correction factor Year,0)
4. forecast investment = FORECAST( Demand (Tons/year) ,3,3)
5. % capex of costs = CAPEX Alk / (NPV total costs electrolysis \* 20 + CAPEX Alk ) \*100
6. BEV share HDT = (EXP(Logit parameter HDT\*(Logit factor BEV/Unit dmnl 3)))/(EXP(Logit parameter HDT \*(Logit factor Diesel/Unit dmnl 3)) + EXP(Logit parameter HDT \*(Logit factor BEV/Unit dmnl 3)) + EXP(Logit parameter HDT \*(Logit factor FCEV/Unit dmnl 3)))
7. Supply demand gap = forecast investment- Total H2 production
8. percentage of BEV trucks = Truck BEV fleet/Total HDT
9. percentage of diesel trucks = Truck Diesel fleet/Total HDT
10. Depreciation Diesel = DELAY1(Investment Diesel,Truck lifetime)
11. test truck percentage = Percentage FCEV trucks of total+percentage of BEV trucks+percentage of diesel trucks
12. Truck BEV fleet = INTEG (Investment BEV-Depreciation BEV,0)
13. Investments in BEV HDT = HDT depreciation \* BEV share HDT
14. Investments in Diesel HDT = HDT depreciation \* Diesel share HDT
15. Depreciation BEV = DELAY1(Investment BEV,Truck lifetime)
16. Electricity costs MWh = Grid connected electricity costs \* MJ to kWh \* kWh to mWh
17. CAPEX electrolysis = SMOOTH( Initial CAPEX of electrolyzer \* Effect of learning on price , Price reduction delay) \* Policy switch electrolyzer CAPEX support
18. Yearly investment rate = Investment reaction to shortage
19. CCS subsidy stop = STEP(20, 2022)\*0
20. CCfD per Tonsteel = (CCfD strikeprice - Carbon costs BF-BOF steel )\*Policy switch CCfD
21. abatement costs steel = Cost HDRI steel- Cost BF-BOF steel
22. Policy switch CCfD = (STEP(1, 2023) - STEP(1,2038))\*0
23. Infrastructure respons to demand = FORECAST(H2 demand, Infrastructure investment response delay , Forecast horizon
24. Production capacity blue TWh = Production capacity CG TWh+Production capacity SMR TWh
25. Production capacity grey TWh = Conversion Tons/day to TWh/year \*Total grey capacity
26. Production capacity Alk TWh = Alkaline production capacity\* Conversion Tons/day to TWh/year
27. Production capacity CG TWh = CG production capacity\* Conversion Tons/day to TWh/year
28. Production capacity SMR TWh = Conversion Tons/day to TWh/year \*SMR production capacity
29. Conversion to TWh = TJ to Tons (LHV) / TJ to TWh \* Day/year
30. Grid connected electricity costs = GET XLS DATA('Scenario\_input.xlsx','ELECGER','A','D3')
31. Conversion Tons/day to TWh/year = TJ to Tons (LHV) /TJ to TWh\* Day/year
32. Diesel share HDT = (EXP(Logit parameter HDT \*(Logit factor Diesel/Unit dmnl 3)))/(EXP(Logit parameter HDT \*(Logit factor Diesel/Unit dmnl 3)) + EXP(Logit parameter HDT \*(Logit factor BEV/Unit dmnl 3)) + EXP(Logit parameter HDT \*(Logit factor FCEV/Unit dmnl 3)))

33. Emission costs truck = Carbon costs diesel\* Carbon intensity Diesel \* Policy switch carbon cost diesel \* Policy switch carbon tax
34. Logit factor BEV = ( TCO BEV (\$/truck) /Total mileage)
35. CCfD price = Cost HDRI steel- Costs BF-BOF w/o carbon costs
36. Total policy costs per year = Policy costs CCfD+Policy costs electricity tax exemption+Policy costs investment subsidies CAPEX + Policy costs infrastructure per year + Policy cost gap NG/blending”+ policy costs carbon costs Diesel
37. policy costs carbon costs Diesel = - Annual mileage long-haul \* Emission costs truck \*Fuel consumption diesel\*Total HDT\* Diesel share HDT \* Policy switch carbon cost diesel/Truck unit
38. Carbon costs diesel = Carbon price transport(Time/Unit correction factor Year)
39. Costs BF-BOF w/o carbon costs = Coal price (per GJ) \* Coal consumption BF-BOF \* Coal energetic value+ BF-BOF steel cost excl. var. costs + Electricity consumption BF-BOF \* Grid connected electricity costs
40. Policy switch carbon cost diesel = STEP(1,2021) Emission costs SMR + CCS (p.a.) = SMR + CCS Emissions \* Emission costs EU \*Policy switch carbon tax / Tons to kg
41. Policy switch carbon tax = 1+STEP(Additional increase ETS,2025)
42. Additional increase ETS = 0.2\*0
43. Initial carbon intensity H2 = DELAY FIXED(Total direct carbon emissions hydrogen production, 40 , Total direct carbon emissions hydrogen production)
44. Emission costs CG +CCS (p.a.) = CG + CCS Emissions \*Emission costs EU \*Policy switch carbon tax/Tons to kg
45. Annual CO2 reduction production = Direct emission reduction in H2 production
46. Total cumulative emission reduction = Cumulative abated emission end-use sectors +Cumulative abated emissions H2 production
47. Cost BF-BOF steel = Carbon emissions BF-BOF steel \* Emission costs EU \* Policy switch carbon tax/ Tons to kg+ Coal price (per GJ) \* Coal consumption BF-BOF \* Coal energetic value+ BF-BOF steel cost excl. var. costs + Electricity consumption BF-BOF \* Grid connected electricity costs
48. Direct emission reduction in H2 production = Initial carbon intensity H2-Total direct carbon emissions hydrogen production
49. Total annual emission reduction = Annual CO2 reduction production+Annual CO2 reduction through H2
50. Cumulative abated emissions H2 production = INTEG (Annual CO2 reduction production,0)
51. Total electrolysis capacity = Alkaline production capacity
52. Policy switch coal in production phase out = RAMP(4, 2020, 2025)\*0
53. Alkaline investments = Investment in Electrolysis
54. Fuel costs Diesel = Diesel costs(Time/Unit correction factor Year)
55. Policy switch construction acceleration = 0
56. Cost gap green-blue = LCOH Alk (\$/kg) -Average blue costs
57. Logit CG = EXP(Logit parameter \* (( LCOH CG (\$/kg) + Policy switch coal in production phase out)/Unit dmnl))
58. Average blue costs = ( LCOH CG (\$/kg) + LCOH SMR (\$/kg) )/2
59. TCO Diesel (\$/truck) = Lifetime truck \* Annual mileage long-haul \*Fuel consumption diesel\*Fuel costs Diesel\*0.8+ TCO Diesel excl. fuel + Emission costs truck\*Lifetime truck \* Fuel consumption diesel \* Annual mileage long-haul
60. H2 demand = ((H2 demand steel sector + H2 demand transport sector +H2 demand blending) + Existing H2 demand in chemical industry and refineries )\* SMOOTH3(STEP (1,2020) , Demand response delay)
61. Annual emissions from hydrogen production = Total direct carbon emissions hydrogen production
62. Cumulative emissions from hydrogen production = INTEG (Annual emissions from hydrogen production,0)

63. Total direct carbon emissions hydrogen production = Annual direct emissions CG+Annual direct emissions SMR+Annual direct emissions WE + Annual direct emissions grey hydrogen
64. Depreciation grey CG = Grey CG capacity/Lifetime grey CG
65. Depreciation grey SMR = Grey SMR capacity/Lifetime grey SMR
66. Annual direct emissions grey hydrogen = ((Grey CG capacity \* Emissions CG \* kg/tons \* Day/year ) + (Grey SMR capacity \*Emissions SMR\* kg/tons \* Day/year )) / kgCO2 to Mtons
67. Grey CG capacity = INTEG (-Depreciation grey CG,Initial grey CG)
68. Grey SMR capacity = INTEG (-Depreciation grey SMR,Initial grey SMR)
69. Total H2 production capacity = Total electrolysis capacity+Total blue capacity + Total grey capacity
70. Annual direct emissions CG = CG production capacity \* Day/year \* kg/tons \* Emissions CG \*(1- CG Carbon capture rate) /kgCO2 to Mtons
71. Carbon intensity of hydrogen = Emissions per unit of hydrogen produced / kg/tons \*kgCO2 to Mtons
72. Total grey capacity = Grey CG capacity +Grey SMR capacity
73. Emissions per unit of hydrogen produced = Total direct carbon emissions hydrogen production/ Total H2 production (Tons/year)
74. Efficiency electrolyzer = Initial electrolyzer efficiency + RAMP((Expected efficiency electrolyzer-Initial electrolyzer efficiency)/(FINAL TIME - INITIAL TIME), INITIAL TIME, FINAL TIME )
75. Learning HDRI steel = RAMP(-( HDRI steel cost excl. var. costs - 381) /(FINAL TIME - 2020), 2020 , FINAL TIME)
76. Retrofit CAPEX = CAPEX retro L\*Share L+CAPEX retro M\*Share M+CAPEX retro S\*Share S
77. Growth rate steel production = BF-BOF replacement \*Annual growth rate steel
78. Growth rate truck fleet = HDT depreciation \* Annual growth rate trucks
79. Policy cost gap NG/blending = IF THEN ELSE(Policy switch blending quota = 0,0,( GJ per Kg (LHV) \*Hydrogen into the grid\* kg/tons \* (Blending costs per GJ + CAPEX blending) ))
80. Pipeline CAPEX = CAPEX new L\*Share L+CAPEX new M\*Share M+CAPEX new S\*Share S
81. Share blending = (EXP(Logit parameter blending \*(Logit blending/Unit dmnl 5)))/(EXP(Logit parameter blending \*( Logit 100% natural gas /Unit dmnl 5)) + EXP(Logit parameter blending \*(Logit blending/Unit dmnl 5)))\* technology switch blending + Blending policy implementation
82. Blending policy implementation = (STEP(Policy switch blending quota ,2025)+ STEP(0,2025))
83. Blending costs per GJ = Blended price (per GJ) - Gas price (per GJ)
84. Emission costs EU = GET XLS DATA('Scenario<sub>input.xlsx'</sub>, 'ETSEU', 'a', 'B2')
85. Policy switch blending quota = 0.2\*0
86. Share of green hydrogen = Total electrolysis capacity/Total H2 production capacity \* 100
87. Policy costs investment subsidies CAPEX = IF THEN ELSE(Policy switch electrolyzer CAPEX support = 1,0,Investment in Electrolysis\* Conversion factor (Tons/day > kW) \*Investment subsidy per kW CAPEX
88. Annual CO2 reduction through H2 = Total emission reduction from hydrogen technologie
89. Investment in pipelines = Infrastructure respons to demand \* KM pipeline per TJ demand required \*Share of new pipelines + Upfront investment pipelines
90. Policy switch electrolyzer electricity tax discount = 1-((STEP(Tax relief electricity,2028)) - (STEP(Tax relief electricity,2038)))
91. Policy switch upfront investment infrastructure = (STEP(1,2022) - STEP(1,2027))\* Upfront investments in infrastructure\*0
92. Retrofit cost per km = (Retrofit CAPEX + (OPEX retrofitted pipeline \* Retrofit lifetime))

93. Retrofit depreciation = DELAY1(Retrofitted pipeline construction,Retrofit lifetime)
94. Pipeline cost per km = (Pipeline CAPEX + Pipeline lifetime \* OPEX new pipeline)
95. Total costs new hydrogen pipeline = Pipeline cost per km\* Investment in pipelines
96. Cumulative policy costs = INTEG (Total policy costs per year,0)
97. Investment subsidy per kW CAPEX = Policy switch electrolyzer CAPEX support \*CAPEX Alk / Normalized electrolyzer input capacity
98. Investment support electrolysis = 0.3\*0
99. Electricity costs = Grid connected electricity costs \* MJ to kWh
100. Cumulative abated emission end-use sectors = INTEG (Annual CO2 reduction through H2,0)
101. Upfront investment pipelines = Policy switch upfront investment infrastructure \* Share of new pipelines
102. Pipeline capacity = INTEG (Investment in pipelines-Pipeline depreciation,Initial H2 pipelines)
103. Tax relief electricity = 0.4\*0
104. Total cost retrofitted pipeline = Retrofit cost per km\* Retrofitted pipeline construction
105. Retrofitted capacity = INTEG (Retrofitted pipeline construction-Retrofit depreciation,Initial H2 pipeline)
106. Retrofitted pipeline construction = KM pipeline per TJ demand required\*Infrastructure respons to demand\*Share of retrofitting+ Upfront investment retrofitting
107. Policy costs CCfD = CCfD per Tonsteel\*Transformation to HDRI
108. Policy costs electricity tax exemption = IF THEN ELSE(Policy switch electrolyzer electricity tax discount = 1, 0, Total electricity costs for electrolysis- Total tax-reduced electricity costs for electrolysis )
109. Policy costs infrastructure per year = Upfront investment pipelines \* Pipeline cost per km +Upfront investment retrofitting \* Retrofit cost per km
110. OPEX electrolysis (p.a.) = (Electricity costs \* Policy switch electrolyzer electricity tax discount \* Electricity required (p.a.) + Water costs + Fixed OPEX electrolysis (p.a.) )
111. Policy switch electrolyzer CAPEX support = 1-(STEP(1,2028) - STEP(1,2038)) \* Investment support electrolysis
112. Pipeline depreciation = DELAY1(Investment in pipelines, Pipeline lifetime )
113. Upfront investment retrofitting = Policy switch upfront investment infrastructure \* Share of retrofitting
114. Total pipeline finished = Pipeline capacity+Retrofitted capacity
115. Supporting impact of infrastructure on FCEV = MIN(Total pipeline finished / (Max pipeline for full capacity ),1)
116. Conversion factor (Tons/day > kW) = kWh to kg (LHV) \* kg/tons /Hours per day \* Capacity rate electrolyzer
117. (Direct) emission reduction from switch to FCEV = Potential abatement FCEV - Emissions FCEV HDT
118. Potential abatement blending = Hydrogen into the grid \* kg/tons \* kWh to kg (LHV) / LHV natural gas \* Carbon intensity NG/ kgCO2 to Mtons
119. Potential abatement FCEV = Truck FCEV fleet \*Fuel consumption diesel\*Carbon intensity Diesel\* Annual mileage long-haul /Truck unit/kgCO2 to Mtons
120. Potential abatement HDRI = HDRI produced steel\* Carbon emissions BF-BOF steel /Unit correction factor Year /kgCO2 to Mton
121. Investments in FCEV HDT = HDT depreciation \* FCEV share HDT
122. Kg H2 per m3 blended = H2 energetic share per m3 blended/ kWh to kg (LHV)
123. Total electricity costs for electrolysis = Costs for electricity per Kw p.a. \*kW to mW\*Electrolysis capacity
124. Emissions BF-BOF = ( Carbon emissions BF-BOF steel \* Annual steel production) / kgCO2 to Mtons
125. BF-BOF H2 share steel = (EXP(Logit parameter steel \*( Logit BF-BOF H2 steel /Unit dmnl 4)))/(EXP(Logit parameter steel \*( Logit BF-BOF H2 steel /Unit dmnl 4)) + EXP(Logit parameter steel \*( Logit BF-BOF steel /Unit dmnl 4)) + EXP(Logit

- parameter steel \*(Logit HDRI steel/Unit dmnl 4)))
126. BF-BOF production capacity = INTEG (Growth rate steel production- BF-BOF replacement , Initial BF-BOF steel production capacity )
  127. BF-BOF replacement required = BF-BOF replacement
  128. BF-BOF replacement = BF-BOF production capacity /Lifetime Blast Furnace
  129. Emissions HDRI produced steel = Emissions per unit of hydrogen produced\*H2 consumption HDRI\*HDRI produced steel / kg/tons /Unit correction factor Year
  130. Emissions HDT Diesel = Carbon intensity Diesel \* Fuel consumption diesel \* Total HDT \* Annual mileage long-haul / kgCO2 to Mtons / Truck unit
  131. Cost BF-H2 steel = Carbon emissions BF-H2 steel (leakage CCS) \* Emission costs EU /Tons to kg+ Coal consumption BF-H2 \* Coal price (per GJ) \* Coal energetic value+ H2 consumption BF-H2 \* Weighted hydrogen market price + BF-H2 steel cost excl. var. costs + Electricity consumption BF-BOF \* Grid connected electricity costs + CCS required BF-H2 \* CCS costs BF-H2
  132. Cost HDRI steel = ( H2 consumption HDRI \* Weighted hydrogen market price + Carbon emissions HDRI steel \* Emission costs EU + HDRI steel cost excl. var. costs +Learning HDRI steel +Electricity consumption HDRI \* Grid connected electricity costs - CCfD per Tonsteel)
  133. Costs for electricity per Kw p.a. = Electricity required (p.a.) \*Electricity costs / Normalized electrolyzer input capacity
  134. Blending TWh = H2 demand blending/TJ to TWh
  135. Direct emission reduction from switch to HDRI = Potential abatement HDRI - Emissions HDRI produced steel
  136. Total emission reduction from hydrogen technologies = (Direct) emission reduction from switch to FCEV +Direct emission reduction from blending+Direct emission reduction from switch to HDRI
  137. Percentage FCEV trucks of total = Truck FCEV fleet/Total HDT
  138. Technology readiness HDRI = STEP(1,2025)
  139. Emissions blended hydrogen = Hydrogen into the grid \*Emissions per unit of hydrogen produced
  140. Carbon costs BF-BOF steel = Carbon emissions BF-BOF steel \* Emission costs EU / Tons to kg
  141. Emissions gas grid = Carbon intensity NG \* Annual NG consumption (volume) / kgCO2 to Mtons
  142. Total tax-reduced electricity costs for electrolysis = Electricity required (p.a.) \*Electrolysis capacity\*kW to mW/Normalized electrolyzer input capacity\*Tax reduced electricity costs
  143. HDRI share steel = (EXP(Logit parameter steel \*(Logit HDRI steel/Unit dmnl 4))) / (EXP(Logit parameter steel \*( Logit BF-BOF H2 steel /Unit dmnl 4)) + EXP(Logit parameter steel \*( Logit BF-BOF steel /Unit dmnl 4)) + EXP(Logit parameter steel \*(Logit HDRI steel/Unit dmnl 4))) \*Technology readiness HDRI
  144. HDT depreciation = Total HDT/Truck lifetime
  145. Direct emission reduction from blending = Potential abatement blending -Emissions blended hydrogen
  146. Tax reduced electricity costs = Electricity costs \* Policy switch electrolyzer electricity tax discount
  147. Emissions FCEV HDT = Emissions per unit of hydrogen produced \* Truck FCEV fleet \* Energy demand FCEV truck / TJ to Tons (LHV)
  148. Total HDT = INTEG (Growth rate truck fleet-HDT depreciation,Initial heavy truck fleet)
  149. Grid electricity emissions = Emission intensity electricity production (grid) \*kW to mW
  150. Emission intensity electricity production (grid) = Steepness of emissions curve \* Share of renewable electricity (grid) + Coefficient emissions curve
  151. Coefficient emissions curve = Initial emission intensity grid electricity - Steepness of emissions curve\* Renewable share 2010

152. Steepness of emissions curve = -Initial emission intensity grid electricity/(Renewable share 2050-Renewable share 2010)
153. Transition curve = Renewable electricity share(Time/Unit correction factor Year)
154. OPEX CG (p.a.) = ( Carbon capture required (p.a.) \* CCS costs CG + Coal costs \* Coal required (p.a.) + Extra electricity costs CG + Water costs CG + Fixed OPEX CG (p.a.) + Emission costs CG +CCS (p.a.) )
155. Share of renewable electricity (grid) = Transition curve
156. CG + CCS Emissions = Annual production CG per kW \* Emissions CG \* (1-CG Carbon capture rate)
157. Annual direct emissions SMR = SMR production capacity\* (1-SMR Carbon capture rate)\* Emissions SMR \* kg/tons \* Day/year /kgCO2 to Mtons
158. Annual direct emissions WE = Grid electricity emissions \*Electrolysis capacity \* Hours per year /kgCO2 to Mtons
159. "Carbon capture required (p.a.) = Annual production CG per kW \* Emissions CG \* CG Carbon capture rate
160. SMR + CCS Emissions = Annual production SMR\*Emissions SMR\*(1-SMR Carbon capture rate)
161. OPEX SMR (p.a.) = ( Carbon capture required SMR (p.a.) \* CCS costs SMR + Gas costs \* Gas required SMR (p.a.) + Extra electricity costs SMR + Water costs SMR + Fixed OPEX SMR(p.a.) + Emission costs SMR + CCS (p.a.) )
162. Transport TWh = H2 demand transport sector/TJ to TWh
163. Existing H2 TWh = Existing H2 demand in chemical industry and refineries/TJ to TWh
164. Steel TWh = H2 demand steel sector/TJ to TWh
165. KM pipeline per TJ demand required = IF THEN ELSE(Total pipeline finished>Max pipeline for full capacity,0,(Distribution pipeline per TJ demand+Transmission pipeline per TJ demand))
166. Weighted hydrogen market price = ( LCOH Alk (\$/kg) \*Market share WE + LCOH CG (\$/kg) \*Market share CG + LCOH SMR (\$/kg) \*Market share SMR) / (Market share CG + Market share SMR + Market share WE)
167. technology switch blending = IF THEN ELSE(Time<2024, 0, RAMP(0.25, 2024, 2028 ))
168. Electrolysis capacity = Total electrolysis capacity \* Efficiency electrolyzer \* Capacity rate electrolyzer \* Conversion factor (Tons/day > kW) /kW to mW
169. LCOH Alk (\$/kg) = NPV total costs electrolysis/NPV production electrolysis
170. TCO BEV excl. fuel = 1.204e+06-1.204e+06\*BEV learning\*(Time- INITIAL TIME)/\$/truck unit
171. Blended price (per GJ) = (Costs hydrogen blending / Mixed lower heating value (kWh) / GJ to kWh)+CAPEX blending
172. Annual new FCEV trucks purchased = Investments in FCEV HDT \* Supporting impact of infrastructure on FCEV
173. Costs hydrogen blending = Hydrogen price (per GJ) \* GJ to kWh \* H2 energetic share per m3 blended + Gas price (per GJ) \* GJ to kWh \* NG energetic share per m3
174. TCO FCEV (\$/truck) = Annual mileage long-haul \*Lifetime truck\*Fuel consumption FCEV\*Weighted hydrogen market price+ TCO FCEV excl. fuel
175. TCO FCEV excl. fuel = 919000-919000 \*FCEV learning\*(Time- INITIAL TIME)/\$/truck unit
176. H2 energetic share per m3 blended = Density H2 (kg) \* kWh to kg (LHV) \* Blending rate volume
177. Mixed lower heating value (kWh) = H2 energetic share per m3 blended + NG energetic share
178. NG energetic share per m3 = (1-Blending rate volume) \* Density NG \* Energetic value natural gas
179. Logit 100% hydrogen = CAPEX blending + Hydrogen price (per GJ)
180. Hydrogen into the grid = Annual NG consumption (volume) \* Blending rate volume \* Density H2 \* Share blending

181. Transformation to HDRI = BF-BOF replacement required \* HDRI share steel
182. Transformation to BF-H2 = BF-BOF H2 share steel \* BF-BOF replacement required
183. BF-BOF share steel = (EXP(Logit parameter steel \*( Logit BF-BOF steel /Unit dmnl 4)))/(EXP(Logit parameter steel \*( Logit BF-BOF H2 steel /Unit dmnl 4)) + EXP(Logit parameter steel \*( Logit BF-BOF steel /Unit dmnl 4)) + EXP(Logit parameter steel \*(Logit HDRI steel/Unit dmnl 4))
184. H2 demand blending = Hydrogen into the grid \* TJ to Tons (LHV)
185. Hydrogen consumption blending = INTEG (Hydrogen into the grid,0)
186. TCO BEV (\$/truck) = Annual mileage long-haul \*Lifetime truck\*Fuel consumption BEV\*Grid connected electricity costs+ TCO BEV excl. fuel
187. Logit denominaor = Logit CG + Logit SMR + Logit WE
188. H2 demand steel sector = ( BF-H2 produced steel \* H2 consumption BF-H2 + H2 consumption HDRI\*HDRI produced steel)\*( GJ per Kg (LHV) /GJ to TJ/Unit correction factor Year)
189. H2 demand transport sector = Truck FCEV fleet \* Energy demand FCEV truck
190. HDRI produced steel = INTEG (Transformation to HDRI,Initial HDRI)
191. Depreciation trucks = DELAY1(Annual new FCEV trucks purchased,Truck lifetime)
192. BF-H2 produced steel = INTEG ( Transformation to BF-H2 , Initial BF-H2 )
193. Truck FCEV fleet = INTEG (Annual new FCEV trucks purchased - Depreciation trucks, Initial FCEV trucks)
194. Total mileage = Annual mileage long-haul \*Lifetime truck
195. Logit factor FCEV = TCO FCEV (\$/truck) /Total mileage
196. Purchase share FCEV heavy road transport = FCEV share HDT
197. Logit factor Diesel = TCO Diesel (\$/truck) /Total mileage
198. FCEV share HDT = (EXP(Logit parameter HDT\*(Logit factor FCEV/Unit dmnl 3)))/(EXP(Logit parameter HDT \*(Logit factor Diesel/Unit dmnl 3)) + EXP(Logit parameter HDT \*(Logit factor BEV/Unit dmnl 3)) +EXP(Logit parameter HDT \*(Logit factor FCEV/Unit dmnl 3))
199. Investment in CG = Investment share CG\*Yearly investment rate
200. Investment in SMR = Yearly investment rate\*Investment share SMR
201. Investment in Electrolysis = Investment share WE\*Yearly investment rate
202. Control output = Investment share CG+Investment share SMR+Investment share WE
203. Control output2 = Market share CG+Market share SMR+Market share WE
204. Gas costs = Gas price (per GJ) \* GJ to kWh
205. Coal costs = Coal price (per GJ) \* GJ to kWh
206. Extra electricity costs CG = Annual production CG per kW \* Electricity consumption CG \* Grid connected electricity costs \* MJ to kWh
207. Extra electricity costs SMR = Annual production SMR \* electricity consumption SMR \* Grid connected electricity costs \* MJ to kWh
208. Total investment costs infrastructure = INTEG (Investment costs infrastructure,0)
209. Investment costs infrastructure = Total costs new hydrogen pipeline + Total cost retrofitted pipeline
210. Energetic value H2 blending = Hydrogen blending potential \* TJ to Tons (LHV) \* Blending of hydrogen
211. Blending of hydrogen = RAMP( 0.005, 2022, 2050 )
212. "Gas required SMR (p.a.) = Capacity rate SMR \* Hours per year \* Normalized SMR input capacity
213. Annual production CG per kW = Capacity rate CG \* Efficiency CG \* Hours per year \* Normalized CG input capacity / kWh to kg (LHV)
214. Annual production SMR = Capacity rate SMR \* Efficiency SMR \* Hours per year \* Normalized SMR input capacity / kWh to kg (LHV)
215. "Fixed OPEX SMR(p.a.) = CAPEX steam methane reforming \* OM fixed SMR
216. CAPEX Alk = CAPEX electrolysis \* Normalized electrolyzer input capacity
217. CAPEX coal gasification = CAPEX CG \* Normalized CG input capacity
218. CAPEX steam methane reforming = CAPEX SMR \* Normalized SMR input capacity

219. Carbon capture required SMR (p.a.) = Annual production SMR \* Emissions SMR \* SMR Carbon capture rate
220. Stack replacement = ((( Lifetime electrolyzer/ (Stack lifetime \* Lifetime electrolyzer) ) \* Stack replacement costs \* CAPEX Alk)/ Lifetime electrolyzer )
221. “Coal required (p.a.) = Capacity rate CG \* Hours per year \* Normalized CG input capacity
222. Investment in new H2 production capacity = INTEG (Yearly investment rate,Initial investments in capacity)
223. Fixed OPEX CG (p.a.) = CAPEX coal gasification \* OM fixed CG
224. Fixed OPEX electrolysis (p.a.) = OM fixed costs \* CAPEX Alk + Stack replacement
225. LCOH CG (\$/kg) = NPV total costs CG/NPV production CG
226. LCOH SMR (\$/kg) = NPV total costs SMR / NPV production SMR
227. Water costs SMR = Annual production SMR \* Water consumption SMR \* Water price
228. Water costs CG = Annual production CG per kW \* Water consumption CG \* Water price
229. Annual production electrolysis = (Efficiency electrolyzer \* Capacity rate electrolyzer \* Normalized electrolyzer input capacity\* Hours per year) / kWh to kg (LHV)
230. Electricity required (p.a.) = Normalized electrolyzer input capacity \* Hours per year \* Capacity rate electrolyze
231. Water costs = Water required \* Water price
232. OPEX new pipeline = OM costs \* Pipeline CAPEX
233. OPEX retrofitted pipeline = OM costs \* Retrofit CAPEX
234. H2 demand Tons = H2 demand/ TJ to Tons (LHV)
235. Share of new pipelines = 1-Share of retrofiting
236. Demand (Tons/year) = H2 demand/ TJ/Ton (LHV)
237. Infrastructure investment response delay = 5
238. Total H2 production (Tons/year) = Total H2 production capacity \* Day/year
239. Gas price (per GJ) = GET XLS DATA('Scenario<sub>input.xlsx</sub>','GASGER','A','B3')
240. Logit SMR = EXP(Logit parameter \* ( LCOH SMR (\$/kg) /Unit dmnl))
241. Logit WE = (EXP(Logit parameter\*( LCOH Alk (\$/kg) /Unit dmnl))
242. Coal price (per GJ) = GET XLS DATA('Scenario<sub>input.xlsx</sub>','COALGER','A','B3')
243. Perceived costs WE = SMOOTH3(Market share WE, Perception delay )
244. Perceived costs CG = SMOOTH3( Market share CG , Perception delay )
245. Price reduction delay = 2
246. Perceived costs SMR = SMOOTH( Market share SMR , Perception delay )
247. Increase experience rate = MAX(Alkaline installation \* Conversion factor (Tons/day > kW) ,0)
248. Alkaline production capacity = INTEG (Alkaline installation-Alkaline depreciation,Initial Alk capacity)
249. CG production capacity = INTEG (CG installation-Depreciation CG,Initial CG capacity)
250. SMR production capacity = INTEG (SMR installation-Depreciation SMR,Initial SMR capacity)
251. Alkaline depreciation = Alkaline production capacity/Lifetime ALK
252. Alkaline installation = Alkaline under construction/Installation time ALK
253. Alkaline under construction = INTEG (Alkaline investments-Alkaline installation,0)
254. CG under construction = INTEG (CG investments-CG installation,0)
255. Depreciated ALK = INTEG (Alkaline depreciation,0)
256. SMR under construction = INTEG (SMR investments-SMR installation,0)
257. Market share CG = Logit CG/Logit denominator
258. Market share SMR = Logit SMR/Logit denominator
259. Market share WE = Logit WE/Logit denominator
260. SMR installation = SMR under construction/Installation time SMR
261. CG installation = CG under construction/Installation time CG
262. Total blue capacity = SMR production capacity+CG production capacity

- 263. Cumulative experience Alk = INTEG (Increase experience rate,Initial cumulative experience)
- 264. Depreciated CG = INTEG (Depreciation CG,0)
- 265. Depreciated SMR = INTEG (Depreciation SMR,0)
- 266. Depreciation CG = CG production capacity/Lifetime CG
- 267. Depreciation SMR = SMR production capacity/Lifetime SMR
- 268. Effect of learning on price = IF THEN ELSE(Cumulative experience Alk <0, 0 , (Cumulative experience Alk / Initial cumulative experience)<sup>(LearningindexAlpha)</sup>)
- 269. Learning index Alpha = LOG((1-Learning rate LR of Alkaline electrolyzers),LOG base learning factor)