Towards a robust European hydrogen network

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Thesis

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by

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Compare yourself to who you were yesterday, not to who someone else is today.

Jordan B. Peterson

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Executive summary

As global climate change concerns intensify, the European Union aims towards the decarbonization of its Member States. Over the last decade, hydrogen has received increasing attention as a vital element to achieve this decarbonization. However, the diffusion of hydrogen in the European Union is critically dependent on the emergence of a pipeline transmission infrastructure. While earlier research has been conducted on this topic, three research gaps exist: 1) a disregard for the international aggregation level, 2) lacking recognition for robustness as a performance measure and 3) a missing link between hydrogen infrastructure development and natural gas pipeline reassignment. This research aims to fill these gaps through the generation of robust network topologies for a European hydrogen infrastructure between 2030 and 2050.

To generate these robust network topologies, a novel methodology combining Exploratory Modelling and Analysis (EMA) and graph theory is proposed. The essence of this methodology is to generate a network that performs well over a wide range of plausible futures. This builds on the idea that uncertainty of the future creates a realm of possible outcomes. Specifically, the development of a European hydrogen infrastructure is dependent on the development of demand and supply in four sectors: transport, built environment, industry and power generation. Additionally, geopolitical uncertainties such as strategies of European Member States to become either hydrogen importers or exporters are of great relevance. By running a large set of computational experiments, EMA facilitates an exploration of the realm of outcomes that is generated by these uncertainties. This research generates optimal networks for all experiments based on existing graph-theoretical heuristics and utilizes a set of three heuristics to generate a robust network based on these results. These heuristics target essential design variables when generating robust network topologies: 1) what connections to build, 2) what capacities to assign and 3) how to factor in future investments. To assess robustness, a regret-based formalisation is used that defines regret as the deviation of the chosen alternative from the optimal alternative in each plausible future. On top of this, the derived network is assured to be financially feasible through an edge removal heuristic, implying that each connected component in the final network features an NPV larger than zero. In doing this, the retrieved network presents a sensible investment opportunity for transmission system operators, which are likely to be responsible for hydrogen network infrastructure investments.

The results of this research highlight that a sizeable European hydrogen network may emerge towards 2050 with Italy and Germany at its core. In 2030, multiple relatively small networks may arise around Italy, Germany and the Benelux. These components can be expected to grow in size by 2040 but nevertheless stay disconnected. As of 2050, a cohesive European network spanning from the Balkan in the East to France in the West may emerge, connecting the previously disconnected networks. The total network size grows from circa 20 connections in 2030 to nearly 100 in 2050, featuring an increase in total network cost from almost 2 billion EUR to over 9.5 billion EUR. When incorporating current efforts of European Member States to stimulate hydrogen, France emerges as a third network pillar in addition to Italy and Germany. Natural gas pipeline reassignment has the potential to increase the size of a European hydrogen network. Specifically the reassignment of pipelines in and surrounding the earlier identified backbone nations of Germany and Italy creates an infrastructure backbone that is feasible in a wide range of plausible futures.

With respect to next steps, this research highlights four policy recommendations. First, the findings of this study should be utilized to activate and inform Member States on the financial feasibility of a European hydrogen infrastructure. Next, cooperation between Member States should be fostered as this study highlights that an international network is most robust. Third, this research highlights initial adoption centres, which can be employed to give direction to resource allocation. Lastly, the developed model is well suited for hypotheses testing and should be employed as a tool in decision-making processes surrounding the development of a European hydrogen infrastructure. For researchers, an expansion on the proposed model can be made by investigating the areas of interest highlighted by this study on a more regional, detailed level. Additionally, the model can be improved by including reliability and redundancy concerns. Moreover, a more extensive consideration of geopolitics can be included, such as strategies of the European Union to import hydrogen from other continents. As a more general, methodological next step, the proposed methodology combining EMA and graph theory can be further tested by applying it to other cases or comparing it to other methodologies aimed at deriving network infrastructures under uncertainty. While this research provides proof-of-concept, other studies may focus specifically on uncovering the true potential of this methodology.

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1 Research introduction

1.1 Europe's need for a hydrogen pipeline network

As the planet is warming up, climate related risks to human health, security and livelihood are increasing due rising sea levels, changing regional climate characteristics and rapidly collapsing biodiversity [1]. Since rising temperatures are attributed to greenhouse gas emissions, governments worldwide have pledged to decarbonize their societies [2]. Hydrogen has the potential to realize this decarbonization as it can be produced sustainably and has applications in industry, transport, built environment and power generation [3]. Therefore, the European Commission [4] identifies it as a 'key priority' to achieve the European transition away from carbon emitting fuels. However, the large-scale penetration of hydrogen in society is highly dependent on an effective transportation infrastructure, which is not yet developed [5]–[8].

Transportation by pipeline is considered the most economical solution in the long term. For example, a pipeline infrastructure is found to be more economical than its alternatives once the market share of fuel cell electric vehicles (FCEVs) reaches 10% and 25% in Germany and France, respectively [7], [9]. As predictions of FCEV penetration rates in these European countries reach between 20% and 75% in 2050, the long term benefits of pipelines become apparent [9]–[11]. Generally, pipelines outperform other alternatives once transportation volumes increase due to economies of scale [7].

A promising pipeline alternative is utilizing the existing natural gas network to transport hydrogen [12]. After all, the necessity of transporting natural gas will be gradually eliminated as European governments are set to phase-out fossil fuels towards 2050 [13]. At this point, reassignment can provide a use for pipelines that may otherwise become stranded assets [14], [15]. The main benefit of pipeline reassignment concerns costs: Cerniauskas et al. [16] concluded for Germany that pipeline reassignment can reduce the costs of a national pipeline network by 20% to 60% compared to a new hydrogen network. Nevertheless, the potential for reassignment towards 2050 will be limited by existing natural gas flows. Most notably, reassigning natural gas pipelines may endanger security of gas supply. This is problematic as security of gas supply has become increasingly important in the European Union ever since the Russia-Ukraine gas disputes of 2006 and 2009 [17], [18]. As a result, a combination of new hydrogen pipelines and reassigned natural gas pipelines seems most promising.

Now, is it worthwhile to investigate effective network topologies as pipeline infrastructures are extremely costly. For example, the single natural gas pipeline of Nord Stream 2 between Germany and Russia costs almost 10 billion euro's [19]. To put this in perspective, the total budget of the European Union allocated to 'address climate change' was 35 billion euro's in 2020 [20]. So, misplacing pipelines is not cheap. Unfortunately, pipeline planning is very intricate due to uncertainty on the role of hydrogen and natural gas in future's society. For example, the European Union (2019) aims to largely remove fossil fuels from its energy mix towards 2050, but Fragkos et al. [21] conclude that the share of natural gas in the European primary energy demand will only decline from 25% in 2010 to 18% in 2050. This is important as the use of hydrogen will determine the necessary new infrastructure, while the use of natural gas will decide the potential for pipeline reassignment.

To complicate matters further, the emergence of a hydrogen infrastructure depends on the geopolitical landscape that will erupt. For example, the European natural gas network is developed to facilitate large inflows from gas exporting nations such as Russia and Norway [22]. In some sense, these relationships are relatively simple because the originate primarily from the geographical distribution of natural resources. Hydrogen is set to transform traditional import-export relations as it can be produced by any country [23]. As a result, the future geopolitical landscape of hydrogen can take on a multitude of forms, leading to massive uncertainty for infrastructure developments.

1.2 Core concepts to hydrogen infrastructure development

To further introduce the topic of this research, three core concepts will be highlighted. These concepts are hydrogen transmission networks, deep uncertainty and natural gas pipeline reassignment.

1.2.1 Hydrogen transmission networks

Hydrogen supply chains consist of five steps, as shown in Figure 1 [5], [24], [25]. To transport hydrogen from producers to consumers, transmission and distribution networks are used. Transmission networks transport substantial volumes over large distances to connect regional hubs, while distribution networks deliver to individual customers such as hydrogen refuelling stations [9], [10]. This research will focus solely on transmission, subsequently giving in on the completeness of the resulting infrastructure. However, due to the large, continental scope of the study, this focus is most appropriate from a practical point of view. Additionally, as argued for in the previous section, this research focuses specifically on the transportation of hydrogen through pipelines.



Figure 1: Five elements of the hydrogen supply chain.

1.2.2 Deep uncertainty

As highlighted in the previous section, the evolution of a European hydrogen network is dependent on a variety of uncertainties such as the development of climate policies. This constitutes a case of deep uncertainty, which is defined as a situation where there exists a range of possible futures while knowledge on the relative likelihood of these futures is absent [26]. Deep uncertainty renders a "best guess" of the future practically useless and requires the consideration of robustness as a performance measure [26], [27]. After all, developing an infrastructure based on a best guess of the future only makes this a desirable solution in that specific scenario, of which the likelihood may as well be zero. Robustness implies finding solutions that perform well in a wide range of futures and are thus relatively insensitive to the specific future that comes to fruition.

1.2.3 Natural gas pipeline reassignment

Within this research, natural gas pipeline reassignment is defined as the alteration of existing natural gas pipelines to transport pure hydrogen. This explicitly excludes mixtures of hydrogen and natural gas through the injection of hydrogen in the natural gas network. As illustrated by Cerniauskas et al. [16], there are four options for reassignment: 1) pipelines without modifications, 2) coating, 3) inhibitors and 4) pipe-in-pipe. However, the specific methods used for reassignment are out of the scope of this research: it is assumed that natural gas pipelines can be utilized to transport hydrogen given a certain cost and if specific conditions are met. The total potential for natural gas pipeline reassignment is considered to be the total set of pipelines that conform to these conditions.

1.3 Current gaps in hydrogen infrastructure research

Based on a review of existing literature, this sub-section pinpoints three research gaps. These gaps provide the starting point for this research and lead up to the research question posed in the next sub-section.

1.3.1 A disregard for the international aggregation level

Numerous studies have looked into the development of hydrogen infrastructures. Andre et al. [7] and Baufume et al. [10] analysed the development of a transmission pipeline network for France and Germany, respectively. Outside of Europe, Johnson and Ogden [28] and Yang and Ogden [29] mapped the development of hydrogen networks in various American states. Various other studies considered pipelines amongst other transportation methods [5], [9], [30]. In mapping the geographical scope of these papers, an emphasis on the national level is found (see Table 1). This fits into the more general notion that hydrogen supply chain studies largely disregard the international level: a recent literature review selected 71 papers on hydrogen supply chains and concluded that only 3 have an international spatial scale [25]. None of these studies consider pipeline networks.

Study	Year	Geographical scope	
[30]	2020	Germany	
[31]	2019	British Colombia, Canada	
[9]	2019	Germany	
[32]	2019	Northern Germany	
[33]	2017	United Kingdom	
[7]	2014	France	
[10]	2013	Germany	
[29]	2013	California, United States	
[34]	2013	United Kingdom	
[28]	2012	Arizona, New Mexico, Colorado & Utah, United States	
[35]	2010	Norway	
[36]	2008	Ohio, United States	

Table 1: Geographical scope of existing hydrogen network studies

As a result of this national focus, scientific papers focusing on the European level are lacking. This is critical as the European level offers both massive opportunities and challenges for hydrogen development. On one hand, cross-border and regional cooperation is essential to achieve the energy transition, as emphasized by the European Green Deal [13]. On the other hand, the European level adds a new level of complexity. For example, let's consider a simple 'make or buy' decision that Member States may face considering hydrogen [37]. If we assume all 27 Member States face this choice, there are over 134 million different outcomes. In turn, these outcomes impact the required infrastructure. So, the interactions between national policy aims of Member States balloon complexity for infrastructure development. This complexity is scientifically important as hydrogen is a blind spot in literature on geopolitics [23]. Through the analysis of a European hydrogen infrastructure, this research aims to tackle the lack of international focus in hydrogen infrastructure research while simultaneously contributing to literature on the geopolitics of hydrogen.

1.3.2 Lacking recognition for robustness as a performance measure

As highlighted in section 1.1, the development of a European hydrogen network resembles a case of deep uncertainty where finding an optimal infrastructure based on a "best-guess" of the future is futile. To tackle uncertainty, hydrogen network studies often employ between 2 to 10 scenarios (see Table 2). In doing this, performance criteria based on optimality are employed to determine the required infrastructure per scenario. Although the terms used differ, most studies focus on minimizing network costs.

Study	Year	Scenarios (#)	Performance criterion
[30]	2020	3	Minimal required delivery distances
[31]	2019	3	Minimal discounted total cost of infras- tructure
[9]	2019	3	Minimal total network length
[33]	2017	7	Minimal discounted total cost
[38]	2016	2	Minimal total energy system costs
[7]	2014	2	Minimal average equivalent annual cost of equipment
[29]	2013	10	Minimal discounted total system cost
[10]	2013	6	Minimal network length
[34]	2013	5	Minimal total supply chain network cost
[28]	2012	5	Minimal total annual cost of produc- tion and pipeline transmission
[8]	2011	3	Minimal sum of the average total cost of the supply chain
[35]	2010	4	Minimal scenario costs, calculated from capital costs, O&M and energy costs
[36]	2008	5	Minimal pipeline network length

Table 2: Scenarios used in hydrogen network studies

This methodology entails the use of "what-if" scenarios that try to predict what will happen given a specific future [27]. For example, through the use of best and worse case scenarios, the borders of the solution space can be mapped (see Figure 2). Now, a fundamental shortcoming of this approach is that it offers little guidance towards determining solid infrastructure investments. At best, the worst case provides an overview of no-regret options if we assume that the relative geographical distribution of supply and demand is constant throughout all scenarios.



Figure 2: Illustration of scenario approach that explores the borders of the solution space.

Contrary to the papers in Table 2, a recent study incorporated the concept of robustness to analyse a European energy system including hydrogen pipelines [39]. However, their robustness analysis focused solely on the consideration of multiple weather years and assumed a 100% renewable energy system based on static assumptions such as a FCEV penetration rate of 75%. As a result, this analysis covers only a range of variations to the best case scenario as shown in Figure 2, hardly informing on truly robust investment decisions. Introducing robustness as a performance criterion to explore the full solution space of a hydrogen infrastructure can significantly improve the usefulness of results. On top of this, it will be a vital addition to the existing bulk of literature focusing on optimality based performance measures.

1.3.3 Missing link hydrogen and natural gas pipeline reassignment

As a third gap, there is a lack of research that integrates natural gas pipeline reassignment in the development of hydrogen pipeline infrastructures. On one hand, some literature papers focus on the reuse of the natural gas network. For example, Cerniauskas et al. [16] analyse the technical and economical potential for natural gas pipeline reassignment in Germany. Speirs et al. [15] test various decarbonization options for gas networks on technical feasibility, costs and environmental impact, including hydrogen. Other papers focus on the injection of hydrogen in natural gas networks [6], [12]. However, these studies do not pair this with an analysis of a hydrogen infrastructure. On the other hand, none of the hydrogen infrastructure studies mentioned in Tables 1 and 2 include natural gas pipeline reassignment. This gap is critical as the specific combination of new hydrogen pipelines and reassigned natural gas pipelines offers a fruitful alternative, as argued for in section 1.1.

1.4 Research questions

Concluding, the development of a robust European hydrogen transmission pipeline network utilizing natural gas pipeline reassignment is a blind spot in the current scientific literature. Through the following research question, the scientific gaps that lead up to this blind spot can be filled:

What is the most robust configuration for a European hydrogen pipeline network between 2030 and 2050, utilizing a combination of new hydrogen pipelines and reassigned natural gas pipelines?

Six sub-questions have been formulated to pinpoint the research activities required to answer the main research question:

- 1. How can energy network infrastructures be modelled?
- 2. How to best deal with uncertainty in the context of network infrastructure development?
- 3. What is a suitable methodology to generate robust network infrastructure configurations?
- 4. What drives the development of a European hydrogen infrastructure between 2030 and 2050?
- 5. What are relevant economic-geographic inputs to model a European hydrogen pipeline network?
- 6. What are critical uncertainties to the development of a European hydrogen pipeline network?

1.5 Research outline

Chapter 2 aims to answer the first two sub-questions by reviewing existing literature on network system design problems and the role of uncertainty in infrastructure development. Next, Chapter 3 tackles the third sub-question through the creation of a methodology for the generation of robust network infrastructure topologies. To allow for the application of this methodology to the case introduced in this Chapter, Chapter 4 analyses the development of hydrogen in Europe more extensively and seeks to provide an answer to the last three sub-questions. The results of this application will be presented in Chapter 5, followed by the discussion, conclusion and recommendations.

2 Theoretical framework

The goal of this Chapter is to review existing literature on network system design problems and approaches on dealing with uncertainty in infrastructure development. This is done by respectively section 2.1 and 2.2.

2.1 Network system design problems

Countless technical and scientific challenges revolve around the analysis of networks and their characteristics, such as finding the shortest path from one point to another or identifying the cheapest way to connect a series of points. Heijnen, Chappin and Herder [40] identify three main approaches to tackle these challenges: graph theory, mixed integer (non-)linear programming (MILP) and agent-based models. Agent-based models rely on Ant Colony Optimisation (ACO), which is utilized to design a wide range of systems that build on the collective behavior of social insects [41]. Initially, ACO models have been applied to find shortest paths between locations of interest [42], although Dorigo highlights that they can also be applied to for example the classical traveling salesman problem. Generally, agent-based models feature a lot of freedom as they are built in a bottom-up fashion that allows for a design based on the decision rules of individual agents [43]. As a second category, MILP studies have been extensively utilized to analyse network systems and their characteristics. Examples include the analyses by Moreno et al. [33], Angolucci and McDowall [44], Andre et al. [7] and Konda et al. [8]. These analyses are often spatially explicit to include the geographical component of network design [28]. The advantage of MILP is that it provides a relatively clear-cut structure to formulate the optimisation problems. As such, it allows for the derivation of an optimal solution given an objective function and set of constraints. As a third category, the most common modelling technique for designing networks is graph theory [45]. This also applies to hydrogen infrastructure research, where the bulk of studies rely on a graph-theoretical approach [9], [10], [30], [46]. Graph theory can be dated back as far as 1736 to Euler and his problem of the seven bridges of Köningsberg [47]. As such, a wide range of heuristics and algorithms has been developed in graph-theoretical literature to analyse networks and their characteristics. Classical algorithms include Dijksta's algorithm to find the shortest path between two points and the Ford-Fulkerson algorithm to assess the maximum flow through a network [48], [49]. Graph theory combines this extensive toolbox with the flexibility to incorporate new elements due to its relatively simplistic structure. Specifically, it strikes a balance between the large flexibility of agent-based models and the relative rigidness of MILP. Additionally, graph theory is specifically designed to analyse networks, whereas MILP and agent-based models have different primary applications and therefore require more effort to be effectively fielded in the domain of network analysis. As such, graph theory seems the most fruitful methodology to model energy networks. More so because the focus of this study lies outside of the direct domain of optimisation, which is the fortitude of MILP. This is line with Heijnen et al. [40], who find that graph theory is the most fitting of the three approaches to analyse infrastructure networks. This is supported by their study comparing a graph-theoretical approach to an agent-based one [43]. As such, this research will utilize this approach.

Graph theory facilitates the analysis of network system design challenges through the formalisation of networks in terms of network points and the connections between them. As such, a graph is defined as the product of a set of nodes $\{n_i\}$ and a set of edges $\{e_{i,j}\}$. If $\{e_{1,2}\}$ is an element of the set $\{e_{i,j}\}$, this implies a connection exists between the nodes $\{n_1\}$ and $\{n_2\}$. Note that this is the case for the simple graph illustrated in Figure 3.



Figure 3: Simple graph consisting of four nodes and edges.

One of the primary characteristics of emerging energy infrastructure networks is their aim to connect multiple sources and sinks, respectively producers and consumers, in a cost optimal way without redundancy [50]. Here, cost optimality is judged based on the weights of the edges, which represent their investment cost. As an example, Figure 4 illustrates such as network system design problem.



Figure 4: Simple network design problem that requires the connection of sources and sinks.

This simple example represents a minimum-weight spanning tree problem, which is one of the best-known problems in graph theory [51]. A tree is a graph that features no cycles, meaning that there exists exactly one path from each node to every other node. To classify as a spanning tree, all nodes should be connected. For every network of more than two nodes multiple spanning trees exist, with the minimum-weight spanning tree featuring the lowest total edge weight. When the weights of edges are assumed to be dependent purely on their length, the minimum-weight network equals the Euclidean minimal spanning tree. Figure 5 illustrates this network for the earlier introduced example. Note that while this network is cost-optimal, it is very susceptible to disruptions as the failure of a single edge is guaranteed to disconnect the network. To decrease this susceptibility, networks may be developed based on rules such as the N-1 criterion utilized in the European natural gas network. As laid out in Regulation (EU) No 994/2010, this implies that in case of a disruption of the largest infrastructure in a region, the remaining infrastructure should still be able to satisfy demand in that area. This exploratory research explicitly aims towards generating an outline of a future hydrogen network. As such, it focuses on the generation of a tree structured network. Because of its wide range of applications, many algorithms have been developed to find minimum-weight spanning trees [52], [53]. Of these algorithms, those discovered by Kruskal and Prim are best-known [54], [55]. Please refer to Appendix A.1 for an illustration of both algorithms. Now, both algorithms are guaranteed to produce optimal outcomes if the edge weights are known in advance [56]. As a distinction, Prim's algorithm generally outperforms Kruskal's algorithm on computational time, although Kruskal's algorithm may be faster for sparse networks [57]-[59]. Both algorithms are readily used in the analysis of energy infrastructures. For example, Reuß et al. [9] utilize Kruskal's algorithm to generate hydrogen infrastructures for Germany while Tlili et al. [30] use Prim's algorithm for a similar analysis applied to France.



Figure 5: Euclidean minimum spanning tree for the problem introduced in Figure 4.

A complication of multi-source, multi-sink networks that aim towards zero redundancy is that edge weights are dependent on the flow between sources and sinks, which in turn is based on the network topology [40]. Specifically, edge capacities can be determined by assigning the supply or demand values of nodes with degree 1 to their neighbouring edges and subsequently removing these edges [60]. Note that a node with degree 1 is connected to exactly one edge. Figure 6 illustrates the capacity assignment procedure, which can be repeated until all edges are removed. Now, if edge weights are dependent on distance only, the minimum-length spanning tree is equal to the minimum-weight spanning tree, irrespective of this complication. However, the investment cost of energy infrastructure connections is also dependent on their capacity (see e.g. Appendix A.3). In this case, the minimum-length spanning tree is not necessarily the lowest cost tree.



Figure 6: Procedure to assign capacities to edges based on supply-demand patterns of nodes.

A first solution to the aforementioned complication is a 'brute force' approach that identifies the optimal tree by enumeration of all possible trees. However, Cayley's formula dictates that the number of possible trees for a network of n vertices is equal to n^{n-2} , meaning that this approach runs to its limits for larger networks [61]. As a result, various heuristics have been developed to find low-cost spanning trees. Brimberg et al. [62] analysed both a Tabu search and Variable neighborhood search approach, concluding that both heuristics produce near-optimal solutions that significantly outperform the minimum-length spanning tree solution. Andre et al. [63] developed a Delta change heuristic based on a tree optimisation procedure developed by Rothfarb et al. [64] and compared this to the Tabu search. They concluded that their heuristic generates 7 - 18% cheaper networks. Heijnen et al. [40] compared this heuristic to three other methods and concluded that is has both the best performance and lowest computational time. As such, the Delta change heuristic seems to be the most fruitful method for finding minimum-cost spanning trees for energy infrastructure networks.

The heuristic starts from a minimum-length spanning tree, which can be derived via Prim or Kruskal's algorithm. Next, the heuristic walks through 2 steps, highlighted in Figure 7. For each node, an edge is added that connects the closest node in Euclidean distance that is not connected to the selected node. This creates a cycle. Next, the other edges of the emerged cycle are removed one by one. If an edge removal improves the network cost, the old network is replaced by the new one. Otherwise, the removal is reverted.



Figure 7: Delta change heuristic to find cost improvements on tree networks [7].

Now, an implicit assumption of the previously discussed heuristics is that all nodes should be connected. However, Heijnen et al. [50] define uncertainty about participants and locations a key characteristic of emerging infrastructure networks. Similar to Bertsimas [65], they assign probabilities to the presence of certain nodes. This is related to the all nodes replacement (ANR) problem, where replacement MST's are calculated for instances in which specific nodes will fail [66], [67]. However, this assumes a reactive approach, which is less fitting to the rigid nature of network infrastructure development, favouring the approach of Heijnen et al. Nevertheless, their method requires an estimation of the probability that specific nodes will not participate, which may be somewhat arbitrary.

Alternatively, Andre et al. [7] utilize an economic criterion to determine node participation. Their heuristic starts from a spanning tree and identifies its leafs. A leaf is a node that is connected by one edge. Each leaf is removed if it violates an economic criterion, after which the set of unvisited leafs is updated (see Figure 8). In their specific case, a pipeline is economically justified if outperforms a predefined alternative.



Figure 8: Edge removal heuristic to remove edges that violate an economic criterion [7].

The advantage of this approach is that node participation is analysed based on a clear criterion rather than the more subjective estimation of probabilities. As such, this approach seems most fruitful to incorporate participant uncertainty in the analysis of emerging network infrastructures. However, the analysis of Andre et al. focuses on single-source, multi-sink networks and guarantees a network topology featuring a single connected component. In reality, energy network infrastructures represent multi-sink, multi-source networks [68]–[70]. As such, this research will apply their approach to this type of network.

A final characteristic of network infrastructures is their growth over time. The European natural gas network illustrates this clearly. Some of the first natural gas pipelines were developed around 1970 in the Netherlands, and still 28 investment projects were commissioned in 2019 and 2020 to foster continuous network improvement [71]. Studies on network infrastructures often incorporate this by deriving an infrastructure for multiple discrete time steps or scenarios. Johnson and Ogden [28] and Thili et al. [30] derive a series of networks based on a proxy for the hydrogen diffusion, implicitly modelling network expansion over time as hydrogen demand increases towards the future. Other studies such as Bique and Zondervan [72] and Almaraz [73] et al. utilize discrete steps of 10 years to map network expansion towards 2050. An essential aspect of modelling network expansion is how to deal with previously built infrastructure. For example, Johnson and Ogden [28] derive multiple networks by continuously expanding on previously built infrastructure. However, they derive networks by purely focusing on the time step at hand and do not correct for possible future capacity expansions. Alternatively, Andre et al. [7] utilize a backward heuristic that first derives the infrastructure in the final time step and subsequently considers the time steps before that [7]. The primary advantage of this approach is that results in initial time steps are generated with the final network in mind. However, their approach ignores the chicken-egg-problem and other dynamics between existing infrastructure and future demand. The chicken-egg-problem refers to a lock-in situation between consumers and infrastructure developers, where each is waiting for the other to act. In recent years, this has gained increasing attention in the development of a refuelling infrastructure for electric vehicles [74], [75]. Based on this phenomenon, future demand values in areas with existing infrastructure can be expected to increase. In addition to the chicken-egg-problem, infrastructure expansions are heavily dependent on existing infrastructure. For example, a hydrogen network is likely to expand from a few initial user centres that serve as a springboard for future expansion [68]-[70]. Thus, a heuristic is required that incorporates the relationship between existing infrastructure and future demand in a forward rather than backward looking manner. Similar approaches have been applied to distribution expansion problems [76], fast-charging location planning [77] and hydrogen refuelling infrastructure planning [78]. However, to the author's best knowledge, no study has utilized a graph-theoretical approach to analyse multi-period pipeline infrastructure design problems with demand dynamics. This research aims to incorporate these dynamics in its analysis.

Concluding, energy network infrastructures can be modelled as 1) multi-sink, multi-source networks without redundancy that 2) feature participant uncertainty and 3) expand over time. This research will utilize a graph-theoretical approach that incorporates these elements, building on existing practices where possible and aiming towards the creation of new methods where necessary. This section purposely neglected a fourth characteristic of network infrastructures, namely supply and demand uncertainty, as this is the focus of the next section.

2.2 Uncertainty in infrastructure development

A critical aspect of network infrastructure development is uncertainty on future supply and demand. This results from a variety of economic-geographic, technical and geopolitical uncertainties. For example, the diffusion of hydrogen is simultaneously dependent on its production potential, the technical development of its applications and efforts by (inter-)national governments. This section will first provide a conceptual basis for decision making under uncertainty and subsequently reviews the analysis of uncertainty in network design problem literature.

The XLRM-framework provides a conceptual basis for structuring decision problems under uncertainty, shown in Figure 9 [79]. It identifies four elements: external factors, relationships or internal factors, policy levers and performance metrics. External factors (X) are exogenous uncertainties outside of the decision maker's control that nevertheless impact the system of interest. Policy levers (L) are alternatives or strategies that the decision may utilize to influence this system. Internal factors and relationships (R) make up the system structure and dictate its dynamic. Lastly, performance metrics (M) represent standards used to judge system outcomes. Given this conceptualization, the goal is to identify strategies that produce desirable outcomes in spite of the existence of external uncertainties. As highlighted by Kwakkel and Van Der Pas, there are three approaches to uncertainty in infrastructure planning, which will be discussed in further detail [80].



Figure 9: XLRM-framework as a means to structure decision problems under uncertainty [81].

A first strategy to decision problems under uncertainty is the "predict-then-act" or static-rigid approach, where the future is anticipated based on best available knowledge [27], [79]. One such category of studies utilizes a number of scenarios to design predictive "what-if" scenarios. Please recall the 13 papers highlighted in Table 2 that utilize between 2 and 10 scenarios to deal with future uncertainty. In the context of decision making under uncertainty, these "best-guesses" of the future are practically useless as their probability may as well be zero [80]. Another category of studies uses probability distributions to dictate the likelihood of future events and find optimal outcomes [82]. These optimal outcomes are determined via a calculation of expected utility. For example, Fodstad et al. [83] utilize a set of 8 scenarios with a known probability to analyse the impact of technology and policy uncertainty on optimal gas pipeline infrastructure investment. Importantly, this builds on the assumption that the probability functions of uncertainties can be estimated [84]. This is problematic as imperfect information and surprises like black swan events make predicting the future a tricky operation [80], [85], [86].

An alternative approach builds on the idea of a great variety of possible futures while knowledge on the relative likelihood of these futures is absent [26]. This concept is introduced as deep uncertainty in Chapter 1. The notion of deep uncertainty refutes the idea of assigning probabilities to future events. Rather than striving for optimality, this approach aims at finding robust strategies that perform well over a wide range of plausible futures [26], [27]. Now, there exists a wide range of robustness metrics. For example, Giuliani and Castelletti [87] identify five classic robustness metrics: maximin, maximax, optimism-pessimism, minimax regret and the principle of insufficient reason. Their analysis concludes that the use of different metrics may have a large impact on research outcomes, emphasising the importance of setting an appropriate robustness metric. Herman et al. [88] make a distinction between regret-based and satisficing measures. The former seeks out alternatives with minimal regret, where regret is based on the relative performance of an alternative to the optimum or a predefined basecase in each scenario. An example of its application to graph theory is the analysis of Conde and Candia, who utilize a minimax regret metric to analyse robust networks under demand uncertainty [89]. Another example is the study by Yang and Jiang [90], who analyse the development of hydrogen refuelling infrastructure under demand uncertainty using a robust regret metric. Satisficing measures identify alternatives that perform sufficiently in a wide range of possible futures. In turn, this requires an explicit definition of what constitutes as sufficient. An example of this analysis is the study of uncapacitated network design problems by Gutiérrez et al. [91], who label network designs that are within p% of the optimal solution as sufficient. In network infrastructure development, (near) optimal solutions can be easily generated utilizing the heuristics discussed in section 2.1. As such, a regret-based approach that focuses on the generation of robust topologies by means of comparison to the optimal network seems most appropriate. Most importantly, this prevents having to define an arbitrary base case or definition of what constitutes as sufficient.

A third approach to decision making under uncertainty focuses on the incorporation of flexibility and introduces multiple decision moments over time [26]. Rather than concentrating on a strategy that remains satisfactory in case of changing conditions, this approach seeks strategies that can flexibly adapt to these conditions. An example is the study by Melese et al. [92], who utilize the concept of real options to incorporate flexibility in infrastructure development. Now, the choice for either a static robust or dynamic approach is dependent on the flexibility of alternatives and the implementation time of alternatives compared to the rate of change of the system [27]. For example, infrastructures are heavily path-dependent and prone to lock-in, limiting options for adaptive planning [93]. Additionally, dynamic approaches require an explicit consideration of timing [94]. As such, the choice for either a static robust of flexible strategy should be considered per case. Irrespective of this choice, static robust and flexible strategies outperform strategies that aim at an optimal alternative.

Now, there are various methodologies for incorporating robust and flexible strategies in the development of network infrastructures, such as robust optimisation, scenario discovery, decision scaling, adaption tipping point approaches and info-gap [27], [94]. The studies mentioned in the previous paragraphs provide examples of the application of some of these methodologies. Important is to match the specific methodology to two characteristics of uncertainty: the level of uncertainty and its dynamic [94]. In the case of infrastructure development, uncertainty can be characterised as deeply uncertain due to the long planning horizon and the multitude of uncertainties that together surround infrastructure development. Additionally, these uncertainties are dynamic as geopolitical, economic technological uncertainties can be expected to vary throughout time. For example, geopolitical pressures on the earlier mentioned Nord Stream 2 suddenly changed since Biden took the Presidential office in the U.S. [95].

A promising methodology to deal with this kind of uncertainty, although neglected in graphtheoretical literature, is Exploratory Modelling and Analysis (EMA). EMA can be utilized to explore robust strategies and gain insight in system behavior. Its core premise is that decision makers should explore a wide range of hypotheses about the system of interest through the use of computational experiments [79]. This is done by broadening the assumptions about the system and investigating system behavior for a wide range of input values (X), model structures (R) and value systems (M) [96]. The wide range of plausible futures that emerges as a result this exploration can be captured in an uncertainty space, highlighted in Figure 10. In this case, the uncertainty space highlights all possible values for a specific uncertainty. An uncertainty space builds on the idea that while the likelihood of future events is unknown, the future is quantifiably uncertain [27]. As such, a distinction is made between plausible and implausible futures.



Figure 10: An uncertainty space dictates the range of possible value for an uncertainty.

Uncertainty spaces can be explored by sampling a large number of values that serve as the input for computational experiments [79]. This is shown in Figure 11, where experiments are sampled based on two exogenous factors. As EMA aims to explore the full range of plausible futures, sampling is utilized to prevent a computational nightmare featuring millions or billions of experiments. The philosophy is that system behavior can be explored accordingly by running a large number of sampled experiments [94]. Various different sampling techniques are available to represent the uncertainty space, most notably Monte Carlo, Factorial Design and Latin-Hypercube [97].



Figure 11: Experiments are created by sampling values from uncertainty spaces.

EMA has been applied aptly outside of the domain of graph theoretical network analysis. Showing its broad applicability, Kwakkel and Pruyt [98] combine EMA with system dynamics and agentbased modelling to investigate cases of metal scarcity and transition dynamics in the electricity sector, respectively. In general, exploratory modelling has found most applications in environmental and water resource literature [27]. Examples include the research by Urich and Rauch [99] and Thissen et al. [100], who applied exploratory modelling to respectively urban water management and fresh water supplies in the Netherlands. Nevertheless, other sectors where exploratory modelling has found its way include coupled human-natural system, airport planning, transport policy and copper scarcity [101]–[104]. The application of exploratory modelling across various domains underlines it validity, further emphasizing its potential in the analysis of emerging infrastructure networks. As such, a methodological aim of this thesis is to develop a novel approach that applies EMA to graph theory and infrastructure design.

2.3 Towards the integration of EMA and graph theory

The starting point for diving in literature on network design problems and uncertainty in infrastructure networks was to answer the first two sub-questions:

- 1. How can energy infrastructure networks be modelled?
- 2. How to deal with uncertainty in the context of infrastructure development?

With respect to the first sub-question, a graph-theoretical approach seems fruitful to formalise energy network infrastructures. This approach can largely build on existing concepts, such as that of multi-source, multi-sink networks and minimum spanning trees. Nevertheless, this research aims to contribute to existing literature by 1) incorporating participant uncertainty based on a economic criterion in multi-source, multi-sink networks and 2) considering demand dynamics in multi-period network infrastructure design. Considering the second sub-question, a novel approach combining graph theory and exploratory modelling and analysis seems promising. As such, this research will add to existing literature by outlining a methodology that utilizes this combination. To the domain of graph theory, this may serve to be an additional means to deal with future uncertainties. On the other hand, the application to graph theory may provide new insights for exploratory modelling practices.

To be precise, this research aims to fill the three knowledge gaps in literature on hydrogen network infrastructures introduced in Chapter 1. These knowledge gaps are case-specific, although they may provide insights that can be applied outside of this specific case. Now, the knowledge gaps highlighted in the theoretical framework have a more methodological nature and aim to improve existing methods that can be applied to a wide range of cases.

Figure 12 provides a high-level overview of the relationship between the theoretical framework and methodology. Based on the theoretical basis of section 2.1, section 3.1 will touch on the generation of optimal networks. Next, section 2.2 will focus on the generation of robust networks by building on both section 2.1 and 2.2. Lastly, section 3.3 addresses the EMA workbench, which will build on the introduction of EMA in section 2.2.



Figure 12: Link between theoretical and methodological sections.

3 Network analysis and modelling

This Chapter lays out the methodology proposed by this research, building on the theoretical foundation of Chapter 2. Section 3.1 focuses on the generation of optimal networks, followed by the derivation of robust networks in section 3.2. Lastly, section 3.3 introduces the EMA workbench.

3.1 Optimal network generation

Section 2.1 highlighted graph theory as a suitable methodology to formalise network infrastructures. To employ graph theory, this research utilizes the Optimal Network Layout Tool, a graphtheoretical tool developed in Python at the TU Delft. [60]. The primary strength of this tool is that it is tailored towards the analysis of energy network infrastructures by focusing on multi-sink, multi-source networks with variable supply and demand patterns. Additionally, it lends itself well for incorporation of natural gas pipeline reassignment through the option to include existing connections. Furthermore, the tool is not tailored to a specific case or geographical scope. As a result, it is favoured above tools that have a fixed scope such as the ECOTRNASHY model utilized by Andre et al. [7], which is tailored towards France. Similarly, Baufume and Reuß [10] utilize a model that focuses solely on Germany. Other models, such as the HyPAT model utilized by Johnson and Ogden [28] do not incorporate the concept of existing connections.

3.1.1 Minimum cost spanning trees

The Optimal Network Layout Tool generates minimum-cost spanning trees in four steps:

- 1. Analyse demand-supply patterns
- 2. Determine representative set of k demand-supply profiles
- 3. Determine minimal spanning tree
- 4. Determine minimum-cost-spanning tree

The tool has two primary inputs: a set of network nodes and their coordinates, and the supply and demand values of these nodes. These values can be specified for multiple time steps to simulate fluctuations in supply and demand. However, finding an optimal network for a large number of time steps requires a sizeable computational effort. To tackle this issue, the tool explores the utilization of a smaller set of representative demand-supply profiles that still captures the dynamic of the underlying supply and demand patterns. To this end, a k-means clustering technique is utilized to map the quadratic relative error of the standard deviation for different numbers of representative sets. Figure 13 shows the output generated by the tool, first giving an indication of the total supply and demand per network node in the left illustration. Consecutively, a plot of the quadratic relative error of the standard deviation is shown in the right illustration, allowing for visual determination of an adequate number of representative sets. The key here is to identify the bending point of the graph, after which only small decreases in the error term are realized. In this example, the bending point is at 9 to 10 clusters.



Figure 13: Output of first step Optimal Network Layout Tool.

In the second step, a chosen amount of representative sets is created and visualised (see Figure 14). These supply and demand sets serve as the input for the generation of optimal networks.



Figure 14: Output of second step Optimal Network Layout Tool.

In the third step, the minimum-length spanning tree is generated based on Kruskal's algorithm (see Appendix A.1). The fourth step tries to improve this network through the Delta change heuristic (please recall section 2.1). Figure 15 illustrates three network alterations made by this heuristic on a small network. Note that the total network cost, shown at the top of each network illustration, decreases. In running this algorithm, the (near) optimal network is generated.



Figure 15: Output of application Delta change heuristic in Optimal Network Layout Tool.

For larger networks, the Delta change heuristic is computationally intensive as the number of possible edge swaps increases severely. In an attempt to reduce this, the heuristic was stopped once the relative improvement fell below a certain threshold. However, a small relative improvement in a specific iteration proved to be a poor predictor for future improvements. Figure 16 highlights the total network cost over 24 improvements rounds for three networks of 150 nodes. This shows that large improvements may follow a series of smaller improvements, making the alteration to the heuristic futile. As such, this research utilizes a timer to prevent the heuristic from taking too long. While a timer may decrease the performance of the heuristic, it allows for control over the computational time.



Figure 16: Decrease in network cost due to Delta change heuristic over 24 iterations in 3 cases.

3.1.2 Multi-source, multi-sink edge removal heuristic

The result of the Optimal Network Layout Tool is a tree network that connects all network nodes. However, Section 2.1 illustrated that it may be desirable to exclude specific network nodes. This research proposes a heuristic to exclude nodes based on an economic criterion. An economic criterion is a decision rule that is grounded in a financial parameter such as the total investment cost or rate of return of connecting a specific node. Economic criteria can be applied to networks on the level of individual edges, connected components and the entire network. This is highlighted in Figure 17. Note that a connected component is defined as a sub-graph of at least 2 nodes for which a path exists from every node to all other nodes.



Figure 17: Financial criteria can be applied to networks on various aggregation levels.

Now, to best simulate the emergence of a network infrastructure, an economic criterion should capture the investment behavior of pipeline transmission system operators (TSOs). These entities are responsible for the investment, operation and maintenance of transmission pipelines. Due to market failure that is inherent to pipeline investment, the transport tariffs charged by these entities are regulated. This regulation has two goals: first, it seeks to stimulate adequate infrastructure investments by providing TSOs with reasonable returns on their investment. Second, it aims to protect users from excessive prices. For more information surrounding infrastructure regulation in the European Union, please refer to Appendix A.2. The key takeaway is that the tariffs charged by a TSO are related to the cost of the pipeline. This implies that pipelines requiring large investments necessitate high tariffs, driving up the cost of the transported hydrogen. If prices are driven above the willingness to pay of consumers, the pipeline will cease to transport hydrogen as demand dries up. As a result, it is reasonable to assume that TSOs only invest in pipelines of which the investment costs can be covered using reasonable tariffs. This research captures this dynamic by conducting a NPV calculation that assumes a reasonable tariff range and weighs this against the cost of each pipeline. For more information on the cost structures of pipelines and the NPV calculation, please refer to Appendix A.3. The key takeaway is that large pipelines are financially more attractive as an increase in a pipeline's diameter significantly increases its capacity relative to its cost. As a result, the maximum length at which a pipeline features a positive NPV increases with its capacity, as illustrated in Figure 18.



Figure 18: Maximum length at which a pipeline is financially feasible given its capacity.

When considering large, international pipeline investments, consortia of both public and private organisations are often set up. Two examples of recent projects include Nord Stream 2 and the the Trans Adriatic Pipeline. These consortia feature their own shareholders and thus require to be financially feasible on their own [105], [106]. As a result, conducting the earlier mentioned NPV calculation on the level of a connected component (please recall Figure 17) seems most appropriate. This implies that every connected component in the final network should feature a NPV larger than zero.

Having defined the economic criterion to utilize, the proposed heuristic will now be discussed. Please refer to Figure 20 and Appendix B.1 for respectively the flow chart and pseudo code of the proposed heuristic. The minimum-cost spanning tree generated by the Optimal Network Layout Tool serves as input for the heuristic, which is labelled as an unvisited connected component. If this component features a NPV above zero, calculated as the sum of the NPV of all individual pipelines, it is added to the final network and the heuristic stops as there are no other unvisited connected components. Otherwise the network connection with the lowest NPV is removed from the network. Removing an edge from a tree may lead to three distinct cases, which will be illustrated using Figure 19. As a first option, one connected component may arise. This is illustrated in the top illustration, where the edge between nodes 4 and 6 is removed. Next, node 6 is removed from the network as this has the largest positive impact on the NPV of the network. Now, the removal of this node impacts the required capacity of the remaining edges in the network. As a result, the Optimal Network Layout Tool is utilized to recalculate the minimum-cost spanning tree. Let's assume the middle illustration of Figure 19 highlights the recalculated minimum-cost spanning tree, but this network still features a negative NPV. Specifically, the connection between nodes 4 and 5 now features the lowest NPV. Upon removing this edge, two connected components arise. In this case, both connected components are labeled as unvisited, implying that a minimum-cost spanning tree will be recalculated for both components. Subsequently, these trees will each be subjected to the economic criterion. Assuming this is done for the component of nodes 5 and 7, it may turn out that the edge between these nodes features as negative NPV. Removing this connection results in zero connected components, in which case both disconnected nodes are discarded. Important to note is that the heuristic ends in case there are no unvisited connected components left, implying that each network node is either part of a connected component with a NPV larger than zero or is discarded.



Figure 19: Removing edges from a connected component creates zero, one or two components.



Figure 20: Flow chart of multi-source, multi-sink edge removal heuristic.

The edge removal heuristic is integrated into the Optimal Network Layout Tool in Python. For verification purposes, toy models are utilized in which both the coordinates and supply and demand patterns of the nodes are randomized. Figure 21 shows the Python output of multiple edge removal iterations on one such model. An important dynamic of the heuristic is that the removal of nodes may create a cascading effect on the feasibility of the rest of the network. After all, this decreases the total supply and demand of the network, requiring lower pipeline capacities. As proven in Appendix A.3, this decreases pipeline feasibility. Additionally, it can clearly be seen from Figure 21 that the longest connections are the first to be removed, which is expected based on the cost structure of pipelines (please recall Figure 18). Lastly, it is important to emphasize the necessity of recalculating the minimum-cost spanning tree after each edge removal. In comparing iteration 4 and 5, removing the edge between nodes 10 and 15 impacts the optimal manner in which to connect nodes 9 and 19 to the rest of the network.



Figure 21: Python output of edge removal heuristic iterations.

The heuristic has been tested by varying the NPV calculation of the pipelines. Figure 22 highlights two pairs of networks, each featuring a different transport tariff value. Higher transport tariffs imply the NPV of a pipeline increases. Note that while all networks start with 20 nodes (top illustrations), the networks featuring a higher tariff value have a significantly larger final network (bottom illustrations).



Figure 22: Python output of edge removal heuristic for two distinct tariff values.

A strength of the heuristic lies in its flexibility with respect to node inputs. Given a specified economic criterion, the heuristic will automatically exclude network nodes that generate an infeasible network. This is a major advantage when designing emerging infrastructure networks, where the set of network points to connect may be uncertain [50]. As such, this heuristic lends itself well for exploratory research. A second advantage is that the heuristic allows for the generation of multiple connected components, which is characteristic for emerging infrastructure networks (see e.g. [70]).

A downside of the heuristic is its computational time as each edge removal requires a recalculation of the minimum-cost spanning tree. This takes time as each iteration requires executing the Delta change heuristic, which is computationally intensive. In part, this is resolved through the earlier discussed timer put on this heuristic. An additional way to decrease the run time is the exclusion of network edges at the start of each experiment (see Appendix A.4). Specifically, certain nodes may be excluded based on the expectation that connecting them is likely to be financially infeasible. In this research, this approach is not utilized as executing it correctly is expected to be computationally intensive on its own. Rather, the edge removal heuristic is altered to remove multiple connections at a time for large networks. After all, the removal of a single edge has a relatively smaller impact on the NPV of a large network. Specifically, multiple edges are removed on networks that feature 40 or more edges, depending on the total network size (see Appendix A.1). In testing this alteration to a network of 150 network nodes, the average run time decreased by 50%.

3.1.3 Incorporation of natural gas pipelines

As a last step towards the generation of optimal networks, the reassignment of natural gas pipelines is added to the model. After all, section 1.3 highlighted the link between hydrogen networks and natural gas pipeline reassignment as a gap in existing literature. The Optimal Network Layout Tool facilitates the incorporation of natural gas pipeline reassignment through the concept of existing connections [60]. Existing connections are included by adding both ends of the pipeline as nodes and specifying the capacity of the connection. Critically, these nodes are only connected if this improves the total network cost. In the original tool, the capacity of existing connections is assumed to be freely available. However, Cerniauskas et al. [16] conclude that the most cost-effective way to reuse natural gas pipelines for the transportation of hydrogen is 60% cheaper than constructing a new pipeline, rather than free. As a result, this research incorporates such a reassignment discount. Figure 23 illustrates a toy model, where the use of the reassignment discount is highlighted. In the left illustration, the possibility for reassignment, depicted by the two salmon-coloured nodes, is not utilized as this requires side-tracking network connections. This features additional costs that are not made up for as the reassignment discount is set to zero. However, the two nodes are incorporated in the network when the reassignment discount is set relatively high. This is shown in the right illustration.



Figure 23: Python output of natural gas pipeline reassignment incorporated in network model.

3.2 Robust network generation

Building on the generation of optimal networks described in the previous section, this section focuses on the creation of robust network topologies. This is grounded in the philosophy that robust and flexible design strategies outperform those aiming towards optimality when facing uncertainty (please recall section 2.2). Specifically, this section proposes heuristic to tackle three design variables that are essential to the generation of robust networks: 1) what network connection to build, 2) what capacities to assign to these connections and 3) how to factor in future time steps.

3.2.1 Edge occurrence

To tackle the first design variable, the concept of edge occurrence is utilized. This builds on the idea of multiple plausible futures as described in section 2.2. For each plausible future, an optimal network can be generated utilizing the methodology described in the previous section. Next, the occurrence of all possible edges can be mapped across these optimal networks. Figure 24 illustrates this idea. This approach is inspired by Heijnen et al. [50], although their analysis is based on the occurrence of specific configurations rather than individual edges.



Figure 24: The occurrence of edges across optimal networks serves as a metric for robustness.

Now, this research utilizes a maximum occurrence heuristic to derive robust network topologies based on edge occurrence. Please refer to respectively Figure 25 and Appendix B.2 for the flowchart and pseudo code of this heuristic. As a first step, the robustness score of each edge is determined as the share of experiments in which it occurs in the optimal network. Subsequently, all edges are labelled as unvisited. Next, the unvisited edge with the highest robustness score is added to the network. If this creates a cycle, the newly added edge is removed from both the network and the list of unvisited edges. Otherwise, the edge is solely removed from the list of unvisited edges. This process is repeated until the list of unvisited edges is empty. Note that this heuristic mimics Kruskal's algorithm in a manner that seeks to maximize the occurrence of edges in the final network.



Figure 25: Flow chart of edge occurrence heuristic.

For verification purposes, toy models are utilized in which both the coordinates and their supply and demand patterns are randomized. The left illustration of Figure 26 illustrates the occurrence of edges of such a model over 20 plausible futures, where the color of each edge indicates its relative occurrence. In the right illustration, the output of the maximum occurrence heuristic is shown.



Figure 26: Python output of maximum occurrence heuristic.

Now, the proposed heuristic guarantees the creation of a spanning tree. However, as described in section 3.1, pipeline investments require connected components that feature a NPV greater than zero. As such, the proposed edge removal heuristic should be applied to the robust network derived from the maximum occurrence heuristic. However, this first requires the assignment of capacities to the derived edges, introducing the second design variable.

3.2.2 Capacity assignment

To assign capacities to the network edges retrieved from the maximum occurrence heuristic, this research utilizes a minimum regret heuristic. Here, regret is defined as the difference between the optimal and chosen alternative (please recall section 2.2). For pipeline investments, regret is caused by either over- or undercapacity. In case of overcapacity, regret assumed to be equal to the difference in the investment costs of the installed and optimal capacity. Alternatively, regret due to undercapacity is equal to the investment cost of expanding the installed capacity to meet the optimal capacity. In this research, it is assumed that capacity expansions are done by constructing an additional pipeline parallel to the existing one, rather than actually expanding the capacity of the existing pipeline. Now, the minimal regret capacity can be determined by finding the capacity for which sum of the regret values over the set of experiments is minimal. A 'brute-force' approach can be applied that takes the minimum and maximum required capacity over all plausible futures and calculates the total regret for every possible value within this range. However, this poses a serious computational challenge. Alternatively, this research applies a minimum-regret heuristic. Please refer to Figure 27 and Appendix B.3 for respectively the flowchart and pseudo code of this heuristic.



Figure 27: Flow chart of minimum regret heuristic.

Based on the cost function of pipelines, the regret associated with undercapacity is significantly higher than that of overcapacity (see Appendix B.3 for an example calculation). With this in mind, the maximum required capacity over all experiments is assigned to a pipeline as a first step. Given this capacity, the regret over all experiments is summed up. In case the total regret is zero, the heuristic stops as this is the lowest possible regret. This happens if the required capacity is identical in all experiments. Otherwise, the capacity of the pipeline is reduced by one tonne hydrogen per day and the total regret is recalculated. This is repeated for as long as the newly found regret value is lower than the previous one. When the newly found value is larger than the previous one, the capacity decrease is reverted and the heuristic stops. While a capacity reduction in steps of one tonne per day is computationally intensive, the time required by this procedure is negligible compared to that of the previously discussed heuristics. As such, the computational cost of performing this procedure accurately are assumed to be worthwhile. The result of this heuristic is a maximum occurrence spanning tree with minimum regret capacities (from hereon 'robust network'). As described in the previous section, this allows for the application of the edge removal heuristic proposed in section 3.1.

3.2.3 Edge removal heuristic applied to robust network

To retrieve a financially feasible robust network, an altered version of the edge removal heuristic proposed in section 3.1 is utilized. In the heuristic used for the generation of optimal networks, the revenue of a pipeline is based on its capacity as this is dictated by the flow of hydrogen. However, the capacity of the robust network is derived by means of the minimum regret heuristic. Since over-capacity generally produces less regret than undercapacity, this capacity is likely to overestimate the total flow of hydrogen through the pipelines. As such, the average flow of hydrogen through the pipeline over the set of plausible futures rather than the pipeline's capacity is considered. Note that this creates a link between the NPV of a pipeline and its occurrence across all plausible futures. After all, the average flow is significantly reduced by experiments in which the required capacity is zero. Additionally, the minimum regret capacity is likely to be lower if the required capacity is zero across a number of plausible futures. As a second alteration, the maximum occurrence tree is not recalculated after each edge removal as this would produce identical results. After all, the occurrence of the edges across the plausible futures is already determined. Now, the derived network applies to a single time step. The next section will touch on the incorporation of multiple time steps.

3.2.4 Investments over time

A European hydrogen infrastructure is expected to expand over time as demand increases (see e.g. [70]). To capture this dynamic, this research assumes three discrete time steps: 2030, 2040 and 2050. These time steps are chosen to match important years in the energy policy goals of the European Union [13], [107]. Each time step is assumed to represent an investment decision and assigns different supply and demand patterns to the network nodes. As described in section 2.1, Andre et al. [7] utilize a backward heuristic, which critically ignores the interaction between existing infrastructure and future demand. Alternatively, this research will propose a forward looking heuristic. Please refer to Figure 30 and Appendix B.4 for respectively the flowchart and pseudo code of this heuristic.

Initially, the three heuristics described in the previous sections are utilized to retrieve a financially feasible robust network for the first time step. Next, the demand patterns in the succeeding time step are updated based on the resulting infrastructure. This is done by first identifying the Member States that are connected by the derived infrastructure. As a second step, the demand values of network nodes present in these Member States are increased by a fixed percentage (see Appendix D.1 for the specific values). In doing this, the Member States that are connected to the network in an earlier stage are more likely to boost the expansion of this network towards the future.

After updating demand patterns based on the derived infrastructure, a network is derived for the next time step. This is done without forcing the model to consider the previously built infrastructure. To understand this choice, it is vital to first consider that this research assumes supply and demand values to either stagnate or increase over time. From this follows that the network derived in the first time step is guaranteed to be financially feasible in the following time step. After all, larger pipelines are financially more attractive than smaller ones, as pinpointed in
Appendix A.3 and Figure 66. Thus, forcing the model to consider previously built infrastructure unnecessarily complicates the model as this is done automatically. An objection to this approach is that the specific tree structure derived in a later time step may vary. However, this research assumes that the interaction between existing infrastructure and future demand is based purely on the nodes connected to the infrastructure. In the example of Figure 28, this implies that demand dynamics are presumed to be identical for both configurations.



Figure 28: Flow chart of minimum regret heuristic.

As supply and demand values are assumed to either stagnate or increase over time, it is likely that pipelines require higher capacities at later time steps. Since larger pipelines are financially more attractive, it is virtually always cheaper to build one large pipeline in advance, than to construct an additional pipeline when a capacity increase is required (please refer to Appendix B.3 for an example calculation). To capture this dynamic, the capacities of pipelines in earlier time steps are automatically updated to match future expansions if this is required. For example, if a pipeline requires a capacity of 20 and 40 tonne per day in respectively the first and second time step, the model assigns a capacity of 40 tonne per day for both time steps.

As with previous heuristics, toy models are utilized to verify the model. Figure 29 highlights the growth of such a model over two time steps. The supply and demand patterns, although randomized, are increased in the second time step to generate a larger final network.



Figure 29: Python output of multi-period model.



Figure 30: Flow chart of multi-period network heuristic.

3.3 EMA workbench

As highlighted in section 2.2, EMA is a promising methodology for dealing with uncertainty in infrastructure development. To apply this methodology, the EMA workbench is utilized. The EMA workbench is developed at the TU Delft and facilitates exploratory modelling by providing support for designing, performing and analysing the results of experiments [97]. As the tool is developed in Python, it is easily linked to the extended Optimal Network Layout Tool described in the previous sections.

The two primary inputs of the Optimal Network Layout Tool are the set of network nodes and the supply and demand values of these nodes. As participant uncertainty is already dealt with by the edge removal heuristic, this research assumes a fixed set of network nodes. Therefore, the EMA workbench is utilized to generate the supply and demand values of these nodes. Specifically, a specified number of plausible futures is generated by sampling values from uncertainty spaces (please recall Figure 10). Each plausible future features specific supply and demand patterns, which shapes the optimal network derived by the Optimal Network Layout Tool. Figure 31 highlights this, where sampling from 2 uncertainties leads to different networks in two plausible futures.



Figure 31: Sampling different values for uncertainties may result in dissimilar optimal networks.

The EMA workbench is set up in accordance with the XLRM-framework introduced in section 2.2. As such, it requires a formalisation of relevant uncertainties (X), policies (L) and performance metrics (M). This necessitates a further investigation of the case introduced in Chapter 1, which is the focus of Chapter 4. First, a test was conducted to verify the integration of the workbench and network model. To this end, a regional model spanning France, Spain and Portugal was developed that incorporates the share of hydrogen vehicles in each province as the sole uncertainty. Specifically, 100 experiments were sampled for the share of hydrogen vehicles between a lower and upper bound of respectively 0.1 and 0.5. Figure 32 highlights the edge occurrence across 100 experiments (left) and the network derived from the maximum occurrence heuristic (right).



Figure 32: Python output of edge occurrence and max. occurrence tree over 100 experiments.

Based on the maximum occurrence spanning tree with minimum regret capacities, the feasible robust network was derived. Figure 33 illustrates this.



Figure 33: Python output of feasible robust network over 100 experiments.

Now, the number of edges and network NPV are picked as two performance metrics to test model behavior. Since the derived network features a tree structure, the number of edges directly correlates to the number of areas that are connected by the network. This is vital as a larger network is likely to stimulate the diffusion of hydrogen in Europe more effectively, which is in the direct interest of the European Union. Figure 34 shows these metrics as a function of the share of hydrogen vehicles in the left and right illustration, respectively. As shown in the left illustration, the total network size decreases at relatively low hydrogen vehicle shares, which is to be expected. Specifically, 15% seems to the threshold below which the optimal network does not connect all network nodes. Similarly, the network NPV increases at higher hydrogen vehicle shares. Additionally, between a hydrogen vehicle share of 0.10 and 0.15, the total NPV of the network is around zero. This can be explained by the left illustration, as these networks have only barely become financially feasible after removing one or more network connections. As a result, the NPV of these networks can be expected to take on a value only slightly higher than zero. From these illustration, it can be concluded that the model performs as expected.



Figure 34: Python output of network size and NPV over 100 experiments.

3.4 Methodology unifying EMA and graph theory

The goal of Chapter 3 is to answer the third sub-question posed in Chapter 1, namely:

3. What is a suitable methodology to generate robust infrastructure networks?

Figure 35 highlights the methodology proposed by this research to generate robust infrastructure networks. This methodology is a synthesis of the heuristics and methods applied in the previous sections. Note that it requires various case-specific inputs, which will be gathered in the following Chapter. Although this research focuses on the development of a European hydrogen infrastructure, the proposed methodology can be broadly applied to a wide range of infrastructure network cases. As such, the case tackled in this research can be seen as a proof of concept from a methodological perspective.



Figure 35: Overview of proposed methodology to generate robust infrastructure networks.

4 A European hydrogen infrastructure

Chapter 1 introduced the case of hydrogen development in the European Union, which is critically dependent on the emergence of a transmission network connecting vital demand and supply centres. For the purpose of applying the methodology laid out in Chapter 3, this Chapter focuses on two activities: 1) defining the set of network nodes and 2) generating supply and demand patterns for these nodes. As highlighted in Figure 35, section 4.1 focuses on the former. Section 4.2 lays the basis for the determination of the latter, which is further developed in sections 4.3 and 4.4.

4.1 Network nodes and geographical scope

As laid out in Chapter 1, the geographical scope of this research entails the European Union. A total of 24 Member States is included, excluding Malta, Ireland and Iceland as these islands are fully disconnected from the European mainland. Now, the number of network nodes and their placement across this geographical scope is critical to the generation of robust network topologies. This research utilizes the Nomenclature of Territorial Units for Statistics (NUTS) as a basis for the generation of these network nodes. Specifically, NUTS level 2 is used, which is a system that splits the European Union in over 200 areas [108]. Figure 36 highlights these areas, pinpointing individual Member States through differing colours.



Figure 36: Geographical scope of this research.

The main advantage of utilizing the NUTS system lies in data availability as Eurostat offers data on a wide range of economic-geographic parameters for each NUTS 2 area [109]. Additionally, it allows for the incorporation of provincial administrative structures since NUTS 2 areas are mostly based on the provincial structure of Member States [108]. As such, this research assumes that distribution networks are developed on the provincial level [110], justifying the creation of a single network node per NUTS 2 area. Lastly, the NUTS 2 system provides a good start for assuring a geographically uniform placement of network nodes across the EU. Nevertheless, some Member States feature a more detailed NUTS 2 formalisation than others. As shown in Figure 36, Germany features significantly more areas than Spain while the total area of Spain easily surpasses that of Germany. To assure more geographical uniformity, a set of modifications is made to the NUTS 2 system. These modifications, aimed towards levelling out the geographical size of the areas, mainly target Germany, the Netherlands and Austria while smaller modifications are made to the Czech Republic, Hungary, Belgium Finland, Poland, Greece and Romania. After modifications, the number of network nodes equals 156. Please refer to Appendix C.1 for the full list of modifications.

4.2 Hydrogen development in Europe

To assign supply and demand patterns to the network nodes defined in section 4.1, internal factors (R) and exogenous uncertainties (X) relevant to the development of hydrogen should be mapped (please recall the XLRM-framework introduced in section 2.2). While in reality few phenomena are truly deterministic, constraints on time and resources require some variables to be considered fixed internal parameters. As such, this research assumes certain economic-geographic variables to be fixed parameters out of practical necessity. In mapping these economic-geographic parameters and uncertainties, of main interest is what could happen rather than how it may happen. This is different from various theoretical frameworks that aim to capture the underlying dynamic of energy innovations and transitions, such as the Multi-Level Perspective (MLP) and Functions of Innovations (FIS) approach [111], [112]. EMA foregoes this as it treats each plausible future as a deterministic outcome (please recall section 2.2). As a result, the realm of possible outcomes caused by the interplay of internal factors (R) and exogenous uncertainties (X) is of interest. An important assumption of this research is that supply will match demand in each of these plausible futures. This is grounded in practical necessity as the Optimal Network Layout Tool introduced in section 3.1 requires supply and demand to be equal. So, this research will focus on mapping plausible levels of hydrogen demand and determining how and where hydrogen may be produced to facilitate this development.

Three literature studies that together reviewed over 140 papers highlight two overarching drivers to hydrogen development: 1) climate change mitigation efforts and 2) security of supply concerns [113]–[115]. Considering the former, four sectors are of interest as they contribute most to the European GHG-emissions. These sectors are transport, built environment, industry and power generation [116], as shown in Figure 37. Additionally, these sectors are widely considered to feature the highest potential for hydrogen development [3], [117], [118]. As a result, this research will focus on the development of hydrogen in these sectors by mapping essential economic-geographic parameters and uncertainties. These elements will be worked out in respectively section 4.3 and 4.4. To incorporate security of supply concerns, additional parameters and uncertainties will be identified following an analysis on the geopolitics of hydrogen. On top of this, security of gas supply concerns are discussed in the context of natural gas pipeline reassignment.



Figure 37: European GHG-emissions by sector in Mton CO2 eq. [116]

4.2.1 Transport

In transport, hydrogen is utilized by Fuel Cell Electric Vehicles (FCEVs). Automotive fuel cells turn hydrogen and oxygen into water, converting chemical into electrical energy [119]. This electrical energy is used to power an electric motor. By the end of 2019, the global FCEV stock was a mere 25.000 units [120]. This small market share is mainly caused by the high costs of the fuel system [121]. Ajanovic and Haas concluded that as of 2016, the total costs of mobility for FCEVs were more than double that of a conventional vehicle [122]. Nevertheless, FCEV costs are expected to drop significantly towards the future [123]. For example, the International Energy Agency forecasts the price of FCEVs to drop from 60.000 USD in 2015 to 33.600 in 2030 [124].

Next to upfront investment costs, four performance criteria are essential for the adoption of hydrogen vehicles: fuel cost, range, refuelling time and environmental performance [125]-[128]. Specifically, its performance on these criteria compared to alternatives such as Battery Electric Vehicles (BEVs), Plug-in Hybrid Electric Vehicles (PHEVs) and Internal Combustion Engine Vehicles (ICEVs) is essential [121], [129]. Competition from the ICEV is fierce due its overwhelming market share and superior technical performance. However, it will likely be phased out as European governments strive for climate-neutrality in 2050 [13]. For example, the United Kingdom has pledged to ban the sale of ICEVs from 2030 onward [130]. Additionally, rising carbon prices will likely increase fossil fuel costs [131]. Towards 2050, hydrogen vehicles are likely to face severe competition from electric vehicles. As of 2019, there were over 7 Million electric vehicles on the road globally, easily surpassing the FCEV stock at that time [132]. Generally, electric vehicles are technologically more mature and benefit from a better developed infrastructure. Nevertheless, hydrogen and electric vehicles may not be mutually exclusive and serve different functions within the transportation sector. For example, Contestabile et al. [129] concluded that BEVs are better suited for smaller vehicle segments, while FCEVs shine in larger segments. This is largely due to the superior range of FCEVs [125].

The uncertainty of interest that is the result of the performance of hydrogen vehicles compared to its competitors is the hydrogen vehicle share. Next to this, the total vehicle fleet and the travel intensity are required to calculate the total demand for hydrogen in transport. After all, the total number of hydrogen vehicles can be calculated by multiplying the share of hydrogen vehicles with the total vehicle fleet. Next, the total demand for hydrogen in transport is the number of hydrogen vehicles times the hydrogen consumption per vehicle. The demand per vehicle is in turn dependent on the travel intensity and the fuel consumption of hydrogen vehicles. To conclude, the factors highlighted in Table 3 are relevant to the development of hydrogen in transport. Note that dependencies are described by the numbering system, where for example the hydrogen vehicle share (1.4) is influenced by the capital cost of hydrogen vehicles (1.4.1).

Key factors	Unit	Type
1. Hydrogen demand in transport	Tonne/day	Output
1.1 Vehicle ownership	vehicles/capita	Parameter
1.2 Travel intensity	km/vehicle/year	Parameter
1.3 Fuel consumption	m kg/km	Parameter
1.4 Hydrogen vehicle share	%	Uncertainty
1.4.1 Capital cost	EUR/vehicle	Uncertainty
1.4.2 Fuel cost	$\mathrm{EUR/km}$	Uncertainty
1.4.3 Range	km/full tank	Uncertainty
1.4.4 Refuelling time	$\min/\text{full tank}$	Uncertainty
1.4.5 Refuelling station density	$\rm stations/km2$	Uncertainty
1.4.6 Environmental performance	g CO2 eq./km	Uncertainty

Table 3: Parameters and uncertainties relevant to hydrogen development in transport.

4.2.2 Built environment

There are various options for the implementation of hydrogen in the built environment, namely 1) Combined Heat and Power (CHP), 2) hydrogen boilers and 3) gas heat pumps converted to run on hydrogen [133]. CHP technologies utilize a fuel cell to convert hydrogen into electrical energy and heat. Hydrogen boilers are very similar to existing natural gas boilers and use combustion to generate heat. However, due to differing physical properties, the utilization of hydrogen boilers requires modifications to various appliances. Existing gas heat pumps are already utilized, which can be be converted to use hydrogen instead of natural gas. A hurdle to all these technologies is the fact that hydrogen applications in heating have not been prioritized in either scientific literature or policy debates [134]. Additionally, although capital costs of fuel cell systems have dropped dramatically in last decade, upfront investment costs a still a major issue [134]. Competitors that claim the spotlight include heat pumps, district heating and solar heating systems [135]–[137].

An essential aspect of decarbonizing the heat sector is the type of infrastructure that is in place. Bertelsen and Mathiesen [138] distinguish two types: large-scale collective infrastructures and individual heat supply. Collective infrastructures include gas and electricity networks and district heating. Individual heat supply systems utilize oil, biomass or coal. One of the major advantages of collective infrastructures is that entire neighbourhoods or cities can be converted at a time. For example, the H21 Leeds City Gate project explored the conversion of the existing natural gas network of Leeds to supply hydrogen [139]. Within dwellings, they installed hydrogen boilers, cookers and gas heaters. However, these projects are highly dependent on the reuse of natural gas pipelines, which will depend on the phase out of natural gas from the energy mix [140]. The pace at which this will be done is uncertain [118]. A major competitor to hydrogen applications in heating is district heating. As of 2013, 11.8% of all EU citizens was served by district heating systems [141]. A 2018 study by Sayegha et al. [142] report that of the 23 EU Member States that utilize district heating systems, the average share was already up to 24.5%. As district heating systems are seen as a solid decarbonization option, their deployment may block the diffusion of hydrogen applications in the built environment. Nevertheless, hydrogen may find a niche in large urban areas. Hydrogen applications are expected to outperform alternatives in areas with a relatively high heat density as the individual heat exchange units are relatively cheap, but the required infrastructure is costly [143], [144].

Thus, the hydrogen demand in built environment is the product of the heating demand per area and the share of dwellings utilizing hydrogen applications. Factors that are relevant to this share include the type of heating infrastructure, the heat density in the area and both the capital and operational cost of the installations. Table 4 summarizes these parameters and uncertainties:

Table 4: Parameters and uncertainties relevant to hydrogen development in built environment.

Key factors	Unit	Type
1. Hydrogen demand in built environment	Tonne/day	Output
1.1 Heating demand per area	kWh/area	Parameter
1.2 Share of dwellings utilizing hydrogen	%	Uncertainty
1.2.1 Type of heating infrastructure	Individual/collective	Parameter
1.2.2 Heat density	kWh/m2	Parameter
1.2.3 Capital cost	EUR/kW	Uncertainty
1.2.4 Operational cost	EUR/kWh	Uncertainty

4.2.3 Power generation

The power generation sector is of main interest to the development of hydrogen from a supply perspective. Most notably, hydrogen production from water is considered capable of producing large amounts of low-carbon hydrogen [145]–[147]. The key principle of electrolysis revolves around the separation of water into hydrogen and oxygen through circulation of a direct current:

$$H_2O \to H_2(g) + 1/2O_2(g)$$

Two vital characteristics of electrolysis are its efficiency and capital cost. The efficiency can be divided in the efficiency of the electrolyser and the power supply [145]. The first is affected by hydrogen losses in the electrolyser, the later by energy losses that occur in the conversion from electrical to chemical energy. Electrolyser efficiencies are expected to increase significantly towards 2050 [148]. Next to low efficiencies, the capital costs of electrolysis currently drive up its production costs, favoring other production methods [3]. Nevertheless, various projections forecast a significant decrease of these costs towards 2050 [146], [147], [149]–[151], as shown in Figure 38:



Figure 38: Capital cost projections of electrolysers towards 2050 in EUR.

One of the major advantages of electrolysis is that it can be coupled to variety of energy sources [152]. Above all, solar and wind energy are considered prime candidates for the production of renewable hydrogen [147], [152]. Over the last decade, the penetration of these technologies in the energy system has significantly increased. Moreover, although highly geographically dependent, there is massive potential for both solar and wind energy in Europe (see e.g. [153], [154]). In turn, this creates massive potential for electrolysis based on these energy sources. Nuclear energy is a second prime contender for the production of low-carbon hydrogen [147], [155]. In part, this originates from the characteristics of the electrolysis reaction. If electrolysis is performed under higher temperatures, the electric energy demand decreases while the thermal energy demand increases [145], [156]. Nuclear power plants have the ability to produce a combination of electricity and heat [157]. Consecutively, heat from nuclear plants can be utilized in high-temperature electrolysis to increase the energy efficiency of the process [158], [159]. On top of this, nuclear power plants do not suffer from the intermittency complication of solar and wind energy while being able to produce energy in large volumes [157]. Nevertheless, although electrolysis on its own is a mature technology, technological improvements are required with respect to high-temperature electrolysis [157], [158]. Apart from high-temperature electrolysis, nuclear energy can also be utilized for conventional electrolysis, resulting in two production pathways [160]. For example, Pinsky et al. [160] researched nuclear hydrogen production systems that utilize Alkaline, PEM and SOEC electrolysers.

As supply is assumed to match demand in this research, the primary uncertainty to hydrogen production from electrolysis is its share in the total production. Furthermore, the geographical distribution of electrolysis potential from wind, solar and nuclear energy is critical. This is highlighted in Table 5:

Table 5: Parameters and uncertainties relevant to hydrogen development in power generation.

Key factors	Unit	Type
1. Hydrogen production from electrolysis	Tonne/day	Output
1.1 Production potential	kWh/year	Parameter
1.2 Electrolysis production share	%	Uncertainty

4.2.4 Industry

The industry sector is relevant to both the demand and supply side of hydrogen. With respect to supply, the vast majority of hydrogen is currently being produced at industrial clusters through steam methane reforming [155]. Primarily, this originates from the significantly lower production costs compared to low-carbon hydrogen production [3]. However, the primary issue with this production method is its carbon intensity. Nevertheless, in combination with carbon capture and storage (CCS), low-carbon hydrogen can be produced by industrial clusters. Navas-Anguita et al. [161] and BP [118] conclude that blue hydrogen may play a sizeable role in the short to medium term.

On the demand side, the three industrial processes reliant on hydrogen are refining and the production of ammonia and methanol. As of today, these processes represent the bulk of hydrogen demand [3]. For ammonia, hydrogen is utilized in the following reaction:

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$

Based on this reaction and the molecular mass of hydrogen and nitrogen of 1 and 14, respectively, circa 177 kg of hydrogen is theoretically required to produce 1 tonne of ammonia. With respect to methanol, the following overall reaction applies:

$CO + 2H_2 \rightleftharpoons CH_3OH$

Based on this reaction and the molecular mass of hydrogen and carbon monoxide of 1 and 28, respectively, circa 214 kg of hydrogen is theoretically required to produce 1 tonne of ammonia. Hydrogen use in refining is a combination of hydrocracking, hydro-treating and biorefinery. However, the measurement of a refinery's hydrogen consumption is a difficult task [162]. The quantities of hydrogen required depend on for example the hydrogen content of the feed and products and the amount of sulfur and nitrogen to be removed [163]. To estimate the hydrogen consumption per refinery, the set of European refineries and their capacities were retrieved from FracTracker [164].

An important uncertainty of industrial clusters is the extend to which their hydrogen consumption is met by internal production. For example, refineries utilize steam methane reforming on-site, foregoing the need of a transmission network that supplies them with externally produced hydrogen. Next, an important economic-geographic characteristic is demand growth or decline of these products, which in turn will influence their hydrogen demand. Lastly, the number of plants and the demand per plant are critical to the geographical distribution of hydrogen demand in industry. On the supply side, the SMR production potential and its relative costs to other production methods is of importance. All these factors are summarized in Table 6:

Key factors	Unit	Type
1. Hydrogen demand in industry	Tonne/day	Output
1.1 Number of plants	#	Parameter
1.2 Demand per plant	Tonne/day	Uncertainty
1.2.1 Baseline demand	Tonne/day	Parameter
1.2.2 Future demand growth	%	Uncertainty
1.2.3 Reliance on internally produced hydrogen	%	Uncertainty
2. Hydrogen supply in industry	Tonne/day	Output
2.1 SMR production potential	kWh/year	Parameter
2.2 SMR production share	%	Uncertainty

Table 6: Parameters and uncertainties relevant to hydrogen development in industry.

4.2.5 Geopolitics of hydrogen and natural gas

As introduced in Chapter 1, an important perspective on the development of hydrogen is a geopolitical one. Within the energy domain, the strategic importance of natural resources, their location, and transportation routes has received significant attention [165]. As such, security of energy supply is a vital element of energy policy and one of the key dimensions of the European Energy Union strategy [22], [166]. Most notably, the importance of energy security was highlighted during the Russia-Ukraine gas disputes of 2006 and 2009 [17], [18]. During these disputes, European Member States faced gas shortages as Russia halted its supply via Ukrainian pipelines. As a result, the dependence on Russian gas is becoming a growing issue in the EU, especially in the most dependent East-European Member States [167], [168]. This is relevant in two ways for this research as energy security concerns may spur the diversification towards new energy sources such as hydrogen but may also halt the reassignment of natural gas pipelines. Additionally, hydrogen development might be halted by security of supply concerns in case it creates new exporter dependencies [169].

Although European developments influence individual Member States, they may have differing views on energy security. For example, Western and Eastern Member States have significantly diverging views on energy security, which finds its origin in differing levels of dependence on Russian gas [167]. On top of this, nations can have very different perspectives on the use of specific technologies or energy sources. For example, since the Fukushima nuclear incident, Germany is phasing out its nuclear power plants, while France still supports its nuclear industry [170]. Thus, is likely that hydrogen will experience a differing levels of enthusiasm from Member States. In fact, these differences are already visible: as of December 2020, six EU Member States had published national hydrogen strategies, 8 others were still developing a strategy, while the rest of the Member States had not taken such measures [171]. This research assumes that each Member States faces a make-or-buy decision, which will shape their role in geopolitical landscape of hydrogen [23]. As such, two geopolitical uncertainties are incorporated: the number of importers/exporters and the import share. Table 7 illustrates these uncertainties. The number of importers dictates the total number of Member States that is designated as an importer. Subsequently, the import share dictates the share of their demand that the importing nations seek to satisfy by means of imports. Note that new groups of importers and exporters are drawn randomly at the start of each experiment. As such, running a large set of experiments creates a multitude of possible geopolitical landscapes.

Table 7: Uncertainties relevant to the geopolitics of hydrogen.

Key factors	Unit	Type
Number of importers/exporters	#Member States	Uncertainty
Import share	%	Uncertainty

This research assumes that the potential for natural gas pipeline reassignment is critically dependent on whether it endangers security of supply. As a result, the topology of the network is of great relevance. Figure 39 illustrates that for each cycle in a network, one network connection can be removed while maintaining a fully connected network. Thus, similar to the approach utilized by the European Backbone initiative [70], this research assumes that pipeline reassignment focuses on looped segments of the natural gas network.



Figure 39: Removing edges from a cycle does not disconnect a graph.

Specifically, it is assumed that each Member State has the option to open their natural gas network to reassignment. This implies that for a share of the cycles in the network of that Member State, one edge is made available for reassignment. Per cycle, the specific edge to be used for reassignment is chosen randomly. Some cycles span multiple Member States. In this case, both Member States are required to open up their gas network for these cycles to be made available for hydrogen transportation. Now, ENTSOG publishes maps of the biggest pipelines of the European natural gas network. Using this map, cycles can be identified, of which an example situated in Spain is given in Figure 40.



Figure 40: Natural gas network cycles can be identified based on visual inspection [172].

Concluding, the uncertainties and parameter related to the reassignment of natural gas pipelines are highlighted in Table 8. Note that the reassignment probability is the probability of a Member State opening up its natural gas network to reassignment, while the reassignment share is the share of the cycles that is made available for reassignment.

Table 8: Uncertainties relevant to the reassignment of natural gas pipelines.

Key factors	Unit	Type
1. Number of reassigned pipelines	#	Output
1.1 Reassignment probability	%	Uncertainty
1.2 Reassignment share	%	Uncertainty
1.3 Number of cycles in network	#	Parameter

4.3 Economic-geographic network inputs

Section 4.2 highlighted the most important economic-geographic parameters for the development of hydrogen across four key sectors: transport, built environment, industry and power generation. Additionally, it listed relevant geopolitical parameters. Table 9 summarises these parameters and highlights both the sources used and the Appendices in which the formalisation of these parameters can be reviewed. For example, Appendix C.2 elaborates on how the number of passenger vehicles for each NUTS 2 area is retrieved.

Parameter	Source	Appendix
Vehicle ownership	Eurostat	C.2
Travel intensity	OECD	C.2
Fuel consumption	H2 Mobility	C.2
Heating demand per area	Eurostat	C.3
Heat density	SEEnergies	C.3
Type of heating infrastructure	Bertelsen and Mathiesen (2020)	C.4
Solar production potential	Solar Atlas	C.5
Wind production potential	Wind Atlas	C.6
Nuclear production potential	World Nuclear Association	C.7
SMR production potential	Fractracker	C.8
Number of refining plants	Fractracker	C.8
Demand per refining plant	Fractracker	C.8
Number of methanol plants	ICIS	C.9
Demand per methanol plant	ICIS	C.9
Number of ammonia plants	CEPS	C.10
Demand per ammonia plant	CEPS	C.10
Number of cycles in network	ENTSOG	C.11

 Table 9: Economic-geographic characteristics

4.4 Uncertainty analysis and experiment design

Section 4.2 highlighted both the vital uncertainties for each of the four most promising sectors for hydrogen application and relevant geopolitical uncertainties. This section builds on this analysis by illustrating the experimental design used to analyse the case of a European hydrogen network in the EMA workbench. The relevant uncertainties are grouped in four categories and highlighted in Table 10.

Table 10: Overview of uncertainties used as input for	experimental	design
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Category	Appendix	Uncertainty
		Hydrogen vehicle share
		Share of dwellings utilizing hydrogen
		Ammonia - Future demand growth
	D 1	Ammonia - Reliance on internally produced hydrogen
Demand	D.1	Methanol - Future demand growth
		Methanol - Reliance on internally produced hydrogen
		Refining - Future demand growth
		Refining - Reliance on internally produced hydrogen
		SMR production share
Supply D	DЭ	Solar production share
	D.2	Wind production share
		Nuclear production share
		Number of importers
Geopolitical	D.3	Import share
		Reassignment probability
		Reassignment share

As pinpointed in Chapter 2, EMA requires the mapping of uncertainty spaces. This is done by determining the minimum and maximum value for each uncertainty. Table 11 illustrates the minimum and maximum values used. For each category of uncertainties, an Appendix is dedicated to describing the methodology used to determine these values (see Table 10).

Table 11: Minimum and maximum values utilized in the EMA workbench

Parameter	2030	2040	2050
Hydrogen vehicle share	1 - 10%	2 - 19%	3 - 27%
Share of dwellings utilizing hydrogen	0 - 1%	0 - 2%	0 - 4%
Ammonia - Future demand growth	2 - $20%$	2 - $20%$	2 - $20%$
Ammonia - Reliance on internal production	0 - 10%	0 - $20%$	0 - 30%
Methanol - Future demand growth	-5 - 5%	-10 - 10%	-15 - 15%
Methanol - Reliance on internal production	0 - 10%	0 - $20%$	0 - 30%
Refining - Future demand growth	-3821%	-6334%	-8347%
Refining - Reliance on internal production	0 - 10%	0 - 20%	0 - 30%
SMR production share	0 - $94%$	0 - $94%$	0 - $94%$
Solar production share	0 - $94%$	0 - $94%$	0 - $94%$
Wind production share	0 - $94%$	0 - $94%$	0 - 94%
Nuclear production share	0 - $94%$	0 - $94%$	0 - $94%$
Number of importers	6 - 18	6 - 18	6 - 18
Import share	25 - $75%$	25 - $75%$	25 - $75%$
Reassignment probability	0 - $20%$	0 - 33%	0 - 50%
Reassignment share	0 - $20%$	0 - 40%	0 - 60%

Note that the hydrogen vehicle share and share of dwellings utilizing hydrogen are percentages of the existing number of vehicles and dwellings, respectively. The future demand growth of ammonia, methanol and refining implies the growth of demand for these products compared to 2020 values. Next, the reliance on internal production implies the share of hydrogen demand that the facilities producing these products can satisfy themselves. The SMR, solar, wind and nuclear share imply the ratio of each method in the total production. With respect to import, the number of importers and import share respectively indicate the number of Member States that are assigned the importer

status and the share of their total demand that they seek to import. Lastly, the reassignment probability and share indicate the odds of a Member State opening up its natural gas network for reassignment and the share of the cycles in their gas network that they seek to reassign.

Based on this experiment design, three explorations have been developed to analyse the development of a European hydrogen infrastructure: 1) broad exploration, 2) targeted exploration and 3) natural gas exploration. The goal of the broad exploration is to embrace the full range of plausible futures. On the demand side, this implies assigning the same uncertainty space to all Member States. So, all Member States on average feature the same level of hydrogen penetration. On the supply side, the probability function of all four production methods is made identical. Now, in reality some Member States are much more likely to facilitate the large scale introduction of hydrogen applications. For example, some Member States have already published national hydrogen strategies while others are lacking behind. The range of demand uncertainties can therefore also be tailored to every individual Member State. However, this level of detail somewhat breaks with the nature of exploratory modelling and analysis. To prevent this, the targeted exploration broadly categorizes Member States in three groups: 1) front-runners, 2) middle of the pack and 3) laggards. Next, distinct demand values are assigned to each of these three groups. On the supply side, the targeted exploration incorporates expectations on the relative share of each production method. Thus, both on the supply and demand side, the targeted exploration has a more narrowly defined uncertainty space. As a third exploration, natural gas pipeline reassignment is added to the design of the broad exploration. Critically, the first two explorations focus on hydrogen pipelines only, which allow for a clear comparison with the exploration in which pipeline reassignment is included. Please refer to Appendix D.4 for the specific alterations to the experiment design in each exploration. Important to note is that 500 experiments are sampled per exploration and time step. Thus, a total of 4500 experiments has been run. As the proper number of experiments is hard to determine upfront, this research performed two sets of 500 experiments with identical input values. Since the results of these experiments did not differ significantly, 500 experiments was deemed to be sufficient.

Next to the uncertainties that serve as the input for the experiment design, a set of five KPI's has been developed to analyse the results of the experiments. Table 12 illustrates these KPI's. These KPIs allow for an exploration of general network characteristics across the set of experiments. As the network features a tree structure, the number of edges directly relates to the number of areas that are connected by the network. Since a larger network is likely to push the diffusion of hydrogen in Europe more effectively, the network size is of interest to policy makers. Next, the network cost and NPV provide crucial financial information to investors. Lastly, the number of connected components implies the set of projects that will have to be developed separately. This guides national parties on potential collaborations with other Member States and gives a general impression on initial adoption centres.

Table 12: Overview of KPI's utilized in experiment design

KPI	Unit
Network size	Number of edges
Network cost	MEUR
Network NPV	MEUR
Connectivity	Number of connected components

4.5 Summarisation of case inputs

The goal of Chapter 4 is to get a better grip on the case of this research by answering three sub-questions:

- 4. What drives the development of a European hydrogen infrastructure between 2030 and 2050?
- 5. What are relevant economic-geographic inputs to model a European hydrogen pipeline network?
- 6. What are critical uncertainties to the development of a European hydrogen pipeline network?

The fourth sub-question serves as an initial step towards answering the fifth and sixth question. As such, it has identified transport, built environment, industry and power generation as the most important sectors for hydrogen development. For each of these sectors, both economic-geographic parameters and uncertainties have been pinpointed in section 4.2. Additionally, a geopolitical perspective on the development of hydrogen has introduced additional parameters and uncertainties. The identified economic-geographic parameters and uncertainties have been described in more detail in respectively section 4.3 and 4.4. Figure 41 summarizes the results of these sections, which provides an answer to the fifth and sixth sub-questions. Note that the relevant Appendix is highlighted for each parameter and uncertainty.



Figure 41: Overview of most important economic-geographic inputs and uncertainties.

5 Model application and results

This Chapter applies the methodology described in Chapter 3 to the case analysed in Chapter 4. First, section 5.1 describes a set of test runs. Next sections 5.2, 5.3 and 5.4 cover respectively the results of the broad, targeted and natural gas exploration.

5.1 Test runs

Before performing the three explorations laid out in section 4.4, the application of the model to the case is tested. While all aspects of the model have been tested in isolation, this provides a final check that the integrated model works accordingly. This is done by sampling 500 experiments from the uncertainty space for 2030 highlighted in Table ?? and ??. In itself, running 500 experiments over 40 hours without errors provides verification that the code in itself does not contain any critical mistakes. Nevertheless, an analysis of the results provides a more clear image. In the left illustration of Figure 42, the relative occurrence of the network edges is highlighted, utilizing a color scheme based on four categories. Subsequently, a robust spanning tree is shown in the right illustration. As can be expected, the left illustration highlights that the network highlighting the edge occurrence has a web-like structure. The right illustration highlights the robust spanning tree, which correctly connects all nodes through a tree-like network.



Figure 42: Test run output: edge occurrence (left) and max. occurrence tree (right).

As a next step, the feasible robust network configuration is derived, shown in Figure 43. The right illustration highlights the emergence of four connected components, which is characteristic of the edge removal heuristic. As expected, the NPV of each of these connected components is positive. Thus, the model correctly manages to determine financially feasible connected components from the robust spanning tree shown in the previous figure.



Figure 43: Test run output: final robust network in perspective (left) and isolated (right).

Figure 44 highlights the number of edges (left) and network cost (right) as a function of the average share of hydrogen vehicles in all EU Member States. It shows through a linear regression that both KPI's are positively correlated to the share of hydrogen vehicles. This is to be expected as a larger demand on average requires more pipeline connections and larger capacity, increasing both network size and cost. Nevertheless, demand in other sectors and factors such as the geographical distribution of demand create differentiation, which can be seen by the scatter in the data points.



Figure 44: Test run output: network size (left) and network cost in MEUR (right).

Figure 45 highlights the number of connected components (left) and network NPV (right) as a function of the average share of hydrogen vehicles in all EU Member States. Considering the former, most experiments lead to either 1 or 2 connected components, with 6 being the maximum. This output is sensible as it is likely that a few initial adoption centres will erupt in 2030. With respect to the network NPV, most experiments produce a result near zero. This is to be expected as the edge removal heuristic removes edge until the NPV of all connected components is larger than zero. Note that this heuristic often 'overshoots', leading to an NPV that is quite a bit above zero. This happens as the network edge with the lowest NPV is removed at each iteration, which may be more negative than the NPV of the connected component itself. For example, if the NPV of the network is -10 MEUR, and the NPV of the edge to be removed is -30 MEUR, the final network NPV becomes +20 MEUR. Thus, there occurs an overshoot.



Figure 45: Test run output: number of con. comp. (left) and network NPV in MEUR (right).

The conclusion of the test run is that the model works accordingly. As a result, the next sections will outline the results of the three explorations proposed in section 4.4.

5.2 Broad exploration

Figure 46 and 47 highlight the results of the broad exploration, pinpointing respectively the relative occurrence of edges over three time steps and the growth of the final network over these time steps. In 2030, four connected components emerge in Germany, Italy, the Netherlands and Belgium. These connected components grow in 2040, with components of Belgium and the Netherlands linking up. In 2050, all components merge into one large network that spans most of the European Union. Note that Scandinavia, Iberia, the Baltic States and Greece are not connected in the final network of 2050. Additionally, a clear link exists between the occurrence of edges and the final network as most edges present in the final network feature an occurrence over 75%.



Figure 46: Edge occurrence of broad exploration over three time steps.



Figure 47: Final robust network of broad exploration over three time steps.

Figure 48 shows the KPI output over the three time steps. First, the total NPV of the network is near zero in all three time steps. This is to be expected as the edge removal heuristic stops after the total NPV is larger than zero. The average regret, total cost and number of edges show similar behavior, doubling both in 2040 and 2050. As pinpointed in Figure 47 the number of connected components decrease to one in 2050, creating an integrated European network.



Figure 48: KPI results of broad exploration (left: in MEUR).

Figure 49 shows the edge capacities of all edges included in the final network of 2050. For edges that occur in multiple time steps, the optimal capacity is highlighted per time step. As such, it becomes apparent that the edges occurring in earlier time steps are amongst the pipelines with the largest capacities in the final network. This result underlines the importance of factoring in future time steps when assigning capacities to pipelines. If this is ignored, pipelines that occur at an early stage likely require various capacity expansions, which significantly increases the investment costs (see Appendix A.3).



Figure 49: Capacity of edges in final network of broad exploration in tonne/day.

Figure 47 highlighted the importance of Italy and Germany as these two nations form the backbone of the network that arises both in terms of the number of edges and their capacity. This is reflected in the correlation between the share of hydrogen vehicles in these Member States and the total network size. This is highlighted in Figure 50.



Figure 50: Link between hydrogen demand in Germany (top) and Italy (bottom) and network size.

Another interesting finding is that there is a strong link between the hydrogen production method and the size of the emerging network, as shown in Figure 51. The share of nuclear and solar energy in the total production mix have respectively a positive and negative effect on the network size. An explanation for this is the fact that nuclear energy production is heavily centralized, which creates clear production hubs that supply to demand centres. Alternatively, solar energy production has a decentralized nature, which satisfies local demand and therefore reduces the need for a transmission network that connects supply and demand hubs.



Figure 51: Link between nuclear (top) and solar (bottom) production share and network size.

5.3 Targeted exploration

Figure 52 and 53 highlight the results of the targeted exploration, pinpointing respectively the relative occurrence of edges over three time steps and the growth of the final network over these time steps. Note that the targeted exploration assumes three time of Member States: front-runners, middle of the pack and laggards (please recall section 4.4). The dynamic of the emerging network is similar to the broad exploration, where relatively small connected components emerge in 2030 that grow larger in 2040 and are ultimately fused into one large network in 2050. Additionally, Germany and Italy play a significant role in the total infrastructure. Nevertheless, this exploration features a larger role for France, which finds its spot amongst these two nations as the backbone of the network.



Figure 52: Edge occurrence of targeted exploration over three time steps.



Figure 53: Final robust network of broad exploration over three time steps.

The bigger role for France in the total network is made apparent by Figure 54. As shown in the left illustration, the hydrogen vehicle share in France has little effect on the total network size. Alternatively, the number of experiments in the targeted exploration which the total network size is between 140 and 160 edges is highly concentrated in the top right corner of the figure, above a hydrogen vehicle share of 0.08. Thus, hydrogen demand in France has a positive effect on network size in the targeted exploration.



Figure 54: Difference in effect hydrogen demand France for broad and targeted exploration.

Figure 55 highlights the differences between the broad and targeted exploration in terms of total network cost (left), number of edges (middle) and total regret (right). Note that the network cost and NPV are in MEUR. It highlights that especially in the first time step, as sizeably larger network emerges, with the relative difference shrinking towards 2050. Additionally, the average regret per run becomes smaller towards 2050 while it is larger than in the broad exploration in 2030. Thus, the results of the targeted exploration are more favourable from the perspective of hydrogen diffusion since a larger infrastructure is likely to stimulate this diffusion more effectively.



Figure 55: Network cost (left), size (middle) and regret (right) for broad and targeted exploration.

5.4 Natural gas exploration

Figure 56 and 57 highlight the results of the natural gas exploration, pinpointing respectively the relative occurrence of edges over three time steps and the growth of the final network over these time steps. Note that this exploration includes the reassignment of natural gas pipelines (please recall section 4.4). The most notable difference compared to previous two explorations is that a large connected network emerges already in 2040, only excluding the Netherlands, Belgium and parts of North-Eastern Germany. Additionally, 2050 features a network that spans all network nodes. Nevertheless, when investigating pipeline capacities it can be seen that the same network core emerges as in the previous two explorations. As such, Germany, Italy and France yet again play a vital role in the total network.



Figure 56: Edge occurrence of natural gas exploration over three time steps.



Figure 57: Final robust network of natural gas exploration over three time steps.

Looking at the KPI's, both the network size and total network cost are larger compared to the other two explorations. In 2030, the network is comparable to that of the targeted exploration, but significant differences emerge in the later two time steps. This stems from the fact that the usage of natural gas pipelines is set to increase in the model. Overall, the reassignment of natural gas pipelines has a strong positive impact on the growth of a European hydrogen network, which is in line with expectations. The average regret per run is between that of the previous two explorations.



Figure 58: Network cost (left), size (middle) and regret (right) for three explorations.

The difference in network size as a result of natural gas pipeline reassignment is especially apparent for the three backbone Member States, namely France, Germany and Italy. Figure 59 compares the total network size with (1) and without (0) the utilization of natural gas pipelines for these Member States in 2030. It can clearly be seen that networks below a size of 40 edges rarely occur in case any of the three backbone nations open up their natural gas network for reassignment.



Figure 59: Comparison of network size with (1) and without (0) natural gas pipeline reassignment.

6 Conclusion

Hydrogen is gaining increasing attention in the European Union as a vital piece of the climate change puzzle. Nevertheless, its development is dependent on the emergence of a European pipeline infrastructure, which is currently lacking. Specifically, a combination of supply, demand and geopolitical uncertainties severely complicates infrastructure development. As such, the main research question of this study focuses on the generation of a robust hydrogen infrastructure network between 2030 and 2050. To this end, a novel methodology combining graph theory and exploratory modelling and analysis (EMA) is proposed. The defining characteristic of this approach is that it generates a financially feasible, low-regret network that performs well in a wide range of plausible futures.

A foremost conclusion of this research is that a sizeable European hydrogen network can be expected to emerge towards 2050. Figure 60 highlights growth of this network in three stages, pinpointing the date of development and capacity through respectively pipeline colour and width. In 2030, the network will likely be characterised by various relatively small connected components that span initial adoption centres. These centres are situated in Germany, Italy, Belgium and the Netherlands. Towards 2040, these components can be expected to grow in size, connecting most parts of central Europe. In 2050, a large connected network may emerge with Germany and Italy at its core, spanning from France in the West and parts of the Balkan in the East. The total network size can be expected to double both in 2040 and 2050, up to a total of nearly 100 pipelines. The derived network is the result of broad exploration based on 1500 experiments that incorporates a wide range of supply, demand and geopolitical uncertainties. Connections in the final network are selected based on their occurrence across this set of experiments, with the average occurrence of edges in the network being 91.61%. Capacities are assigned to minimise regret, which emerges in case of over- or undercapacity. On average, the regret of the final network represents 40% of its total investment cost, which represents the average cost of altering the network to the optimal network in each experiment. This regret value is relatively high due to the large variety in required capacities across the set of experiments. Nevertheless, it provides an indication of the risks associated with the development of a European hydrogen infrastructure, which is plagued by a large set of uncertainties.



Figure 60: Growth of robust network derived from this research between 2030 and 2050.

The core of the network mostly corresponds to the Blue Banana, a geographical construct of densely populated areas spanning Northern Italy, Southern Germany, North-Eastern France and the Benelux [173]. Due to high population density, hydrogen demand in both transport and built environment is expected to be relatively high in these areas. Additionally, Italy, Germany, the Netherlands and Belgium are well-represented in terms of ammonia, methanol and refining production facilities. For example, industrial clusters in Antwerp, Rotterdam and the Ruhr area create potential for an early hydrogen cluster. Also, Germany and Italy are favourably located within the European Union to form the link between Eastern and Western Member States. In this sense, the conclusion of this research aligns with previous research on the Blue Banana as a hydrogen corridor [174]. When incorporating current political efforts of Member States to stimulate hydrogen, France emerges as a third backbone nation. Especially if hydrogen production from nuclear energy takes off, France features a set of dedicated production areas that help stimulate the development of a transmission infrastructure. After all, transmission infrastructures thrive on dedicated supply and demand centres, rather than areas where local demand and supply cancel each other out. For example, this research shows that a high share of decentralized hydrogen production from solar energy on average decreases the total network size. When incorporating the reassignment of natural gas pipelines in hydrogen infrastructure development, the average network size over the set of experiments grows. Specifically, the earlier mentioned backbone is further solidified as most opportunities for reassignment exist in Italy, France, Germany and the Benelux. After all, the Netherlands historically played a large role in the development of a European natural gas network due to their ample production capacity. Additionally, Italy's natural gas network is well-developed as it facilitates large imports from North-African states. The increase in average network size due to reassignment primarily stems from a decrease in the occurrence of relatively small networks.

In reflecting on the impact of hydrogen on the relative geopolitical influence of European Member States, some similarities can be drawn to the world of natural gas. For example, the Baltic states and parts of the Balkan are at risk of becoming poorly connected to Central and Western European Member States. With respect to the Balkan, a combination of sparsely populated areas in combination with relatively low wind potential and average solar potential creates a tough environment for hydrogen development. For the Baltic States, solar potential is even worse. Especially a focus on natural gas pipeline reassignment creates similarities between the worlds of hydrogen and gas, with the Benelux, Germany, Italy and France likely becoming most well-connected. Especially Germany and Italy are set to become pillars of a future hydrogen network, and may receive the geopolitical power that accompanies this role.

Concluding, this exploratory study has proposed a network topology to answer the main research question posed in Chapter 1. As such, it aims to contribute to the development of a European hydrogen infrastructure by providing insight in how such an infrastructure may be developed in a financially feasible and robust manner.

7 Discussion

The development of a European hydrogen network is plagued by a host of complexities due to its societal importance, large financial cost and long life cycle. On top of this, little is currently known on what a European hydrogen network may look like. As a result, investments can quickly be considered too risky or ill-advised, hampering the development of hydrogen in Europe. To prevent this, research is required that helps shape this pivotal network. The added value of this research is that it does so by presenting a topology for a European hydrogen network that is robust to future uncertainty. Here, robustness is quantified in terms of regret, which provides an indication of the financial risks associated with investing in the proposed network. This is vital information to investors and policy makers as investments boil down to a weighing of expected benefits and risks. On top of this, the network topology presented in this research features financially feasible connected components. As such, the results of this study provide a clear exploration of a potential backbone for a future European hydrogen network. This assists policy makers in the planning of such an infrastructure in two ways. First, this research highlights Italy, Germany and France as backbone nations for a future hydrogen network. The initial topology derived from this research can be utilized to stimulate cooperation between these Member States by providing an objective starting point for further research and planning. Second, it pinpoints potential early adoption centres, namely 4 clusters in Belgium, the Netherlands, Germany and Italy. This paves the way for the creation of policies to stimulate hydrogen development in these areas. In fulfilling these functions, the derived network should be interpreted as an outline rather than a detailed blue print of a future hydrogen network. Most notably, the network features a tree structure that foregoes redundancy and reliability criteria and thus primarily serves as the starting point for a more comprehensive network. Also, local characteristics have not been considered in the placement of network nodes, which implies that the geographical placement of network connections is primarily an indication. Nevertheless, this indication is critical at this point in the development of a European hydrogen network.

Now, the novelty of this research complicates the validation of its results. Nevertheless, these results show clear similarities with both the Hydrogen Backbone and the topology derived by Caglayan et al. [39]. First, the general development of the infrastructure derived in this study matches that of the Hydrogen Backbone, with multiple clusters emerging in 2030 that grow together towards 2040 and 2050. Additionally, both the initial cluster spanning the Netherlands, Belgium and North-Western Germany and the one emerging in Italy matches with the results of the Hydrogen Backbone. The most apparent dissimilarity between the results of this study and that of the Hydrogen Backbone is that this research downplays the role of Spain. From an economic-geographic standpoint this makes sense as Spain is relatively sparsely populated and primarily has solar energy potential to produce hydrogen in a decentralized manner. However, this study neglects constraints on production capacity while Spain features very high production capacity [175]. Additionally, this study assumes that the European Union internally produces all its required hydrogen and thus foregoes the role of imports. As in the world of gas, Spain may prove to facilitate these imports by building import terminals, similar to their development of LNG terminals. Also, Spain is geographically well-located to import hydrogen from North-African states, similar to Italy. Thus, arguments can be made both for and against an important role for Spain in a future hydrogen network. With respect to the study of Caglayan et al., a shared importance is assigned to Italy, Germany and France. Additionally, the vital North-South connection found in this research also occurs in their results. In their case, this connections runs through France rather than Germany, which is likely due to the inclusion of Great Britain in their geographical scope. Overall, the results of this study align in a general sense with existing findings and can therefore be utilized to fulfill an exploratory function in search of a European hydrogen infrastructure.

To the domain of hydrogen infrastructure literature, this study is the first to investigate a network topology on a European scale over multiple time steps. This is a vital addition to the existing bulk of nationally focused research. After all, this study shows an integrated European network to be most robust. Already in 2030, initial hydrogen adoption centres are likely to cross national borders. An example of this is the cluster of Member States in North-Western Europe spanning the Netherlands, Belgium and Germany. This motivates a more international view on infrastructure development that is missing in current literature. As a second addition, this research has incorporated a more extensive review of uncertainty in its network design. Most existing hydrogen infrastructure studies utilize between 2 to 10 scenarios, barely covering the realm of possible out-

comes. This research has considered thousands of experiments, which allows for the generation of a robust rather than optimal network. By providing a clear example of how to incorporate robustness in infrastructure design, it may spark a much needed reorientation from optimality towards robustness as a performance metric.

As a more general contribution, this research identifies a combination of graph theory and exploratory modelling and analysis (EMA) as a promising methodology for generating robust network infrastructure topologies. On its own, graph theory offers an effective toolbox of existing heuristics and algorithms to analyse network infrastructures and their characteristics. Additionally, its simple structure in terms of nodes and edges provides ample opportunity for the development of novel heuristics to tackle a wide variety of challenges. Critically, smart heuristics allow for the creation of computationally inexpensive models. This pair expertly with EMA, which allows for the generation of hundreds to thousands of experiments. As a result, a clear advantage of this pairing is that it creates a virtual sandbox that allows for the investigation of a near limitless amount of hypotheses. In the exploratory phase of infrastructure development, this is a vital trait as parties involved may seek to test their initial assumptions of the network. With the proposed model, policy makers can easily explore these assumptions by generating hundreds of additional experiments in the span of a day. In doing this, the proposed methodology may assist in decision making processes surrounding the development of a European hydrogen network. Additionally, the proposed methodology can be applied to a wide range of other network problems. As such, it offers a more extensive way to incorporate uncertainty compared to existing methods utilized in graph-theoretical research. On a more detailed level, this research has proposed a set of heuristics. In the generation of optimal networks, an expansion of the edge removal heuristic proposed by Andre et al. [7] has been made towards multi-source, multi-sink networks. The primary strength of this heuristic is that it breaks with the assumption of a fixed set of nodes that characterises many graph-theoretical procedures. In the analysis of energy infrastructure networks, this is a convenient way to tackle uncertainty on the necessity or financial feasibility to connect specific areas. Furthermore, utilizing an economic criterion to remove edges on the level of connected components has proven to closely imitate the development of an emerging network infrastructure. To facilitate the generation of robust networks, three heuristics have been proposed by this research. Since the execution of these heuristics relies on the consideration of a large set of plausible futures, their application is primarily restricted to a methodology that incorporates EMA. Additionally, they should be considered within the integrated methodology aimed at retrieving robust network topologies. Nevertheless, they provide an illustration of how robustness can be defined in infrastructure design, which may spark further research. Especially since robustness can be operationalized in a multitude of ways, various alternative heuristics may be developed.

8 Recommendations

This section discusses recommendations to both policy makers and researchers for building on the insights delivered by this research. For policy makers, four next steps can be identified. First, the results of this study can be utilized to activate and inform both European Member States and non-state stakeholders. As illustrated in the introduction of this research, the current lack of a hydrogen infrastructure holds back its diffusion. Nevertheless, this research underlines that a European hydrogen network connecting large parts of the European Union is both financially feasible and robust in 2050. This projection can be utilized to support the expectation that a European hydrogen infrastructure will emerge and hydrogen is worth investing in. Germany and Italy are identified as infrastructure backbone nations, which should be steered towards a favourable stance on hydrogen. Second, the results of this research should be employed to stimulate coordination among European Member States. This study illustrates that a robust hydrogen network is likely to cross national borders from the start, underlining the fruitfulness of cooperation amongst European Member States. Specifically, the proposed network gives an indication of probable interdependencies between Member States, for example between Belgium, the Netherlands and Germany. These results provide a fruitful motive to foster collaboration between such groups of Member States. Third, the results of this study should be utilized to support the allocation of resources towards the development of a European hydrogen infrastructure. Specifically, this research identifies four initial adoption centres. The European Union can stimulate infrastructure investments in these areas by identifying them as Projects of Common Interest (PCI's) and allocating resources from the Connecting Europe Facility (CEF) fund. Fourth, the model developed in this study should be employed to support future decision-making processes. While the results of this research provide a solid exploration, the developed model can be utilized to test a wide variety of alternative hypotheses. For example, Member States can test the impact of specific policies on the network and its characteristics by updating model inputs. Jointly exploring such hypotheses can foster cooperation amongst European Member States and other stakeholders.

For researchers, three primary avenues exist to expand the network model proposed in this study. First, the results of this study provide a basis for investigating fruitful network topologies on a regional scale. For example, this research has utilized a relatively straightforward approach with respect to pipeline routing. In part this stems from the assumption that each geographical area features a single network point located at its centre. Additionally, routing restrictions arising from mountains, lakes or other geographical obstructions are disregarded. These choices are founded in practical necessity due to the broad geographical scope of this study. Rather, studies focusing on a local level have the capability to perform a more detailed analysis without ballooning its data requirements. The earlier mentioned initial adoption centres provide a promising selection of areas to research on a more detailed level. Additionally, this research provides motive for reviewing existing scientific papers that have developed national or regional infrastructure topologies. On one hand, this may help point out areas in which the model developed in this research lacks detail. On the other hand, it helps to illustrate how these national networks may be designed to fit better into an international network. Second, future research can build upon the network generated in this study by including reliability and redundancy considerations. The derived topology features a tree structure as these networks are relatively easy and computationally inexpensive to generate. Additionally, tree networks feature low costs and are well suited to provide a first outline for a network. Nevertheless, they are inherently vulnerable as the failure of a single network connections leads to a disconnected network. Third, geopolitics can be included in future research more extensively. Namely, this research neglects the role of import towards the European Union and rather assumes that the European Union as a whole will be self-sufficient. Import-export relations with nations outside of the European Union may serve as an additional class of uncertainties, broadening the analysis of the case. Also, this research neglects connectivity constraints in the generation of the final network. For example, Member States may desire multiple import nations to decrease reliability on a single exporter, as is currently the case in the world of natural gas. Important to note is that these avenues for future research are a logical sequence to exploratory research, which aims at identifying fruitful ways forward.

A secondary avenue for future research is further testing and developing the novel methodology proposed in this study. First and foremost, this can be done by applying it to other cases. While the basic components of the methodology are a graph-theoretical network model and experiment design based on EMA, there exists a lot of flexibility to shape these components. Another way to test the methodology's effectiveness is by comparing it to other methods such as mixed-integer linear programming (MILP) and agent based models. Specifically, a comparison can be made on criteria such as the quality of the results, data requirements and computational efficiency. Another way towards developing the proposed methodology is by tapping into the variety of methods that EMA offers to analyse the results of computational experiments. These methods include amongst others PRIM, dimensional stacking and scenario discovery.

As part of building on the proposed methodology, an avenue for future research is to further investigate and validate the heuristics proposed in this research. Out of practical necessity, this research has taken a straightforward approach towards the generation of these heuristics. With respect to the edge removal heuristic, a limitation is its sole focus on economic performance, neglecting connectivity. Thus, a fruitful avenue for future research may be to incorporate connectivity constraints to this heuristic. Another practical issue it its computational time. The current heuristic requires the recalculation of a minimum-cost spanning tree after each iteration, which is computationally intensive in combination with the Delta change heuristic that is utilized by the Optimal Network Layout Tool. Considering the robustness heuristics, the networks derived deviate on average 40% from the optimal solution. While deviations in plausible futures inherently drive up regret, this signals room for improvement. As such, future research is encouraged to find alternatives to the proposed heuristics to explore whether they can improve upon this regret value. Additionally, the proposed heuristics can be compared to alternatives to further test their validity and effectiveness.

A Networks and their characteristics

This section contains a series of Appendices dedicated to specific elements of networks and their characteristics. These Appendices have been grouped to promote a cohesive report structure.

A.1 Prim's and Kruskal's algorithm

Section 2.1 highlights that Prim's and Kruskal's algorithm are best-known to find a minimum spanning tree. This Appendix describes the specific procedure of both these algorithms. Figure 61 illustrates Kruskal's algorithm on a simple network. Kruskal's algorithm starts by adding the lowest weight edge. Consecutively, the lowest weight edge from the remaining set of potential edges is added as long as this does not create any cycles. This process is repeated until all nodes are connected.



Figure 61: Illustration of Kruskal's algorithm on simple network.

Figure 62 highlight the use of Prim's algorithm. Prim's algorithm starts from an arbitrary node, in this case node 2. Thereafter, the lowest weight outgoing edge of the already present network is added. This process is repeated until all nodes are connected.



Figure 62: Illustration of Prim's algorithm on simple network.

A.2 Regulation of pipeline infrastructures

Section 3.3 described that different economic criteria can be applied to network infrastructures. To decide on what specific economic criterion to use, it is required to asses what party will or should invest in large infrastructure pipeline projects. This Appendix makes this assessment. In practice, large energy infrastructure are often maintained and operated by regulated transmission system operators. These parties are also responsible for adequate investment in capacity expansions. Specifically, Directive 2009/73/EC specifies the tasks of transmission system operators of gas. These include:

"a) operate, maintain and develop under economic conditions secure, reliable and efficient transmission (...) to secure an open market, with due regard to the environment, ensure adequate means to meet service obligations. b) refrain from discriminating between system users or classes of system users, particularly in favour of its related undertakings"

To cover operating costs and facilitate new investments, TSOs charge tariffs to users of the network. These tariffs regulated via Regulation (EC) No 715/2009, which states that:

"In calculating tariffs for access to networks, it is important to take account of the actual costs incurred, insofar as such costs correspond to those of an efficient and structurally comparable network operator, and are transparent, as well as of the need to provide appropriate return on investments and incentives to construct new infrastructure"

To understand the regulation of these transmission systems operators, the case of market failure in infrastructures should be elaborated upon. Specifically, infrastructures represent a case of market failure due to the presence of a natural monopoly that provides essential services. As a result, a monopolistic party may abuse its power and charge excessive prices. These excessive prices hurt consumers and are socially undesirable. Consecutively, the government steps in and regulates these entities, resulting in the regulatory schemes of Directive 2009/73/EC and Regulation (EC) No 715/2009. Based on these regulatory schemes, this research assumes TSOs will invest in specific network connections as long as this does not prohibit them from covering their costs, in line with the goals laid out in Directive 2009/73/EC. As a result, this research will consider the Net Present Value (NPV) as an economic criterion. Moreover, the NPV of connected components will be assessed. This stems from the international nature of the used case, where a connected component may span multiple countries. In this case, it is assumed that the national TSOs invest in the network as a group and consider the NPV of this connected component as a whole. Now, it is hard to pinpoint a specific investment cycle as the specific nature of pipeline investments depend largely on the regulatory scheme [176]. Within the EU, Regulation (EC) No 715/2009 forces the development of Community-wide ten-year network development plans, which makes 10 years a natural investment period to consider. Additionally, climate goals are often formulated on a 10 year basis, supporting this approach (see e.g. [13], [177]. As such, this research will consider three discrete time steps: 2030, 2040 and 2050.

A.3 Cost and NPV of hydrogen pipelines

As described in section 3.3, the generation of robust networks required a formalisation of the cost and NPV of hydrogen pipelines. This Appendix analyses both these elements. The material costs of a pipeline are in large dependent on its length and diameter. Now, a pipeline's cost is proportional to its length, implying a relatively simple linear relationship. Alternatively, the relationship between a pipeline's diameter and its cost is quadratic. The left graph of Figure 63 shows the relationship between a pipeline's cost and diameter as estimated by three studies. In the right graph, a second order polynomial is fitted to the average values of these three studies. Note that the R-squared value of the trendline equals 1, implying a perfect fit.



Figure 63: Cost of a hydrogen pipeline as a function of its diameter in MEUR.

Now, the capacity of the pipeline is also dependent on the diameter. Figure 64 applies an identical methodology to the one utilized in Figure 63. Note that the R-squared value of the trendline equals 0.99, practically implying a perfect fit.



Figure 64: Capacity of a pipeline as a function of its diameter in tonne/day.

An additional cost source to pipelines are compression stations. Compression stations are required to counter the pressure drop in pipelines as a result of for example friction and elevation to maintain a steady flow over long distances. The pressure drop in a pipeline is inversely related to its diameter, favoring larger pipelines. Figure 65 highlights the pressure drop per 100 km as a function of a pipeline's diameter.



Figure 65: Pressure drop per 100 km as a function of diameter in bar.

The following formula is utilized to calculate the power necessary to increase the pressure from the inlet pressure P_1 to the outlet pressure P_2 [45], [46]:

$$W = m * \frac{R * T_1}{M_w} * \frac{\gamma}{\gamma - 1} * \frac{Z_1 + Z_2}{2} * \frac{1}{\eta_s * \eta_m} * \left(\left(\frac{P_2}{P_1}\right)^{\frac{\gamma - 1}{\gamma}} - 1 \right)$$

- m: mass flow [kg/s]
- R: universal constant of ideal gas (8.314) [J/(K mol)]
- T_1 : inlet temperature of the compressor [K]
- M_w : molecular mass of hydrogen (2.016) [g/mol]
- γ : specific heat ratio (1.4) [-]
- Z: hydrogen compressibility factor at 1) suction and 2) discharge (1) [-]
- $-\eta_s$: isentropic compressor efficiency (80%) [-]
- η_m : mechanical losses from the driver (98%) [-]

Both Yang and Ogden [46] and Andre et al. [45] use in- and outlets pressures of 70 and 35 bar, respectively. This research similarly utilizes these numbers. As such, the total pressure drop is calculated for each pipeline by multiplying the pressure drop per km as highlighted in Figure 65 by the total length of the pipeline. Next, the total required compressor capacity is calculated, for which the costs are calculated using the following proposed by Andre et al. [45]:

CAPEX = 2,655.04 * W

With respect to the NPV of hydrogen pipelines, TSOs can be expected to charge tariffs that allow them to cover their costs based on the regulatory schemes laid out in Directive 2009/73/ EC and Regulation (EC) No 715/2009 (see Appendix A.2). If this principle were applied perfectly, the NPV of pipelines would always be zero and pipelines would never have to be excluded based on a negative NPV. In practice, this doesn't hold up as the network tariffs are charged to end consumers, increasing the total hydrogen price. If network tariffs skyrocket the hydrogen price, demand will decline and the pipeline will not be able to pay itself back. Thus, network tariffs should vary within a range for which end consumers deem the hydrogen price acceptable. However, the dynamic between network tariffs, the hydrogen price and subsequently hydrogen demand is uncertain. As a simplification, this research assumes a fixed tariff for all pipeline investments in each plausible future. This fixed tariff is sampled from a range that is based on a review of existing literature and varies for each plausible future between 0.50 and 1.00 €/kg [7], [46]. Now, having defined both the cost and revenue structure of pipelines, NPV calculations can be made.
For each pipeline, the investment costs are incurred in the first year. Consecutively, network tariffs generate revenue based on the capacity of the pipeline over the total lifetime of the asset. Future cash flows are discounted using a discount rate of 5% and the lifetime of the asset is set to 30 years to span the entirety of the research scope. Now, important to these calculations is the threshold at which the NPV is positive. In comparing Figures 63 and 64, it becomes apparent that the slope of the latter is much steeper. This implies that while larger pipelines are more expensive, they are expected to make more than up for this in increased capacity. For example, expanding a pipeline's capacity from 10 to 20 inch increases its cost by 37.8% while its capacity increases by 412.7%. The same dynamic applies to compressor costs, which favour larger pipelines. Figure 66 highlights the maximum length for each capacity at which the NPV is positive. Now, the specific values shown are dependent on the chosen values of for example the tariffs. Nevertheless, the dynamic is clear: the higher the pipeline capacity, the higher the maximum length.



Figure 66: Maximum length at which a pipeline is financially feasible given its capacity.

A.4 Exclusion of network nodes

As highlighted in section 3.1, an edge removal heuristic is applied in the generation of optimal networks. One of the downsides of this method is the computational effort required. As mentioned earlier, the removal of one or more network connections requires the recalculation of the remaining network's capacities. This may have a cascading effect that necessitates several more iterations, further increasing the computational burden. When investigating a larger network over a broader set of scenarios, the removal of infeasible connections may lead to a sizeable increase in the overall computation time, especially if similar cascading effects occur.

One way to prevent the necessity of a large number of iterations is by evaluating the set of network nodes. For example, when evaluating the selection of nodes in Figure 67, the three nodes highlighted in green can be identified as outliers based on the geographical proximity of the network. Instinctively, they may be removed to prevent the exclusion of their network connections later on. However, their supply and demand values are essential in determining whether this is wise. For example, if the three green nodes are the only supply nodes in the network, their removal renders the remaining network completely ineffective. However, when these nodes have a more balanced supply and demand pattern, their removal is hard to instinctively determine. After all, the impact of their removal is dependent on the infrastructure that will arise and the presence of other nodes in the selection.



Figure 67: Possible nodes to exclude may be identified based on their geographical location.

Now, the exclusion of nodes can be evaluated based on the expected feasibility of the network connections that will be potentially connected to them. In the simple example of Figure 69, the two nodes can potentially be connected by a pipeline with length x, transporting a volume of y. The transported volume stems from the total demand and supply of the two nodes, respectively y and -y. If this network connection is infeasible on its own, both nodes can be excluded from the network as there are no potential network connections stemming from these nodes that are expected to be feasible.

However, when expanding this network, the connection between the initial two nodes may become feasible as a transit connection. This is illustrated in the bottom graphic of Figure 69. As a result, network nodes cannot be excluded purely on the feasibility of connections to neighbouring nodes. Rather, the surrounding network should be evaluated.



Figure 68: Network connections may become feasible as a transit connection.

As a first step towards a broader analysis on the exclusion of network nodes, various circles may be formed around the center of the network. Now, network nodes that lie in the outer ring are unlikely to be used as a transit hub as virtually all the other network nodes lie on the same side of it. As a result, these nodes can be excluded if the connections to the nodes in their closest proximity are infeasible.



Figure 69: Transit nodes may be identified by drawing circles around a network's centre.

Now, if a node has a potential connection that is feasible, it can remain in the network. To analyse the next ring in the network, the demand and supply profiles of the nodes that remain in the outer layer can be added to the nodes that are on the other side of their feasible potential connections. For example, if the outer node has a net demand of x while the inner node has a net supply of 2x, the net supply of the combination of nodes is x. This is similar to the existence of a single node with a net supply of x. As shown in Figure 70, each layer can be analysed by consistently peeling off the most outer layer. When getting closer to the center, the probability of having to exclude a network decreases as the center nodes are generally closer to other nodes and may serve as transit hubs for the network around them. Consecutively, a quick & dirty method of eliminating a relatively large share of nodes is evaluating only the outer rings of the network.



Figure 70: Nodes may be excluded by systematically peeling off outer circles.

While the approach described may be fruitful to initially remove a portion of the network nodes, it is deemed to be computationally intensive on its own. Additionally, it requires a further complication of the model described in sections 3.2 and 3.3. As such, this research does not incorporate this approach. Nevertheless, it provides an illustration of a possible avenue for decreasing computational time.

B Pseudo code network analysis heuristics

This section contains the pseudo code of four heuristics proposed in section 3.1 and 3.2 of this research. These Appendices have been grouped to promote a cohesive report structure.

B.1 Multi-source, multi-sink edge removal heuristic

The following pseudo code applies to the edge removal heuristic proposed in section 3.2 of this research. Note that CC is an abbreviation of connected component, which implies a set of nodes for which a path exists to all other nodes. The goal of this heuristic is to derive a network in which all connected components feature a NPV larger than zero.

- 1. Add initial network to list of CC (from hereon 'CC_list')
- 2. WHILE number of CC in CC_list > 0
- 3. FOR all CC in CC_list DO
- 4. WHILE NPV of CC < 0

5.	IF number of edges > 39 THEN
6.	Remove (number of edges/20) edges with lowest NPV \sim
7.	ELSE
8.	Remove edge with lowest NPV
9.	END IF
10.	IF number of CC in remaining network > 1 THEN
11.	Add CC to CC_list
12.	ELSE
13.	IF number of CC in remaining network $= 0$ THEN
14.	Remove CC from CC_list
15.	ELSE
16.	Recalculate optimal network
17.	Calculate NPV of found network
18.	END IF
19.	END IF
20.	END WHILE
21.	END FOR
22.	END WHILE

B.2 Maximum occurrence heuristic

The following pseudo code applies to the maximum occurrence heuristic introduced in section 3.2. Its goal is to define a spanning tree containing edges that feature the largest occurrence across a set of plausible futures.

- 1. Define a network with all network nodes and no edges
- 2. Define the occurrence of all possible edges across experiments and delete the edges with zero occurrence
- 3. WHILE number of edges left in list > 0
- 4. Pick edge with highest occurrence score
- 5. IF addition of selected edge creates a cycle THEN
- 6. Remove edge from list
- 7. ElSE
- 8. Add edge to network
- 9. END IF
- 10. END WHILE

B.3 Minimal regret capacity heuristic

The following pseudo code applies to the minimal regret capacity heuristic introduced in section 3.2. Its goal is to assign capacities with minimal regret to network edges.

- 1. Set the capacity equal to the largest required capacity over all runs
- 2. Calculate the regret of the chosen capacity over all runs and take the sum
- 3. IF the total regret > 0 THEN
- 4. WHILE new regret is smaller than previous regret
- 5. Lower the capacity by 1
- 6. Calculate the regret of the chosen capacity over all runs and take the sum
- 7. END WHILE
- 8. Assign previous capacity increased by 1
- 9. ELSE
- 10. Assign maximum capacity
- 11. END IF

The heuristic is initiated by assigning the largest required capacity to each edge. This stems from the consideration that overcapacity leads to more regret than undercapacity, as illustrated by the following example. Let's assume a specific network connection with a capacity of 500 tonne/day. However, two plausible futures may require a capacity of 300 and 700 tonne/day. Based on the pipeline cost functions highlighted in Appendix A.3, the regret in the first scenario is equal to:

 $Regret = cost_{cap: 500} - cost_{cap: 300} = 64.52 - 53.90 = 10.63 Meur$

In the second scenario, regret equals:

 $Regret = cost_{cap: 200} = 46.34 Meur$

B.4 Multi-period network heuristic

The following pseudo code applies to the multi-period network heuristic proposed in section 3.2. Its goal is to derive robust network topologies for multiple time steps, simulating infrastructure expansion over time.

- 1. Set time equal to 2030
- 2. Determine the optimal network in each experiment for the given time step
- 3. Derive the maximum occurrence tree (see Appendix B.2)
- 4. Assign minimal regret capacities (see Appendix B.3)
- 5. Apply economic criterion to found network (see Appendix B.1
- 6. Update supply and demand patterns of the next time step based on derived network
- 7. Increase time by 10 years
- 8. IF time > 2050 THEN
- 9. STOP
- 10. ELSE
- 11. Go to step 2
- 12. END IF

Section 3.2 states that initially building an excess of capacity is cheaper than having to expand initially built infrastructure. The following calculation illustrates this, where a 250 km pipeline may require a capacity of 250 tonne/day. Based on the cost function of pipelines described in Appendix A.3, this amounts to the following cost:

$Cost_{cap: 250} = 140.56 Meur$

If we assume that the required capacity doubles in the next time step, a second pipeline is placed in parallel to the existing one. Recall from section 3.2 that this research assumes no capacity modifications can be made to existing pipelines. Now, the difference between this capacity expansion and the initial construction of 1 pipeline with a capacity of 500 tonne/day amounts to:

$$Regret = 2 * Cost_{cap: 250} - Cost_{cap: 500} = 140.56 * 2 - 190.34 = 90.79 Meur$$

Although the specific values differ per case, this example illustrates the immense upside to initially constructing an excess of capacity. Now, initially constructing overcapacity brings additional operations & maintenance (O&M) costs. However, Andre et al. [7] utilize a fee of 2% of the total CAPEX, which is negligible compared to the upside of constructing an excess of capacity. In this specific calculation example, the extra O&M costs outweigh the upside after 23 years. As this research considers a time horizon between 2030 and 2050, capacity will never be constructed 23 years in advance.

C Economic-geographic input data

This section groups the modifications made the to the NUTS 2 system that is utilized to generate network nodes (see section 4.1) with various economic-geographic parameters that serve as an input for the network model. These parameters are further described in section 4.2 and summarized in section 4.3. These Appendices have been grouped to promote a cohesive report structure.

C.1 Modifications to NUTS 2

Table 13 highlights the modifications made to the NUTS 2 classification that is utilized as a basis for the formalisation of network nodes. The goal of these modifications is to retrieve a more geographically uniform set of network nodes, as elaborated upon in section 4.1. For each Member States, the merged areas are shown. This implies that one network node is assigned to each of these merged areas, reducing the total set of nodes compared to the initial NUTS 2 classification.

Member State	Merged areas
	DE11, DE12
	DE13, DE14
	DE22, DE23
	DE24, DE25, DE26
	DE21, DE71
	DE72, DE73
Germany	DE91, DE92, DE93
	DE94, DE50
	DEA1, DEA2
	DEA3, DEA4, DEA5
	DEB1, DEB2
	DEB3, DEC0
	DED2, DED4, DED5
Netherlands	NL11, NL12, NL13
	NL21, NL22, NL23
	NL32, NL33, NL34
	NL41, NL42
	AT11, AT12, AT13
Austria	AT21, AT22
Austria	AT31, AT32
	AT33, AT34
	CZ01, CZ02
Czech Republic	CZ05, CZ06
	CZ07, CZ08
	EL63, EL65, EL54
Greece	EL61, EL64
	EL51, EL52, EL53
Belgium	BE21, BE22, BE23, BE24, BE25
Boigium	BE31, BE32, BE33, BE34, BE35
Denmark	DK01, DK02
	DK03, DK04
Poland	PL81, PL82
	PL91, PL92, PL72
Hungary	HU11, HU12
	HU21, HU22
Romania	RO21, RO22
	RO31, RO32
Finland	FI1B, FI1C
Italy	ITH1, ITH2, ITH3, ITH4
Slovakia	SK01, SKO2

Table 13: Modifications to NUTS 2 system

C.2 Vehicle ownership, travel intensity & fuel consumption

Section 4.2 highlighted that two vital parameters to the development of hydrogen in transport are the travel density and number of vehicles. Table 14 highlights the values of these parameters per Member State. Figure 71 provides a histogram of the distribution of these parameters across the NUTS 2 areas. Eurostat provides complete data on the number of passenger vehicles on NUTS 2 level [178]. The number of kilometers travelled per Member State is retrieved from the Organisation for Economic Co-operation and Development (OECD) [179]. To retrieve values on a NUTS 2 level, the total value of the corresponding Member State is multiplied by the region's share in the nation's total population. There a few outliers in both the number of passenger vehicles and kilometers travelled per vehicle. Considering the former, Île de France (Paris area) in addition to Andalusia (Southern Spain) and Lombardia (North Italy) are the highest ranking values. For the number of kilometers travelled per vehicle, Berlin, Île de France and Stockholm score the highest. These outliers make sense as these areas represent densely populated regions.



Figure 71: Histogram of vehicles per area and average kilometers travelled per vehicle (x1000/year).

Member State	Passenger vehicle movements (in Million vehicle-kilometers)	Passenger vehicles (x1000)
Austria	89719	4979
Belgium	120069	5854
Bulgaria	8588	2773
Croatia	3843	1663
Czechia	88921	5748
Denmark	70635	2594
Estonia	2924	746
Finland	74800	3482
France	861944	32879
Germany	1000302	46475
Greece	44776	5283
Hungary	82607	3641
Italy	826284	39001
Latvia	2156	708
Lithuania	32702	1431
Luxembourg	2300	415
Netherlands	144700	8531
Poland	268386	23429
Portugal	97217	5170.611
Romania	19937	6453
Slovakia	34699	2322
Slovenia	34699	1143
Spain	372744	24074
Sweden	126730	4870

Table 14: Economic-geographic parameters in transport per Member State

Data on the passenger vehicles movements of six Member States are missing for the year 2018. To fill these gaps, the most recently available data was gathered and extrapolated based on the average travel intensity growth rate of the other Member States. Table 15 illustrates this.

Member State	Reference year	Reference data	Extrapolated to 2018
Austria	1992	68200	89719
Denmark	2016	66544	70635
Portugal	2008	96756	97217
Belgium	2016	119500	120069
Greece	2008	42182	44776
Slovenia	2010	28819	30411

Table 15: Data on the utilized extrapolation

By multiplying the travel intensity and number of vehicles per region, a first impression can be gathered of the geographical distribution of the potential for hydrogen (see Figure 72). It can be seen that Italy, France, the Netherlands and Germany feature relatively high potential. On the contrary, the Balkan nations show relatively little potential.



Figure 72: Geographical distribution of hydrogen demand if all passenger vehicles run on hydrogen.

A last parameter of importance to the development of hydrogen in transport is the fuel consumption. This research utilizes the fuel consumption of the Toyota Mirai II [180]. Based on Ajanovic and Haas [121], an fuel consumption decrease of 20% and 40% is assumed for respectively 2040 and 2050. In doing this, technological advances of hydrogen vehicles are incorporated.

C.3 Heating demand per area & heat density

Section 4.2 highlighted the heating demand of households as a vital parameter to the development of hydrogen in the built environment. Table 16 illustrates the value of this parameter per Member State. Figure 73 provides a histogram of the distribution of this parameter across the NUTS 2 areas. The data is retrieved from Eurostat [181].



Figure 73: Histogram of heating demand per area (PJ/year).

Marshan State	Water heating	Space heating	Cooking
Member State	(x1000 TJ)	(x1000 TJ)	(x1000 TJ)
Austria	40393	187754	7230
Belgium	40210	249269	5780
Bulgaria	16802	49433	7981
Croatia	9670	65745	6240
Czechia	51138	205465	18756
Denmark	40813	119808	3123
Estonia	4653	28637	1913
Finland	35924	159352	2329
France	185417	1061537	90489
Germany	391090	1528162	150606
Hungary	24783	88860	10176
Ireland	31269	174761	11915
Italy	165767	893196	88080
Latvia	9498	33927	3651
Lithuania	5532	43946	4011
Luxembourg	1602	16579	540
Netherlands	67410	255985	8514
Poland	134186	534537	67670
Portugal	21256	34411	43443
Romania	43953	204322	31758
Slovakia	12024	57628	4910
Slovenia	7489	27313	1911
Spain	107584	272244	46838
Sweden	44128	171832	4834

Table 16: Heating demand per Member State and category

Figure 74 gives an indication of the spatial variety of heating demand, calculated as the sum of the three aforementioned categories. Northern Italy and Southern France form the highest demand area, while Spain, Portugal and parts of the Balkan represent some of the lowest demand areas.



Figure 74: Geographical distribution of hydrogen demand if all households utilize hydrogen applications.

A second parameter essential to the development of hydrogen in the built environment is the heat density. To make a distinction between low and high density heat demand, the European heat map developed by sEEnergies is used [182]. This map contains data on all areas with a heat demand density of 500GJ/ha and above. Figure 75 gives an illustration for Spain and Portugal, where areas with a high heat density are represented in orange. Based on the geographical location of these high heat density locations, they are assigned to NUTS 2 areas.



Figure 75: Illustration of sEEnergies heat map indicating high heat density areas.

Figure 76 shows a histogram for the low and high density heat demand of the NUTS 2 areas. Both categories show the same dynamic, where the number of areas decreases as the total heat demand increases.



Figure 76: Histogram of low and high density heat demand per area (in PJ).

Figure 77 shows the distribution of low and high density heat demand over all areas. This highlights that there exists a wide variety between the NUTS 2 areas as there are both areas that are made up of 100% and 0% high density heat demand.



Figure 77: Distribution of low and high heat density demand over set of areas.

Figure 78 illustrates the spatial variety of heating demand, only incorporating high density heat demand. In this research, the hydrogen demand in low density heat areas is multiplied by a factor of 0.5 to mimic the expectation that hydrogen will likely develop mostly in high density heat areas [143], [144].



Figure 78: Geographical distribution of high heat density areas.

C.4 Type of heating infrastructure

A third parameter of interest to hydrogen development in the built environment is the type of heating infrastructure. Here, a distinction is made between collective and individual heating infrastructures, in line with section 4.2. Figure 79 illustrates that the share of these two options varies greatly amongst Member States. The data is retrieved from Bertelsen et al. [138]. This research assigns the hydrogen demand in built environment to these two categories, based on their relative share in the respective Member State. For example, as Spain features 60% individual heating infrastructure, 60% of total hydrogen demand is assumed to originate from dwellings utilizing a individual heating infrastructure. In this research, the hydrogen demand assigned to collective infrastructure is multiplied by a factor of 1.5. This mimics the expectation of easier hydrogen diffusion in collective infrastructures [139].



Figure 79: Relative share of individual and collective heating infrastructures across Europe.

C.5 Solar potential

Section 4.3 highlighted the potential for electrolysis coupled with solar energy as an important economic-geographic parameter (see Table 9). Figure 80 highlights the geographical distribution of solar energy potential across the European Union. The data is retrieved from the Global Solar Atlas [153]. For each Member State, the total required production of hydrogen from solar energy is divided across its areas based on this potential. So, if the potential is equal in all areas of a Member State, production is divided equally across these areas.



Figure 80: Geographical distribution of solar energy potential across Europe.

C.6 Wind potential

Section 4.3 highlighted the potential for electrolysis coupled with wind energy as an important economic-geographic parameter (see Table 9). Figure 81 highlights the geographical distribution of wind energy potential across the European Union. The data is retrieved from the Global Wind Atlas [153]. For each Member State, the total required production of hydrogen from wind energy is divided across its areas based on this potential. So, if the potential is equal in all areas of a Member State, production is divided equally across these areas.



Figure 81: Geographical distribution of wind energy potential across Europe.

C.7 Nuclear potential

Section 4.3 highlighted the potential for electrolysis coupled with nuclear energy as an important economic-geographic parameter (see Table 9). Figure 82 highlights the geographical distribution of nuclear reactors across the European Union, which is utilized as an indicator for the potential to produce hydrogen from electrolysis coupled to nuclear energy. For every Member State with nuclear reactors, the total hydrogen production from nuclear energy is divided equally over these reactors. In case a Member State has no nuclear reactors, the required production is divided equally over all its areas.



Figure 82: Geographical distribution of nuclear reactors across Europe.

C.8 SMR production potential & refinery hydrogen demand

Section 4.3 highlighted the demand for hydrogen from refining as an important economic-geographic parameter. Figure 83 highlights the geographical distribution of refining facilities. Table 17 highlights the full list of European refineries used in this research including their production and hydrogen demand. The data is retrieved from Fractracker [164].



Figure 83: Geographical distribution of refining plants across Europe.

Refinery	Production	Hydrogen demand
	(in BPD)	(in TWh)
OMV Schwechat Refinery	175000	2,141
Vitol Antwerp N.V. Refinery	35000	0,428
Total Antwerp Refinery Belgium	360000	4,405
Petroplus BRC Antwerp Refinery Belgium	107500	1,315
ExxonMobil Antwerp Refinery Belgium	270000	3,304
LUKEOIL Neftokhim Burgas Refinery Bulgaria	208000	2,545
INA Group Rijeka Refinery Croatia	102000	1,248
INA Group Sisak Refinery Croatia	61000	0,746
PARAMO Pardubice Refinery Czech	15000	0,184
Ceska Rafinerska Kralupy Refinery	66000	0,808
Ceska Rafinerska Litvinov Refinery	110000	1,346
SHELL Fredericia Refinery Denmark	68000	0,832
StatOil Kalundborg Refinery	110000	1,346
Fortum Oyj Porvoo Refinery	160000	1,958
Fortum Oyj Naantali Refinery	40000	0,489
Shell Reichstett Refinery	77000	0,942
BP Lavera Marseilles Refinery	220000	2.692
ExxonMobil Fos-sur-Mer Refinery	140000	1.713
Shell Berre L':Etang Refinery	80000	0.979
Total Provence Marseilles Refinery	155000	1.897
Total Donges Refinery	231000	2.827
Total Flandres Mardyck Refinery France	160000	1.958
Total Feyzin Refinery	119000	1.456
Total Grandpuits Refinery	99000	1.211
ExxonMobil Port Jerome-Gravenchon Befinery	270000	3 304
Total Gonfreville lOrcher Befinery	343000	4 197
Shell/ExxonMobil/Bubr Oel/Conoco Karlsruhe Befinery	285000	3 487
Bavernoil Ingolstadt Refinery	262000	3 206
ExxonMobile Ingolstadt Refinery	106000	1 297
OMV Burghausen Refinery	70000	0.857
PCK Baffinerie GmbH Schwedt Befinery	210000	2 570
Shell Elbe Mineral Iwerke Hamburg-Harburg Refinery	110000	1 346
Tamoil Holborn Hamburg Refinery	95000	1,040
Louis Drevfus Group Wilhelmshaven Befinery	220000	2 602
Buhr Oel (BP/PDVSA) Emsland Lingen Befinery	80000	0.070
Ruhr Oel (BP/PDVSA) Colsenkirchen Horst Refinery	246000	3 010
Shell Bheinland Werk Codorf Cologne Befinery	162000	1 082
Repsol VPF Bilbao Refinery	22000	2 692
CEPSA Tenerife Befinery	90000	1 101
Repsol VPF Puertollano Refinery	140000	1,101
Repsol VPF Tarragona Refinery	160000	1,715
Repsol VPF a Coruna Refinery	120000	1,558
Repsol VPF Cartagena Refinery	100000	1,400
Nyp0 s Potroloum Nyposhamp Rofinory	90000	1,224
Proom Potroloum Cothonburg Refinery	90000	1,101
Proom Potroloum Lucolul Pofinory	90000 910000	1,101 2 570
Pompetrol Detromidie Definery	210000	2,570
Potrom /OMV Potrobragi Ploiosti Rofinory	100000	1,224
Rompotrol Voga Ploiosti Rofinery	20000	0.245
Mol Slovnaft Bratislava Pafinary	20000 110000	0,240
CEDSA Cibrelton Definery	240000	1,040
CEDCA DI LI D'ALLI D'A	240000	⊿,901 1.004
CEPSA Palos de la Frontera La RA bida Refinery	100000	1,224

Table 17: List of refineries including production and hydrogen demand

Refinery	Production	Hydrogen demand
Tomory	(in BPD)	(in TWh)
Dow Chemical Buna SOW Leuna Refinery	222000	2,716
TOTAL Raffinerie Mitteldeutschland Spergau Refinery	227000	2,778
Shell Erdoelwerk Holstein Heide Refinery	84000	1,028
Hellenic Petroleum Aspropyrgos Refinery Greece	135000	1,652
Hellenic Petroleum Elefsina Refinery	100000	1,224
Motor Oil Hellas Corinth Refinery	100000	1,224
Hellenic Petroleum Thessaloniki Refinery	66500	0,814
Mol Szazhalombatta Refinery	161000	1,970
API Falconara Marittima Ancona Oil Refinery Italy	85000	1,040
Saras SPA Sarroch Oil Refinery Italy	300000	$3,\!671$
ENI Gela Oil Refinery Italy	100000	1,224
Tamoil Cremona Oil Refinery Italy	96000	1,175
Iplom Busalla Oil Refinery Italy	40000	0,489
ENI Livorno Oil Refinery Italy	84000	1,028
Italiana Energia Servizi (IES) Mantua Oil Refinery Italy	55000	$0,\!673$
ENI/Kuwait Petro Milazzo Oil Refinery Italy	80000	0,979
ExxonMobil/Erg Trecate Oil Refinery Italy	200000	2,447
ENI Sannazzaro de Burgondi Oil Refinery Italy	170000	2,080
Total/ERG Rome Oil Refinery Italy	90000	1,101
ExxonMobil Augusta Oil Refinery Italy	190000	2,325
ISAB ERG Impianti Nord Oil Refinery Italy	160000	1,958
ISAB ERG Impianti Sud Oil Refinery Italy	214000	2,619
ENI Taranto Oil Refinery Italy	110000	1,346
ENI Porto Marghera Oil Refinery Italy	80000	0,979
ExxonMobil Antwerp Refinery	265000	3,243
Total/DOW Chemical Vlissingen Refinery	160000	1,958
BP ChevronTexaco Nerefco Refinery	400000	4,894
ExxonMobil Rotterdam Refinery	190000	2,325
Rafineria Trzebinia Refinery	4000	0,049
Mazovian Refinery & amp; Petrochemical Works Plock Refinery	260000	3,181
Lotos Gdansk Refinery	120000	1,468
Lotos Czechowice Refinery	10000	0,122
Galp Energia Porto Refinery	100000	1,224
Galp Energia Sines Refinery	200000	2,447
Petrom/OMV Arpechim Pitesti Refinery	70000	0,857
Petrotel-LUKOIL Pitesti Refinery	68000	0,832

C.9 Methanol production EU

Section 4.3 highlighted the demand for hydrogen from methanol production as an important economic-geographic parameter (see Table 9). Figure 84 highlights the geographical distribution of methanol producing facilities. This data is retrieved from the Independent Commodity Intelligence Services [183].



Figure 84: Geographical distribution of methanol plants across Europe.

Plant	Location	Capacity (x1000 tonnes/year)
BASF	Ludwigshafen, Germany	480
BIOMCN	Delfzijl, Netherlands	870
BP refining & petrochemical	Gelsenkirchen, Germany	300
Doljchim	Craiova, Romania	230
Mider-Helm Methanol	Leuna, Germany	660
Nafta Lendava	Lendava, Slovenia	165
Shell & DEA Oil	Wesseling, Germany	400
Viromet	Victoria, Romania	225

Table 18: List of methanol plants including capacity

C.10 Ammonia production EU

Section 4.3 highlighted the demand for hydrogen from ammonia production as an important economic-geographic parameter (see Table 9). Table 19 illustrates the ammonia production potential per Member State. Figure 85 highlights the geographical distribution of ammonia producing facilities. This data is retrieved from the Centre for European Policy Studies [184].



Figure 85: Geographical distribution of ammonia plants across Europe.

le	19: Distribution of	of ammonia production pote
	Member State	Capacity (x1000 tonnes)
	Germany	5500,8
	Poland	3852
	Netherlands	2717
	France	1495
	Belgium	1360
	Lithuania	1118
	Finland	948
	Bulgaria	749,06
	Spain	609
	Italy	600
	Austria	485
	Croatia	474
	Portugal	474
	Slovakia	429
	Hungary	383
	Romania	363
	Czech Republic	350
	Estonia	200
	Greece	165

 Table 19: Distribution of ammonia production potential

C.11 Natural gas network cycles

Section 4.3 highlighted cycles in the natural gas network as an important economic-geographic parameter. Table 20 illustrates the areas that are included in the identified cycles. Figure 86 shows the geographical distribution of these areas across the European Union. The source for identifying network cycles is ENTSOG, which has published a map of the European transmission network [172].



Figure 86: Geographical distribution of areas included in cycles in European natural gas network.

Note that each cycle in Table 20 has between 1 and 4 connections. This stems from the fact that different cycles may occur in a network, as illustrated in Figure 87. The underlying dynamic of removing edges from these cycles is identical, namely that each node is still connected to all other nodes in the cycle after the removal of a single edge.



Figure 87: Network cycles spanning two to four areas.

Number	#1	#2	#3	#4
1	(ES52, ES51)	(ES51, ES24)	(ES42, ES52)	(ES42, ES24)
2	(ES21, ES22)	(ES21, FRI1)	(ES22, FRI1)	
3	(FRI1,FRI3)	(FRJ1, FRK2)	(FRK2,FRK1)	(FRI2,FRI1)
4	(FR10, FRB0)	(FRC1, FRB0)	(FRC1, FR10)	
5	(FR10, FRB0)	(FRG0, FR10)	(FRB0, FRG0)	
6	(FR10, FRF2)	(FRE2, FRF2)	(FRE2, FR10)	
7	(FRF1, FRF3)	(FRC2, FRF3)	(FRC2, FRF1)	
8	(NE41, BE21)	(NE41, BE31)	(BE10, BE21)	
9	(NE11,NE21)			
10	(NE21, NE41)			
11	(NE31,NE21)			
12	(DE24, DE21)			
13	(DEA1, BE31)	(DEA1, DEA2)	(DEA1, NE21)	(NE21, BE31)
14	(DEB1,DEA1)			
15	(DEA2, NE21)	(NE21, NE11)	(NE11, DE94)	(DE94, DEA2)
16	(DE91, DE30)	(DE80, DE30)	(DE91, DE80)	
17	(DEE0, DED1)	(DE40, DED1)	(DEE0, DE40)	
18	(ITH1,ITH5)			
19	(ITH5,ITC4)			
20	(ITI4,ITF2)	(ITF3,ITI4)	(ITF3, ITF2)	
21	(ITF3, ITF5)			
22	(ITF6,ITG1)			
23	(CZ01,CZ06)	(CZ01, CZ04)	(CZ04, CZ03)	(CZ03,CZ06)
24	(PL41, PL61)			
25	(PL81,PL91)	(PL91, PL71)	(PL72, PL81)	(PL71, PL91)
26	(HU32,HU11)	(HU33,HU32)	(HU33,HU11)	
27	(RO21,RO31)	(RO12,RO31)	(RO12,RO21)	
28	(BG33, BG34)	-		
29	(BG34,BG42,BG41)			

Table 20: NUTS 2 areas within each natural gas network cycle

D Experiment design

This section groups three Appendices containing a further investigation of demand, supply and geopolitical uncertainties introduced in section 4.2 and summarized in section 4.4.

D.1 Demand uncertainties

Section 4.4 highlighted demand uncertainties as an important category of uncertainties to the development of hydrogen in Europe. This Appendix further elaborates on the uncertainties in this category. The critical uncertainty to hydrogen demand in transport is the share of hydrogen vehicles in the total fleet. To retrieve the range of plausible values, the share of hydrogen vehicles in the total vehicle fleet is modelled through a Multinominal Logit (MNL) model. This method is often applied to model decisions of individual consumers based on vehicle preferences [127], [185]. The model presents a choice between three vehicle types: FCEVs, BEVs and ICEVs. The probability of consumer i choosing alternative j is based on the relative utility of the alternatives:

$$P(x = a_i) = \frac{e^{U(a_i)}}{\sum_{j=1}^3 e^{U(a_j)}}$$

 $j \in \{FCEV, BEV, ICEV\}$

In turn, the total utility is determined based on the Willingness To Pay (WTP) to pay for the vehicle's characteristics. WTP is used to define a singular scale on which the various characteristics can be expressed and compared. A total of five vehicle characteristics are included:

$$U(a_i) = \sum_{a=1}^{5} WTP_a$$

 $a \in \{Capital, Fuel, Range, Refuelling, Environmental\}$

These characteristics have been selected based on a review of various choice experiments [126], [127], [185]. Table 22 highlights the WTP values utilized. Because the purchase price is measured in present Euros, the WTP is equal to the marginal utility of of a Euro of income, which is assumed to be 1.

Parameter	Unit	Willingness to pay	Sources
Capital cost	EUR	-1	-
Fuel cost	EUR/100 km	-433.84, -1055.74	[128], [127]
Charging time	EUR/min	-182, -193.85	[126], [127]
Refuelling stations			
Detour time	EUR/min	-234	[126]
Fuel availability	%	249	[127]
Range	$\mathrm{EUR/km}$	19, 19.64	[126], [127]
Environmental performance			
CO ₂ emissions	g/km	-36.70	[128]
CO2 emissions	%	28.64	[127]

Table 21: Willingness to pay utilized in MNL model

It is assumed that an investment decision takes place at the start of each year. The new sales for each of the alternatives equals the probability of consumers choosing that alternative times the total sales:

$$S_i = P(x = a_i) * TS$$

The total sales equals the existing fleet times the ratio of new sales to the total fleet:

$$TS = TF * RS$$

The total number of vehicles declared end-of-life equals the total new sales minus the product of the total fleet and the fleet's growth rate:

$$TEOL = TS - (TF * GR)$$

It is assumed that the end-of-life vehicles in each segment are proportional to the existing market share of each segment. As a result, the number of vehicles in each segment in a given year equals the number of vehicles in the previous year plus the number of new vehicles minus the end-of-life vehicles:

$$TV_{jt} = TV_{jt-1} + S_{it} - EOL_{it}$$

Based on this conceptualisation, the diffusion of hydrogen vehicles in the transport sector can be determined with data on the relative performance of the various alternatives on the various criteria. This research utilizes the data provided by Senkpiel, Berneiser and Baumann [125]. For each alternative, a starting value and learning rate is determined per characteristic, both for a worst and best case. Please refer to Table 22 and 23 for the starting values and learning rates utilized.

Table 22: Starting values used per vehicle type and characteristic in MNL model

	FCEV		ICEV		BEV	
	min	max	min	max	min	max
Capital cost	65400	76800	26969	35983	28714	39130
Fuel cost	5.45	9.5	6.48	9.72	3.57	5.14
Range	658	428	1996	1196	328	260
Refuelling time	5	5	2	2	30	10
Detour time	20	30	5	15	0	0
CO2 emissions	0	266	163	205	0	76

Table 23: Learning rates used per vehicle type and characteristic in MNL model

	\mathbf{FC}	EV	IC	EV	BEV	
	\min	\max	\min	max	\min	max
Capital cost	1.70%	1.90%	-0.20%	-0.20%	0.4%	0.4%
Fuel cost	0.32%	1.20%	0.40%	0.80%	0.2%	0.5%
Range	0.60%	0.60%	0.00%	0.00%	2.2%	2.4%
Refuelling time	0.00%	2.50%	0.00%	0.00%	0.00%	6.00%
Detour time	2.00%	2.50%	0.00%	0.00%	0.00%	5.00%
CO2 emissions	0.00%	0.00%	1.00%	2.00%	0.00%	0.00%

Figure 88 shows the output of the model. In the left illustration, the upper limit of the uncertainty space is mapped by taking the best case values for hydrogen vehicles and the worst case values for BEVs and ICEVs. Alternatively, the right illustration portraits the lower limit of the uncertainty space, where the worst case values are taken for hydrogen vehicles while the best case values are applied to BEVs and ICEVs.



Figure 88: Market share of each vehicle type in best (left) and worst (right) case.

In built environment, the key uncertainty is the share of dwellings that utilize hydrogen based applications for heating purposes. To estimate the uncertainty space of this parameter, the results of three studies have been combined. Sgobbi et al. [38] estimated the application of hydrogen in this sector through the JRC-EU-TIMES model. Additionally, a collaboration of 17 companies under the name Hydrogen Europe also published an estimation [117]. Lastly, an estimation by the Oxford Institute for Energy Studies is considered [186]. The uncertainty space following from these estimations is shown in Figure 89.



Figure 89: Uncertainty space of market share hydrogen applications in built environment.

The decline for refining demand, as shown in Figure 90, is based on the BP Energy Outlook 2020 and IEA 2021 Oil Analysis [118], [187]. Similarly, the demand for ammonia and methanol is based on forecasts of the International Energy Agency [188]. As conclusive data on the development of these chemicals is missing, their uncertainty spaces have been chosen conservatively.



Figure 90: Uncertainty space of demand change refining, ammonia and methanol towards 2050.

The dependence on externally produced hydrogen is an uncertainty for which no direct data is available. As such, an estimation is made based on the relative expected share of green hydrogen since sustainable hydrogen production is likely to be located outside of industrial clusters. BP [118] forecasts that the share of green hydrogen is circa 20% and 50% in 2030 and 2050. Nevertheless, it is also uncertain how this relates to the production specific for industrial demand. As such, this research utilizes a conservative uncertainty space with 0% as the minimum and 10%, 20% and 30% as the maximum in 2030, 2040 and 2050 respectively.



Figure 91: Uncertainty space of industry dependence on external hydrogen as share of total.

As highlighted in section 3.2, interaction effects exist between existing infrastructure and future demand. Specifically, this research incorporates these effects on a national basis, in accordance with the values illustrated in Table 24. This implies that all demand values of Member States featuring one or more pipeline connections in a previous time step will be increased by the illustrated percentages.

	2030	2040	2050	
Demand increase	10%	15%	20%	

D.2 Supply uncertainties

As illustrated in section 4.4, supply uncertainties represent as an important category of uncertainties to the development of hydrogen in the European Union. This Appendix further elaborates upon the uncertainties in this category. In this research, four hydrogen production methods are considered: steam methane reforming (SMR) and electrolysis combined with nuclear, solar and wind energy. The methodology to determine the share of each production method differs per exploration. For more information on these explorations, please refer to section 4.4. In the broad exploration, the share of each production method is determined by drawing four random numbers that together add up to 100. Figure 92 gives an indication of the relative production share for each method over 5000 rolls. On average, this results in a 25% share for each production method. Now, this assumes a broad number of plausible futures as the share of each production method theoretically lies between 0% and 96%.



Figure 92: Probability distribution of production share for each production method.

In the targeted exploration, a more focused approach to production shares is applied. This is based on the expected ratio of sustainably produced green hydrogen and fossil-based blue and green hydrogen published by BP [118]. Table 25 illustrates the uncertainty ranges utilized. Note that the range described for green hydrogen implies the sum of hydrogen production from nuclear, solar and wind energy. To this end, three values are randomly drawn that together add up to 100 minus the value for grey and blue hydrogen. This assures that sum of all production shares equals 100.

Table 25: Production bounds per production method in targeted exploration.

	2030	2040	2050
Grey + blue hydrogen	70 - 100%	60 - 90%	40 - 70%
Green hydrogen	0 - 30%	10 - $40%$	30 - $60%$

D.3 Geopolitical uncertainties

Section 4.2 highlighted geopolitical uncertainties as an important category of uncertainties to the development of hydrogen in Europe. With respect to the geopolitics of hydrogen, two uncertainties are of importance: the number of importers and the import share. Now, as every European Member State has the potential to produce hydrogen, import-export roles are less clear than in the world of fossil energy [169]. As such, this research applies a wide range with respect to the number of exporters, shown in Table 26. This excludes relatively extreme cases where almost all Member States are either importers or exporters.

Table 26: Uncertainty space number of importers and import share

	2030	2040	2050
Number of importers	6 - 18	6 - 18	6 - 18
Import share	25 - $75%$	25 - $75%$	25 - $75%$

Figure 93 highlights the current energy import dependency of European Member States. This highlights that import dependencies can widely vary between nations. As such, this research assumes that Member States assigned as import nations feature an import share between 25% and 75%. Similar to the number of importers, a wide range is assumed to compensate for the relatively scarcity of information on these uncertainties.



Figure 93: Energy import dependency of European Member States.

Section 4.2 highlighted two vital geopolitical uncertainties related to the reassignment of natural gas pipelines. The reassignment probability implies the odds of a Member State opening up its natural gas network to reassignment. Next, the share of a Member State's total cycles that is reassigned is dictated by the reassignment share. Please refer to section 4.2 for more information on the reassignment of network cycles. Now, although direct data on these uncertainties is lacking, an estimation can be made based on the relative change of demand for natural gas in the European Union. Figure 94 illustrates the uncertainty space of this development based on estimations by the IEA [187] and BP [118]. Based on the trend of this uncertainty space, the reassignment probability and reassignment share are chosen relatively conservatively in 2030 and increased towards 2040 and 2050.

Figure 94: Trajectory of natural gas demand in Europe



Table 27 highlights the uncertainty space utilized to map the reassignment probability and reassignment share.

Table 27: Uncertainty space reassignment probability and reassignment share

	2030	2040	2050
Reassignment probability	0 - 20%	0 - $33%$	0 - $50%$
Reassignment share	0 - $20%$	0 - $40%$	0 - 60%

D.4 Exploration designs

Section 4.4 highlighted this research utilizes three explorations to analyse the development of a hydrogen pipeline infrastructure in Europe. Specifically, it described that the targeted exploration deviates from the broad exploration by identifying three categories of Member States: front-runners, middle of the pack and laggards. Table 28 highlights the categorization utilized and the percentage with which all demand values are altered per category and time step. This categorization is made based on the current efforts of Member States to develop national hydrogen strategies and set hydrogen related targets. This is based on a study of Hydrogen Europe [171].

Table 28: Design targeted exploration

Member State	Category	2030	2040	2050
Netherlands				
France				
Spain	Front-runners	20%	30%	40%
Portugal				
Germany				
Italy				
Austria				
Slovakia				
Poland	Middle of the pack	0%	0%	0%
Sweden				
Romania				
Greece				
Belgium				
Bulgaria		-10%	-15%	-20%
Czechia				
Denmark				
Estonia				
Croatia	Lommonda			
Latvia	Laggarus			
Lithuania				
Luxembourg				
Hungary				
Slovenia				
Finland				

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