Modelling Ammonia-Based Hydrogen Network Development Using a Threshold and Optimization Approach

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TU Delft – MSc Complex Systems Engineering and Management

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Acknowledgements

Dear reader,

This report represents the conclusion of my master thesis from my master Complex System Engineering and Management at the Delft University of Technology.

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Modelling Ammonia-Based Hydrogen Network Development Using a Threshold and Optimization Approach

by

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Executive Summary

The decarbonisation of industrial clusters is a key priority for achieving Europe's climate targets for 2040 and 2050 [49]. Hydrogen is expected to play a central role in this transition, however, large-scale infrastructure planning remains highly uncertain [29]. As European nations navigate competing demands between defence expenditure and environmental commitments, industrial clusters must pursue efficient investment strategies to avoid stranded assets or costly delays. Project developers face the challenge of aligning firm-level investments with long-term infrastructure objectives. Existing models do not adequately capture how adoption spreads among firms through interdependencies, nor how these dynamics shape the development of hydrogen infrastructure over time [39] .

This study aims to simulate the development of hydrogen infrastructure in industrial clusters by integrating firm-specific characteristics, interdependencies, and investment decisions with network development over time. It addresses the central question of how individual firm attributes and interdependencies influence the rollout of hydrogen infrastructure, using the Port of Rotterdam as a representative case study.

To address this question, a dynamic modeling framework was developed that combines a threshold logic adoption model with the Optimal Network Layout Tool (ONLT) to simulate how infrastructure evolves over time. Firm level data, including hydrogen trade volume, grid capacity, and plot size, were normalized and incorporated into the model to represent how adoption spreads among firms with different characteristics. This method allows for scenario analysis under varying levels of hydrogen demand and ammonia import, making it possible to identify network segments that are robust across uncertain futures. The approach improves significantly on static planning models, which often overlook behavioral dynamics among firms in industrial clusters.

Results show that adoption dynamics are shaped by a combination of firm-specific characteristics, interdependencies, and the configuration of early adopters. Strategic hubs such as Air Liquide and Eneco emerged across multiple scenarios, highlighting their importance in accelerating network development. In contrast, late adoption by firms like Air Products often resulted in inefficient, long, and costly connections. Moreover, the low hydrogen demand scenarios frequently led to fragmented sub-networks within the industrial cluster, whereas high demand scenarios supported more cohesive, highly interconnected, and cost-effective layouts. Across all scenarios, a set of robust network segments was identified that consistently appeared under different conditions. These segments are critical for guiding infrastructure planning, as their repeated occurrence suggests a lower risk of becoming stranded assets, and can potentially function as a backbone in the industrial cluster..

The developed framework provides project developers, such as Power2X, with a scalable decision-support tool to inform coordinated infrastructure planning. It highlights where early investments can accelerate broader adoption and offers a means to evaluate hydrogen infrastructure opportunities across various industrial clusters. By identifying strategic early adopters and robust network segments, the model enables investment strategies that minimise cost and support more efficient decarbonisation pathways aligned with pressing climate objectives.

In conclusion, this modelling approach offers valuable insights into network development and is applicable across multiple industrial clusters. Power2X can apply the same criteria and methodology to other clusters by incorporating the appropriate firm-level data, industrial layout, and spatial context. This enables the simulation of alternative adoption pathways and the identification of robust network segments in clusters with different characteristics.

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Introduction

1.1 Background

In recent years, climate change has become one of the most urgent challenges facing societies worldwide. Global awareness and the need for decarbonization are driving a fundamental transformation across all sectors, especially the energy and industrial sectors [34]. Climate targets such as the European Union's 90 percent emissions reduction goal for 2040 are rapidly approaching [49]. However, European nations face increasing challenges in maintaining decarbonisation priorities amid shifting global agendas that threaten progress. Although the 2040 targets underscore the urgency of action, governments are increasingly redirecting resources toward defence and security in response to ongoing conflicts, often at the expense of climate efforts. This has contributed to a weakening of climate policies and highlights the growing need for efficiency in resource planning. To meet decarbonisation goals, a targeted and cost effective strategy is essential within the constraints of limited time and budget, to prevent misaligned investments and ensure that all measures contribute meaningfully to long term climate objectives [49].

In 2019, annual global carbon dioxide (CO_2) emissions reached 34.2 gigatonnes (Gt), largely due to the extensive and unrestricted use of fossil fuels to meet approximately 80% of the world's energy demand, which stood at around 585 exajoules (EJ) per year [34]. These concerns are particularly pressing given the current rate of population growth and associated increases in energy consumption. It is projected that global energy demand will increase by at least 50% by 2050 [34]. In practical terms, this means that in 25 years, the world will require at least 875 EJ annually, equivalent to adding the current energy use of the entire United States and China combined [34]. As the global energy system transitions to renewable electricity, one of the key challenges is the efficient transmission and storage of this energy. This has led to a growing need for energy carriers, which are substances capable of storing and releasing renewable energy, particularly for use in hard-to-abate sectors.

In response, international agreements such as the Paris Agreement have set targets like achieving net-zero greenhouse gas emissions [53]. To meet these goals while minimizing environmental impacts, the large-scale deployment of low-carbon renewable energy sources is essential. Within this evolving energy landscape, hydrogen (H_2) is gaining significant momentum [6]. In recent years, hydrogen has become a focus point in many economic and political strategies [6]. As a carbon-free energy carrier, hydrogen offers a promising pathway for decarbonizing the energy and industrial sectors [6], especially since it does not produce CO_2 emissions when used for heat or electricity.

Hydrogen has the potential to replace conventional fossil fuels such as natural gas and oil, thereby reducing carbon emissions. This is particularly relevant in hard-to-abate sectors like the chemical industry, petroleum refining, steel production, and heavy transport [62].

Hydrogen is typically classified into three types based on its production method:

1. **Grey hydrogen:** produced from hydrocarbons without carbon capture,

2. **Blue hydrogen:** grey hydrogen with integrated carbon capture,

3. **Green hydrogen:** produced via water electrolysis powered by renewable electricity.

Currently, the majority of hydrogen production (62%) comes from natural gas through steam methane reforming [62]. To better illustrate the distinction between the different hydrogen production methods and their relative environmental impact, Figure 1.1 provides an overview of the technological shift from the conventional production method towards the sustainable hydrogen production routes. The figure highlights the feedstocks, processes, and CO_2 implications associated with each method.

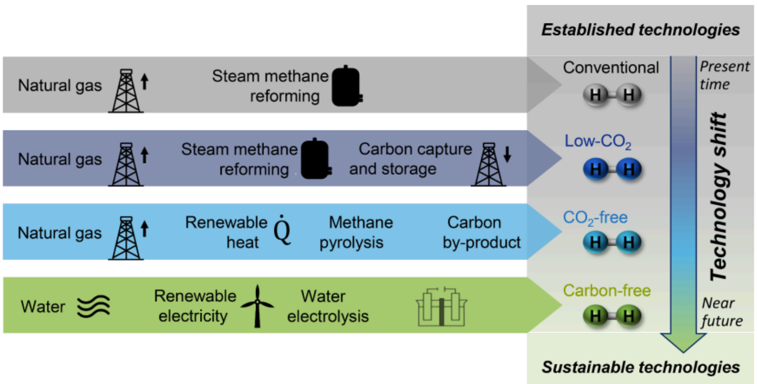

Figure 1.1: Common differentiation of hydrogen production pathways. Source: [20].

More than 100 countries have now set net-zero carbon emissions targets, requiring technological innovation in heavy industries such as oil and gas. Hydrogen is increasingly seen as a critical component in this transition. Investments in hydrogen infrastructure and low-emission hydrogen projects are rising globally [62], primarily because hydrogen offers long-term solutions for decarbonizing oil and gas operations.

Specifically, green hydrogen can be used in:

- Refinery hydrotreating units,

- Space heating (as a natural gas replacement),

- Steam generation for thermal processes,
- Fuel for transportation (e.g., trucks, rail, and marine vessels in the oil and gas sector).

However, while hydrogen offers many opportunities, it also presents significant challenges, particularly in storage and transport. One major issue is its low volumetric energy density under ambient conditions [35], making it difficult to store and transport large quantities efficiently [51]. To increase density, hydrogen can be compressed or liquefied [35], but both methods are energy-intensive and expensive. For example, hydrogen liquefaction requires more than 45% of the energy stored in the hydrogen itself, resulting in considerable energy losses [35].

Scaling up hydrogen production also raises infrastructure challenges. Although existing natural gas pipelines offer some potential, converting them to transport pure hydrogen requires significant modifications [62].

To overcome these challenges, hydrogen carriers are being developed as alternative solutions for storage and transport [51]. A hydrogen carrier is a substance or method used to store and transport hydrogen more efficiently. These carriers are specifically designed to mitigate the difficulties of handling pure hydrogen, such as energy losses and low density. The core idea is to store hydrogen within another substance that is easier and more energy-efficient to handle [35].

Within the energy sector, two primary types of hydrogen carriers have emerged:

1. Liquid Organic Hydrogen Carriers (LOHCs): where hydrogen is chemically bound to a liquid molecule through hydrogenation.
2. Ammonia (NH_3): which has a high hydrogen content and energy density. When decomposed, ammonia yields hydrogen and nitrogen, with no CO_x emissions, making it advantageous for hydrogen purification [51].

Table 1.1 compares ammonia with LOHCs, highlighting its advantages in terms of volumetric density, storage conditions, and energy efficiency.

Table 1.1: Comparison of Hydrogen Carriers by Key Properties

Property	**Ammonia (NH_3)**	**LOHC**
Hydrogen content (wt%)	17.6%	˜6%
Volumetric density ($g\,L^{-1}$)	120	˜50–60
Storage temperature	-33 °C	Ambient
Liquefaction energy loss	Low	Medium

One of the most promising hydrogen carriers is ammonia, which can be synthesized using renewable electricity and nitrogen. This synthesis occurs through the Haber-Bosch process. Ammonia can be transported using existing infrastructure and later be converted back into hydrogen. Figure 1.2 illustrates the ammonia to hydrogen supply chain.

Hydrogen is first produced from renewable electricity through water electrolysis. It is then combined with nitrogen to produce ammonia. After transportation, hydrogen will be released from ammonia through a thermal cracking process, after which it can be used for end-use applications.

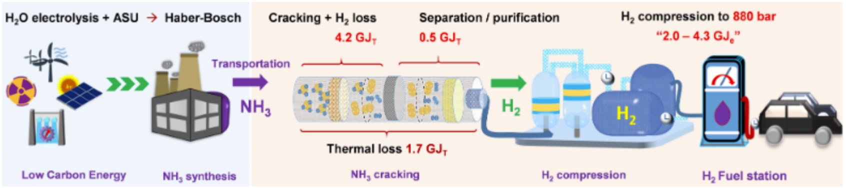

Figure 1.2: Schematic overview of ammonia as a hydrogen carrier[7].

Essentially, hydrogen carriers act as a bridge technology, enabling the transport of hydrogen from remote production sites (with abundant renewable energy) to demand centers. This makes the decarbonization of hard-to-abate sectors more feasible and economically viable [35].

Industrial clusters often serve as strategic locations for deploying ammonia-based hydrogen infrastructure. These clusters typically contain a high concentration of energy-intensive industries, which are major sources of greenhouse gas emissions and are difficult to decarbonise. In addition, their dense spatial configuration enables the development of shared infrastructure, such as pipelines and storage facilities. This density creates opportunities for economies of scale, making the adoption of hydrogen carriers such as ammonia more feasible and cost-effective.

The Rotterdam Industrial Cluster (RIC) provides a concrete example of such a setting. With its concentration of hard-to-abate industries, large port access, and existing energy infrastructure, the RIC illustrates both the challenges and opportunities involved in developing an ammonia-based hydrogen network. Chapter 4 will elaborate further on the specific case of the Rotterdam Industrial Cluster. In this study, an ammonia-based hydrogen network refers to a hydrogen pipeline system supported by nearby ammonia infrastructure, such as import terminals, storage tanks, and cracking units. This infrastructure enables the conversion of imported ammonia into hydrogen. Although ammonia is used as a carrier for international transport and storage, only hydrogen flows through the pipeline network. While the analysis focuses on the Rotterdam Industrial Cluster (RIC), the modelling approach and key insights are broadly applicable to other industrial clusters. Throughout this thesis, the term hydrogen infrastructure or hydrogen network is used to refer to both hydrogen systems and ammonia based hydrogen infrastructure, unless stated otherwise.

1.2 Ammonia as Hydrogen Carrier and its Role in Industrial Cluster Decarbonization

While the technical feasibility of using ammonia as a hydrogen carrier is well established, the deployment of hydrogen infrastructure depends critically on firm-level decision-making within industrial clusters. Firms are interdependent: many hesitate to invest in hydrogen or ammonia-related assets in the absence of supporting infrastructure, while infrastructure development is often delayed until there is sufficient certainty regarding hydrogen demand and ammonia import volumes [46, 10]. This strategic uncertainty and mutual dependence can lead to hesitation, thereby slowing the adoption and development of hydrogen infrastructure.

Consider a storage company evaluating the construction of an ammonia cracker at its site within an industrial cluster. This investment involves substantial capital expenditure and is only viable if sufficient volumes of imported ammonia are available [13]. At the same time, import terminals are unlikely to commit to constructing large-scale ammonia facilities without a guaranteed level of demand. Although both parties have an interest in proceeding, each waits for the other to act first. This results in stalled progress, even when the collective benefits are clear.

This coordination problem is common in the development of shared infrastructure systems, such as hydrogen pipeline networks, import terminals, and storage facilities. These assets require high upfront investment and depend on the participation of multiple actors to ensure economic viability. As no more firms become involved, the risk increases that early investments may become stranded or that infrastructure will be underutilised [22, 8]. This further discourages firms from taking the first step. Yet, such shared infrastructure is essential for enabling the energy transition in industrial clusters.

Without sufficient coordination or intervention, the dynamics between firms in an industrial cluster can lock the system into a low-investment equilibrium. When firms postpone investment due to strategic uncertainty, the cluster may fail to build momentum toward large-scale adoption [14]. This can ultimately delay the energy transition and the decarbonisation of industrial clusters, even when the technical readiness of ammonia as a hydrogen carrier is well established [39]. In such cases, clusters risk becoming locked into existing fossil fuel-based infrastructure pathways. Understanding these dynamics requires models that account for firm-level interdependencies and how infrastructure emerges from decentralised investment decisions.

To better understand this coordination problem, it is essential to analyse the actors involved, along with their incentives, roles, and constraints. The next section outlines how different stakeholders and their objectives influence the development of infrastructure within industrial clusters.

1.3 Stakeholders and Design Objectives in Industrial Clusters

Addressing this coordination challenge requires a clear understanding of the key stakeholders, the factors that drive their decisions, and the extent to which their objectives align or conflict in shaping hydrogen infrastructure development. As noted earlier, the development of hydrogen infrastructure in industrial clusters involves a complex interplay of decisions made by multiple stakeholders, each with distinct objectives and constraints. This stakeholder analysis clarifies the assumptions underlying infrastructure design objectives, including cost efficiency and robustness under uncertainty.

Each actor brings distinct priorities, and their interactions shape both the constraints and opportunities for system development. The key stakeholders are listed in Table 1.2 [31]. Industrial firms, including hydrogen suppliers and consumers, primarily seek affordable, reliable, and low-carbon energy while minimising investment risk [10]. Infrastructure operators, by contrast, focus on the long-term viability of their assets and require sufficient and stable demand to justify capital-intensive investments. The port authority oversees infrastructure within the cluster and facilitates development to sustain economic competitiveness and meet decarbonisation targets. In addition, various levels of government are involved in setting policy, regulating markets, and offering incentives. Finally, local communities influence the development process through concerns related to safety, environmental impacts, and spatial planning. Each of these stakeholders operates under a different set of priorities, which shapes the governance and design of hydrogen infrastructure.

Table 1.2: Overview of Key Stakeholders and Their Objectives

Stakeholder	**Primary Objectives**
Industrial firms (e.g., refineries, chemical producers)	Secure affordable, reliable, and low-carbon energy; minimize investment risks.
Infrastructure operators (e.g., pipeline or terminal owners)	Ensure long-term asset viability and cost recovery; require sufficient and predictable demand to justify investments.
Cluster and port authorities (e.g., Port of Rotterdam)	Maintain cluster competitiveness; facilitate decarbonization through coordinated planning and infrastructure provisioning.
Government bodies (national/regional)	Meet climate goals, reduce emissions, and ensure energy resilience; provide regulation, incentives, and public funding.
Local communities and civil society	Influence political acceptance; raise concerns about safety, environmental impact, and spatial planning.

Based on the interests of these stakeholders, several key design objectives can be identified. These objectives represent the criteria that any hydrogen infrastructure must meet to be considered viable [31]. Table 1.3 summarises these objectives and explains how they inform the design and evaluation of hydrogen networks. Together, they help explain what a successful outcome looks like for an industrial cluster. Given the high upfront capital investments, cost efficiency is a central design objective. A viable network must minimise both capital expenditure and operational costs to reduce investment hesitation among firms. As hydrogen demand is expected to increase over time, the infrastructure must also support incremental expansion to accommodate future needs. In addition, the network must demonstrate robustness under uncertainty by performing consistently across a range of plausible future scenarios, particularly in the context of fluctuating import volumes and variable demand. To address the coordination challenges discussed earlier, the network should enable sufficient utilisation and distribute investment risks across multiple stakeholders. Finally, to align with the concerns of local communities and civil society, the infrastructure must achieve environmental and spatial acceptability by limiting negative impacts on surrounding areas.

Table 1.3: Design Criteria for Hydrogen Infrastructure

Criterion	Description
Cost-efficiency	The network should minimize capital expenditure and operating costs to reduce investment hesitation and enable competitive energy pricing.
Scalability	Infrastructure must be able to expand over time to accommodate growing demand and changing technology without requiring complete redesign.
Robustness under uncertainty	The network must perform well across a range of future scenarios, especially in the face of fluctuating import volumes and adoption rates.
Utilization and risk-sharing	The system should be used sufficiently by multiple actors to avoid stranded assets and enable shared ownership or funding.
Network connectivity	The infrastructure should result in a cohesive network with minimal fragmentation. High connectivity improves efficiency, supports risk-sharing, and reduces the likelihood of isolated or underutilized segments.

This study focuses exclusively on the behaviour of firms within an industrial cluster, as their investment decisions are likely to influence both other firms and the development of hydrogen infrastructure. While the roles of governments and local communities are recognised as important, they are treated as contextual factors rather than dynamic actors within the modelling framework.

1.4 Problem Statement

1.4.1 Limitations of Centralized Models in Capturing Firm-Level Dynamics

This coordination problem reveals a deeper scientific gap in existing infrastructure models, which are not well equipped to capture the complex interdependencies and behavioral dynamics within industrial clusters. The current energy infrastructure models take a centralized and static approach, focusing instead on cost minimization or achieving a supply-demand equilibrium under different scenarios.

While this is suitable for macro-level studies, it fails to represent how the strategic decision-making of individual companies influences other firms under interdependency and uncertainty [5]. Most of these studies rely on fixed firm behavior or top-down planning logic, which overlooks the complexities of decision-making, meaning future conditions are predefined rather than emerging from interactions in the model. They typically depend on a fixed set of scenarios, reinforcing their centralized, static structure [39].

Such an approach is particularly inadequate under uncertainty, which characterize the energy transition. Fixed scenarios provide little actionable insight for robust infrastructure investment, especially in industrial clusters, where infrastructure is shared and inter-firm coordination is essential. In the absence of a model that captures interdependencies and peer influence among firms, infrastructure plans that appear optimal on paper may lead to misaligned investments and delayed development. To address this, modelling approaches must be extended to incorporate the strategic behaviour of firms as they respond to one another over time.

1.4.2 Real World Systems Dynamics

Bridging this gap requires recognizing how infrastructure investments occur in practice and how such infrastructure develops over time. Investment decisions, particularly in energy systems, unfold gradually and are shaped by expectations, interdependencies, and mutual influence. These decisions often consider horizons of up to 40 years, which makes early-stage uncertainty highly consequential [13]. In the Rotterdam Industrial Cluster (RIC), firms do not act independently. Their investment strategies influence, and are influenced by, those of other firms, resulting in a dense network of mutual dependencies and uncertainties. Individual firms often cannot anticipate how their decisions are conditioned by others in the cluster [10].

As previously illustrated, a company may postpone investment in a large-scale ammonia cracker if future ammonia import volumes remain uncertain [13]. Similarly, renewable infrastructure projects are typically developed on a project-to-project basis [22]. This practice, where each project is treated as a separate investment decision rather than part of a coordinated long-term strategy, introduces significant risk. When too few projects are initiated, the result can be underutilized infrastructure and a increased risk of stranded assets due to the high upfront capital requirements [22]. Traditional models often overlook these interdependent dynamics within industrial clusters [8]. Since the developments in renewable energy are rapidly increasing, it is essential to incorporate these nonlinear relationships in current energy models [8].

1.4.3 Case Context: Power2X

Power2X is a consultancy and project developer specialising in green molecules, with a strong focus on enabling the energy transition in industrial contexts. As the host organisation for this research, Power2X plays a dual role. First, it provides insights into firm behaviour and interdependencies within industrial clusters involved in decarbonisation, based on its advisory experience. Second, the company actively invests in large-scale decarbonisation projects across multiple industrial clusters worldwide, including initiatives related to hydrogen, ammonia, and pipeline networks.

Operating at the intersection of strategy and execution, Power2X combines a deep understanding of technical feasibility with practical knowledge of coordination challenges, regulatory environments, and infrastructure planning. This perspective is particularly relevant to the topic of this thesis, which examines the development of hydrogen pipeline networks shaped by decentralised investment decisions within industrial clusters.

1.5 Research Objective

To address the limitations of existing infrastructure and energy models, this study's objective is to simulates how firm-level investment decisions unfold under conditions of uncertainty and interdependence, and how these decisions influence the development of a cost-effective and robust hydrogen network within an industrial cluster.

To operationalise this objective, the study is guided by the following research question and sub-questions, which explore the mechanisms, outcomes, and design implications of an hydrogen network in industrial clusters.

1.6 Research Questions

To examine how the strategic investment decisions of firms shape the development of a hydrogen network in an industrial cluster, this research addresses the central question:

How do corporate interdependencies and investment decisions in ammonia infrastructure determine the optimal topology of a hydrogen pipeline network in industrial clusters?

To address this complex research question, the study is structured around four interrelated themes. Each theme captures a necessary component for understanding how decentralised firm behaviour influences infrastructure development. The sub-questions align with these themes, progressing from the identification of interdependencies and firm-specific attributes to their integration in network design, and finally to the assessment of external incentives. Together, these themes provide a comprehensive foundation for modelling firm interdependencies and the formation of hydrogen infrastructure under uncertainty.

1.6.1 Research Themes and Sub-Questions

Theme 1: Interdependency Mapping

Industrial firms do not make investment decisions in isolation. Their actions are highly interdependent and contribute to the complex coordination challenges inherent in shared infrastructure development. To simulate these dynamics, it is first necessary to map the interdependencies between firms and identify the firm specific attributes that shape these relationships. These attributes define how firms are connected within the social network, which reflects the structure of interdependencies, and they also inform each firm's individual threshold for investment.

Sub-question 1: Which company-specific attributes determine interdependencies and threshold values within Industrial Clusters?

Theme 2: Behavioral Dynamics

Building on the mapping of interdependencies and threshold values from Subquestion 1, Subquestion 2 focuses on capturing the behavioural dynamics of firms and examining how these interdependencies influence actual investment behaviour. Understanding these dynamics is essential for realistically simulating when and why firms choose to invest in hydrogen infrastructure [41].

Sub-question 2: How do threshold values and interdependencies impact firms' investment decisions?

Theme 3: Network Implications

The infrastructure network does not emerge independently, but is shaped by the investment decisions of firms within industrial clusters. This theme investigates how these decisions influence the development of the physical hydrogen infrastructure. Building on the outcomes of the threshold model, which simulates firm adoption over time, this theme connects firm level dynamics to spatial outcomes and examines how different adoption patterns translate into different hydrogen network topologies.

Sub-question 3: How do threshold model outcomes under different scenarios shape the optimal hydrogen pipeline layout?

Theme 4: Policy Sensitivity

The final theme focuses on policy sensitivity and examines how external policy instruments, such as subsidies or incentives, influence the development of hydrogen infrastructure in industrial clusters. Since firms operate under uncertainty, governments may introduce such measures to accelerate investment. These interventions can shape the pace and pattern of infrastructure development. In conclusion, this subquestion assesses which early adopter strategy leads to the most cost-efficient and robust network topology. In this thesis, the early adopter strategy refers to the selection of initial firms that are assumed to invest first. The choice of these early adopters influences the adoption dynamics and plays a critical role in determining the overall cost efficiency of the resulting hydrogen network.

Sub-question 4: How do external incentives (e.g., subsidies) influence firm behavior and network development?

1.7 Key Concepts and Definitions

To understand the dynamics analysed in this study and how they influence the network topology of hydrogen infrastructure in industrial clusters, it is essential to define a set of key concepts that are used throughout the analysis.

1.7.1 Investment Dynamics

Early Adopter

An early adopter refers to a firm that makes an initial investment decision in hydrogen infrastructure. This involves committing to become a future user or supplier of hydrogen by preparing the necessary infrastructure, such as securing a pipeline connection or constructing an on-site conversion unit like an ammonia cracker. Such a decision represents a formal commitment that enables network connectivity. Early adopters play a critical role in initiating network development and can influence the behaviour of other firms through their actions.

Threshold

In this study, a threshold represents the minimum level of external influence from neighbouring firms that must be present before a firm decides to invest [41]. Each firm is assigned an individual threshold based on specific attributes, including hydrogen trade volume, grid connection, plot size, and other relevant factors. These attributes are further detailed in Section 6.1. Thresholds are central to the diffusion model, as they determine how investment decisions spread through the network over time.

Tipping Point

A tipping point occurs when a sufficient number of firms have invested, causing adoption to accelerate rapidly across the network. More specifically, it refers to a critical moment when a small change, such as a single firm reaching its threshold, triggers widespread adoption throughout the network [33].

Cascasding Effect

In this study, a cascading effect refers to a chain reaction that describes the rapid and widespread changes unfolding in the network once a tipping point is reached. In the context of infrastructure, this means that initial investments by early adopters can reduce the thresholds of other firms, thereby initiating further rounds of investment [47].

Interdependency

Interdependency in industrial clusters means that a firm's investment decision depends on the decisions of others [47]. These relationships imply that firms do not act in isolation, but that their choices directly or indirectly influence those of other firms. This reflects a real-world coordination challenge, where firms are often unwilling to act first without sufficient assurance of future network use or demand.

1.7.2 Evaluation Criteria

Robustness

Finally, robustness is a key concept throughout this study. Robustness refers to the ability of a hydrogen pipeline network to perform well and retain its value across a wide range of uncertain future scenarios. A robust network performs consistently under uncertainty and reduces the risk of stranded assets [40].

Cost-Efficiency

In this study, cost efficiency refers to the objective of minimizing the total cost associated with the development of a hydrogen network. This objective serves to reduce investor hesitation, lower economic risks, and support competitive energy pricing.

Scalability

In this thesis, scalability refers to the ability of the hydrogen infrastructure to accommodate future expansion through the addition of late adopters, without requiring a complete redesign. This is assessed using a dynamic modelling approach that examines how new firms connect to the network over time and how the layout evolves. The analysis identifies whether the resulting network configurations are adaptable to continued growth.

Utilization and risk-sharing

Another design criterion concerns utilization and risk sharing, assessed by observing how many firms make use of specific pipeline segments. High-utilization segments typically form well-connected hubs within the network, where infrastructure is shared among multiple firms. These hubs enhance economic viability by lowering the risk of stranded assets. In contrast, more isolated segments tend to serve fewer users and may lead to less efficient outcomes.

1.8 Scope and Limitations

This section outlines the scope of the study and clarifies the key assumptions and limitations. These boundaries are necessary to ensure analytical focus and maintain the tractability of the model.

The study focuses specifically on hydrogen pipeline infrastructure supported by ammonia-based hydrogen carriers. Ammonia is selected due to its favourable properties, including high volumetric hydrogen density and ease of liquefaction [51]. While ammonia plays a critical role in the transport and storage of hydrogen, the study assumes that imported green ammonia is converted into hydrogen through a cracking process at local facilities. As such, the primary focus is on the optimal topology of the hydrogen pipeline network rather than the logistics of ammonia transport. Other hydrogen carriers and maritime shipping considerations are excluded from the scope.

The Rotterdam Industrial Cluster (RIC) is used as an illustrative case study due to its strategic location and industrial profile. While the focus is on the RIC, the study's dynamic modelling framework and resulting insights are generalisable to other industrial clusters facing similar coordination and infrastructure challenges.

Firms in the model are grouped by type and are assumed to behave homogeneously within each group. This means that all firms of the same type follow identical decision rules. An investment is defined as a firm's commitment to become a future hydrogen user by adopting the necessary infrastructure, such as securing a pipeline connection or installing an ammonia cracker. This commitment is critical, as it dynamically shapes the evolving hydrogen network over time.

Finally, the model operates under several important simplifications and limitations. It does not explicitly account for environmental permits, safety regulations, or complex spatial planning constraints that affect the construction of real-world pipelines. Government interventions, such as subsidies, are treated as external incentives that influence firm behaviour, rather than being modelled as detailed policy mechanisms. In addition, the model does not simulate real-time economic variables such as energy prices or global trade effects. Instead, it assumes that firms make investment decisions based solely on their static attributes.

1.9 Alignment with Complex Systems Engineering and Management

This study aligns with the MSc program in Complex Systems Engineering & Management (CoSEM), Energy track. Within this program, courses such as Engineering Optimization and Integrating Renewables in Electricity Markets (SEN1522), Sociotechnology of Future Energy Systems (SEN1541), and Design in Networked Systems (SEN124A) have equipped me with the skills to analyze and optimize ammonia pipeline networks while considering both physical and non-physical connections between stakeholders. These insights will guide this research in creating solutions to improve and better understand ammonia networks and accelerate the energy transition.

1.10 Research Outline

This study investigates how adoption dynamics and interdependencies among firms influence hydrogen network development within industrial clusters under uncertainty. It addresses the strategic challenge of coordinating firm level investment decisions, firm specific attributes, and infrastructure planning in an environment characterised by fluctuating demand and import scenarios. The adoption outputs from the threshold model were combined with a network optimisation tool (ONLT) to generate multiple cost optimal infrastructure layouts under different conditions. By simulating both firm level adoption and infrastructure development, the analysis identifies key adoption patterns and network outcomes, providing insights into robust network formations. Ultimately, this study contributes to a clearer understanding of strategic adoption behaviour, investment timing, the role of early adopters, and offers practical guidance for infrastructure planning under uncertainty.

2

Literature Review

2.1 Introduction

To address and understand the challenges in hydrogen infrastructure development in industrial clusters, particularly considering the connection with ammonia as a hydrogen carrier, a thorough review of the existing literature is essential. The global transition towards low carbon energy systems involves not only technological and economic factors but also the dynamic interactions of firm-level behavior [5]. In industrial clusters, shared infrastructure and interdependencies between firms further complicate infrastructure planning and investment dynamics. This literature review positions the research within a multidisciplinary field, identifies relevant knowledge gaps, and provides the theoretical foundation for the modelling approach applied in this study. Specifically, the study addresses a gap in the literature by integrating a threshold-based adoption model with spatial network optimisation tools. This integration enables a dynamic representation of how hydrogen infrastructure evolves in response to interdependent firm behaviour and uncertainty within industrial clusters.

This chapter is organized thematically, focusing on several core concepts that are central to this study, focusing first on the current state of research into the ammonia infrastructure, and specifically into its integration into broader hydrogen networks. It then assesses energy system modeling approaches and highlights their limitations in representing firm-level investment behavior and infrastructure interdependencies. The review then discusses the theoretical and methodological contribution of a threshold model in analyzing cascading adoption behavior. This approach supports a more realistic illustration of how investment decisions unfold over time and influence the development of a hydrogen pipeline network in industrial clusters. Finally, this section reviews literature on network optimization tools, like graph theory, minimum spanning trees, and mixed integer linear programming models, which connect the threshold model with infrastructure layout.

In addition to reviewing the existing knowledge and identifying the current gaps in the literature, this chapter also functions as a theoretical framework for this study. It bridges the gap between real-world observations and existing modeling approaches and supports the development of a new framework that combines the behavioral dynamics of companies in industrial clusters with network planning of hydrogen pipelines.

2.2 Search Strategy

This section outlines the systematic approach used to identify and select relevant literature for this review. This ensures transparency and reproducibility in building the theoretical foundation of this study.

The search strategy used in this literature review primarily focused on published literature from academic databases. The literature search was conducted primarily through Google Scholar due to its broad accessibility. Where relevant, other academic databases were used, such as Scopus or Web of Science. Additionally, expert knowledge from Power2x and industry documents were reviewed to include practice-based insights.

This search strategy mainly focuses on articles published between 2014 and 2025 to ensure relevance to hydrogen and ammonia infrastructure development, with one article from 1996 included for its theoretical framework based on graph theory, despite not focusing on hydrogen or ammonia developments. An overview of the articles and their publication years is shown in the figure below.

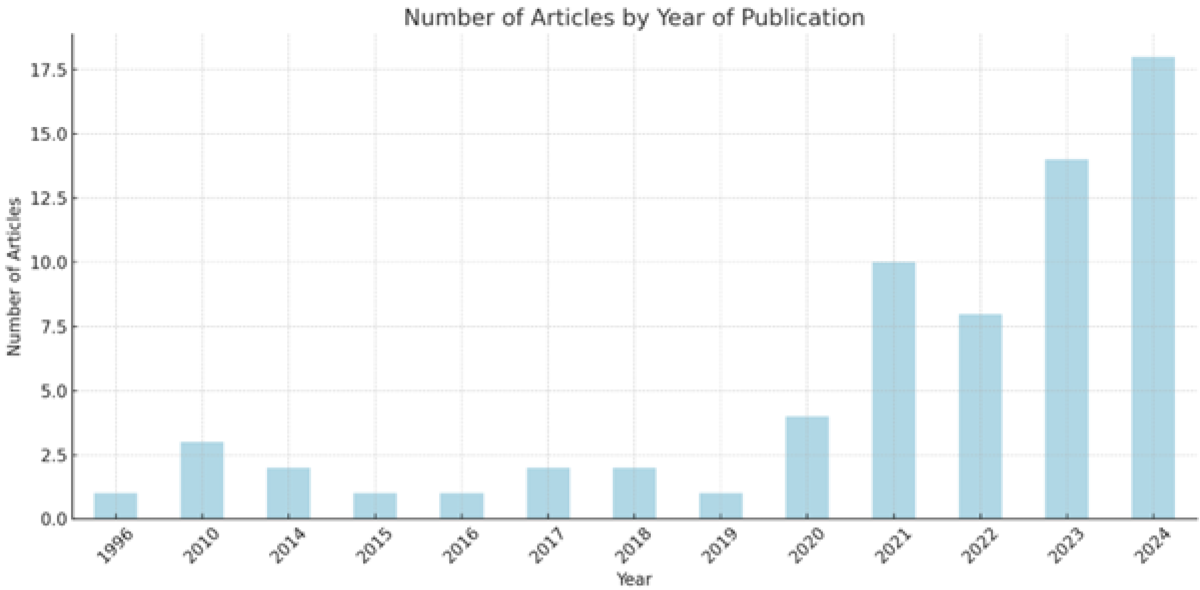

Figure 2.1: Article Year of Publication

The search terms were grouped into conceptual categories relevant to this study, including: ammonia, hydrogen, ammonia as a hydrogen carrier, pipeline infrastructure, hydrogen networks, infrastructure development, threshold, interdependencies, investment dynamics, cascades, and tipping points. Boolean operators such as AND and OR were used within these categories to generate relevant search results.

Eventually, this review included studies on ammonia and hydrogen supply chains, as well as specific research focused on firm interdependencies, shared infrastructure, and threshold-based adoption models, particularly those applied within industrial clusters. Studies were excluded if they focused solely on small-scale infrastructure pilots, on specific technologies, or lacked relevance to network development.

2.3 Thematic Analysis of Literature

2.3.1 Criteria

This section outlines the search criteria used to narrow down the literature and provide relevant context for the study. Six core criteria were defined based on the conceptual scope of the thesis. These criteria were selected to reflect the key concepts introduced earlier and to ensure alignment with the study's objectives. This structured approach supports both the relevance and comprehensiveness of the literature review.

Ammonia Infrastructure

This criterion supports the study's aim to understand how physical infrastructure components influence network development and investment patterns. In this research, ammonia infrastructure is defined as the various logistical components of the ammonia supply chain, from import to ammonia cracking. This includes, for example, large ammonia import terminals, storage solutions, and ammonia crackers. The objective of this study is to analyze how the interdependencies between companies influence their investment decisions in this ammonia infrastructure and how this affects the layout of a hydrogen network.. Relevant literature is needed to study the existing ammonia infrastructure within industrial and energy systems. A thorough understanding of these infrastructures will provide key insights that can contribute to the development of a possible ammonia infrastructure [10].

Ammonia as Renewable Hydrogen Carrier

The second criterion ensures inclusion of studies that recognize ammonia's role in long-distance hydrogen transport and its implications for supply-side network infrastructure [34]. However, other energy vectors offer distinct advantages over hydrogen as an energy carrier. Ammonia, in particular, demonstrates significant potential to play a key role in the energy transition, especially as a hydrogen carrier. Green ammonia is assumed to be imported into European ports in large volumes to supply the demand for green hydrogen [42]. Therefore, in this study ammonia is recognized as a renewable hydrogen carrier, which means that ammonia can be used as an efficient storage medium for hydrogen. This is mainly because ammonia (NH_3) has a high volumetric hydrogen density [25]. Furthermore, ammonia does not emit CO_2 when used as a hydrogen source, unlike hydrocarbons or alcohols [25]. Hydrogen will likely be produced in regions where renewable energy is inexpensive. It can then be efficiently stored and transported as ammonia to and in industrial clusters.

Pipeline Infrastructure

To capture the physical layout of the hydrogen network, this criterion emphasises the role of pipeline infrastructure in transporting hydrogen within industrial clusters. The focus of this study will be exclusively on pipelines as a form of infrastructure. The pipeline will primarily be used for the transport of hydrogen. At this moment, initial investments are being made, focusing on small-scale hydrogen. However, in the coming years, large-scale hydrogen pipelines will be required to support the growing demand [55].

Interdependencies

This criterion includes studies that examine how investment decisions are influenced by neighbouring firms, particularly within shared infrastructure contexts. These interdependencies may include economic, supply chain, and technical relationships between companies operating within industrial clusters.

Economic interdependencies arise from shared investments, competitive pressures, and market dynamics that affect the entire ammonia and hydrogen supply chain. Supply chain interdependencies involve the physical flow of ammonia and hydrogen between firms. Technical interdependencies refer to shared use of infrastructure, including ammonia cracking units and storage facilities.

A key challenge in this study is to define and categorise interdependencies based on firm-specific attributes and to assess how these relationships influence network dynamics.

Firm Behavior Modeling

This search criterion focuses on studies that apply threshold logic to model firm behaviour under uncertainty. Agent-based simulation models are also included, as they capture cascading investment dynamics in which the actions of one firm can trigger others to invest, thereby reducing their effective thresholds. By incorporating this criterion, the study moves beyond static and centralised modelling assumptions, offering a more realistic representation of infrastructure development in industrial clusters [54].

Network Optimization Approaches

The final criterion focuses on studies that apply network optimisation approaches, including graph theory, Mixed Integer Linear Programming (MILP), or related methods for designing efficient infrastructure. These approaches translate firm-level adoption behaviour into feasible and cost-effective pipeline network layouts.

2.4 Ammonia Infrastructure in Industrial Clusters

Ammonia infrastructure, including import terminals, cracking units, and storage facilities, plays a critical role in the decarbonisation of industrial clusters. This is particularly relevant in port-based clusters such as Rotterdam, where large volumes of ammonia are expected to be imported. A large body of literature focuses on the feasibility of ammonia as a hydrogen carrier. As stated by Negro et al. [34] and Chatterjee et al. [7], ammonia presents significant advantages for hydrogen storage and transport. Key benefits include its high hydrogen density, as it contains 17.8% hydrogen by weight. Furthermore, the volumetric hydrogen density of ammonia is almost 2.5 times higher than that of liquid hydrogen, allowing for more hydrogen storage per unit volume [26].

A second important advantage is that ammonia can be stored and transported under mild conditions, such as $-33\,^{\circ}\mathrm{C}$ and moderate pressure (~ 10 bar) [34]. However, most studies focus on techno-economic evaluations and do not model how ammonia infrastructure develops as part of a co-evolving hydrogen system within an industrial cluster [34]. This type of modelling remains underdeveloped. Existing studies rarely examine how firms coordinate their investments or how this coordination influences investment decisions in ammonia specific infrastructure.

The majority of these studies focus on small-scale projects, with limited investigations into large-scale industrial ammonia systems. A project is considered large scale if it involves multiple interconnected users, such as hydrogen consumers, storage providers, and import terminals, and supports flows of 100 to 1000 tonnes of ammonia per day. In addition, it requires substantial transport infrastructure, such as pipelines or import terminals, and involves the use of shared infrastructure. An overview of these articles and their scope is presented in Table 2.1. While ammonia is already widely used in the fertilizer and chemical industries, its growing potential as a hydrogen carrier is expected to increase its utilization [56]. Consequently, its adoption in large-scale energy systems presents several unresolved challenges that warrant further study [56].

The integration of ammonia into large hydrogen infrastructure networks is crucial for two main reasons: the growing demand for hydrogen, which will require large-scale infrastructure, and the economies of scale that can make large-scale systems more cost-effective. The import volumes of green ammonia are expected to increase rapidly, as its cost primarily depends on the availability and price of renewable energy [42]. Countries such as Spain, Portugal, Chile, and Australia have high renewable energy potential, making ammonia imports more cost-effective compared to domestic production. To accommodate large-scale green ammonia imports, dedicated terminals, storage facilities, and other infrastructure components will be necessary.

Additionally, while shipping logistics for ammonia transportation have been extensively studied, research on large scale pipeline networks that integrate ammonia into hydrogen systems remains limited [10]. According to Cui and Aziz [10], pipelines could potentially offer cost advantages over maritime transport, but their feasibility, economic benefits, and integration into existing energy systems remain underexplored. This study focuses exclusively on infrastructure within an industrial cluster. As a result, shipping logistics are not considered, since the distances within the cluster are too short to warrant maritime transport.

Economies of scale also play a crucial role in the transition toward hydrogen systems [10]. Large-scale hydrogen infrastructure benefits from economies of scale, meaning that the cost per unit of transported ammonia decreases as the number of participants in the system increases [10]. For example, high initial investment costs can act as a critical threshold for companies considering whether to invest, particularly given the uncertainty surrounding infrastructure planning. While building pipelines with enough capacity to meet the supply and demand of all participants can help distribute costs, there is a risk that the pipeline will be underutilized. Cui and Aziz [10] present a techno-economic analysis showing that scaling up ammonia infrastructure can lead to reduced transport costs over time. However, additional research is needed to examine how economies of scale emerge in hydrogen network development when driven by investment decisions in ammonia-related assets.

Study	Year	Scope
[25]	2008	Focuses only on large-scale automotive distribution of ammonia
[42]	2021	Focuses only on large-scale shipping distribution
[21]	2024	Focuses on small-scale storage and transport methods
[15]	2023	Conceptual comparison of pipeline and shipping logistics for large-scale ammonia transport; lacks detailed modeling
[26]	2022	Focuses on large-scale ammonia systems for transportation and storage, particularly in marine tankers
[10]	2023	Feasibility study of ammonia for short-distance hydrogen transport
[46]	2023	Focuses solely on the technological feasibility of repurposing natural gas pipelines for ammonia
[30]	2024	Focuses solely on risk analysis of large-scale ammonia networks
[34]	2023	Economic and technical evaluation of small- and large-scale ammonia networks; large-scale analysis focuses on shipping

Table 2.1: Studies Investigating Small- and Large-Scale Ammonia Systems

2.5 Limited research on integrating ammonia into hydrogen infrastructure networks

Building on the infrastructure challenges discussed in the previous section, another key gap concerns the limited research on how ammonia infrastructure integrates with broader hydrogen energy systems. Ammonia has long been used in the fertilizer and chemical industries, according to Galimova et al. [15]. These sectors account for about 70% of global ammonia consumption [15]. In many industrial clusters, ammonia is emerging as a key component of hydrogen supply systems. It functions both as a transport vector and a supply buffer, supporting stable hydrogen availability for industrial applications. This indicates potential synergies between ammonia and hydrogen systems in practice. However, realising this synergy requires coordinated infrastructure planning that aligns with projected hydrogen demand and ammonia import volumes [36].

Despite its promise, there remains a major gap in the literature on how infrastructure elements such as crackers, import terminals, storage facilities, and hydrogen pipelines are connected in a co-evolving system. To effectively integrate ammonia into large hydrogen-based energy systems, it must first be decomposed into hydrogen and nitrogen [56]. According to Trangwachirachai et al. [52], there is a lack of research on the integration of ammonia crackers within large-scale energy networks, particularly when considering crackers as a shared investment within the network.

Finally, Kojima and Yamaguchi [26] state that little research exists on the interaction between large-scale ammonia networks and hydrogen infrastructure networks. A large body of studies focuses solely on hydrogen supply chains, neglecting ammonia's potential integration into industrial and energy networks [46]. This highlights the absence of a joint modeling framework that simulates how ammonia and hydrogen infrastructure could co-develop over time in response to investment behavior in industrial clusters. Given that ammonia imports are expected to increase significantly, future research should explore how ammonia could complement other energy systems, identifying synergies and potential challenges in large-scale adoption.

Makhloufi and Kezibri [32] respond to the growing interest in ammonia by assessing the feasibility of large-scale cracking systems for producing high-purity hydrogen suitable for fuel cell applications. This underscores ammonia's importance as a hydrogen carrier. However, Makhloufi and Kezibri [32] do not explore how large-scale ammonia cracking systems influence the hydrogen pipeline network. Their article only presents a detailed design for a large-scale ammonia-to-hydrogen plant. Nonetheless, they do mention that the integration of ammonia cracking into a hydrogen supply chain requires further research.

The current status of hydrogen infrastructure has been widely reviewed, with studies focusing on production methods, storage technologies, transportation, and refuelling infrastructure [24]. However, these reviews, including that by Kim et al. [24], generally treat hydrogen and ammonia infrastructure as separate systems and often overlook their potential integration and interaction.

Despite valuable contributions to both ammonia and hydrogen infrastructure, most studies examine these systems in isolation. Reviews such as Kim et al. [24] focus primarily on technical aspects, including production and storage, but rarely address how investments in ammonia infrastructure, such as cracking units or import terminals, affect the spatial layout and development of hydrogen networks in industrial clusters. The need for coordinated infrastructure planning that incorporates for interdependencies across different assets remains insufficiently addressed.

2.6 Current analysis of energy systems

To understand and address these integration challenges, it is not only necessary to develop physical infrastructure, but also to adopt efficient modeling approaches capable of capturing the complexity within industrial clusters. This complexity arises from interdependencies between firms and the strategic investment behavior that characterizes modern energy systems. The energy transition is driving fundamental changes in both system design and modeling. This requires new approaches that go beyond traditional optimization frameworks. Existing models must be re-evaluated to assess how new energy vectors like ammonia integrate with infrastructure, and how decentralized investment behavior impacts infrastructure development.

A wide variety of models have been developed to analyze energy systems, many based on top-down, system-level optimization techniques. These techniques assume a central planner makes all decisions to optimize outcomes such as cost. However, new energy vectors and decentralized systems are increasing complexity, driven by renewable integration, distributed generation, and diverse energy carriers [39]. Yet energy models remain limited by computational constraints due to their level of detail. It is essential to capture interdependencies and non linear dynamics between actors in energy models, yet these interactions are often excluded to reduce complexity. Understanding these limitations is essential for effectively analyzing future energy systems [39].

To manage complexity in industrial hubs, it is important to align model purpose with detail. Ridha et al. [39] propose a framework for categorizing traditional models. While these models are useful for high-level planning, they overlook firm-level decision dynamics, especially in emerging areas like ammonia and hydrogen infrastructure. They often ignore uncertainties in company decisions and how these shape cascading investment effects. Key elements such as interdependencies, thresholds, and peer influence are vital for advancing model realism.

Ridha et al. [39] reviewed 145 energy system models and identified trade-offs between model detail and computational feasibility. Their study categorizes models into four types, summarized in Table 2.2. However, these models assume firms act independently or follow system-wide optimization. They do not account for interdependencies, even though one firm's decision can strongly influence another's [39].

Model Type	Description
Unit Commitment Models	Used for power plant deployment planning, optimizing power generation scheduling and dispatch.
Electrical Grid Models	Analyze and optimize electrical grids, including load flows and grid stability.
Policy Assessment Models	Assess the effects of energy policies on economic and environmental outcomes.
Future Energy System Models	Conduct scenario analysis for energy system transformations and long-term energy planning.

Table 2.2: Energy System Model Classification [39]

To evaluate shared infrastructure systems effectively, models must account for interdependencies. In industrial clusters, many firms coordinate investments in pipelines, terminals, and storage facilities, all of which require high capital and long-term planning. Investment cascades are also common, when a key player commits to ammonia, others might follow. Capturing these dynamics is essential for assessing the viability of infrastructure investments. Since traditional models do not incorporate strategic firm behaviour, alternative approaches are needed, particularly those that reflect non-linear adoption patterns and peer influence.

One such approach is the threshold model. It evaluates how firms adjust decisions based on the actions of connected neighbors [54]. At each timestep, a firm decides whether its threshold is met based on network influence. Chen et al. [8] used threshold models to study how renewable energy consumption affects economic growth. They showed that linear models miss non-linear effects, while threshold models capture them. Their results found that the impact of renewables varies based on whether a country has crossed a threshold in renewable energy use [8].

The table below, based on Ridha et al. (2020), summarizes key differences between traditional and threshold-based energy system models.

Table 2.3: Comparison Between Traditional Energy Models and Threshold-Based Models [39]

Aspect	Traditional Models (Unit Commitment, Grid, Policy, Future Systems)	Threshold-Based Model
Decision-Making Process	Centralized (system-level optimization)	Decentralized (firm-specific adoption choices)
Interdependencies	Ignored; Companies are modeled independently	Captured; Companies react to each other's decisions

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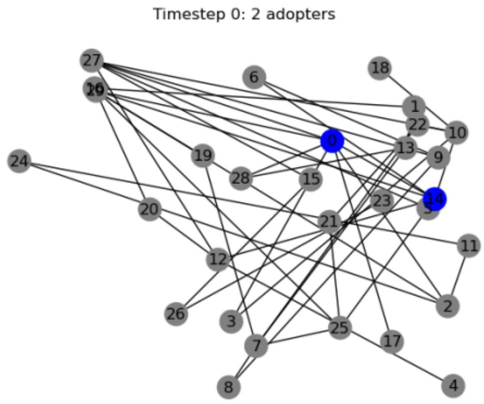
Aspect	Traditional Models	Threshold-Based Model
Adoption Dynamics	Assumes smooth, policy-driven adoption	Captures tipping points, investment hesitations, and cascading effects
Policy Influence	Simulates high-level policy impacts (e.g., carbon pricing, subsidies)	Models how companies react to policy incentives & infrastructure investment trends
Infrastructure Development	Exogenous (assumed to develop if needed)	Endogenous (companies invest only if conditions are favorable)
Mathematical Framework	Linear/mixed-integer optimization, system dynamics	Threshold-based agent modeling (firms adopt only when certain conditions are met)

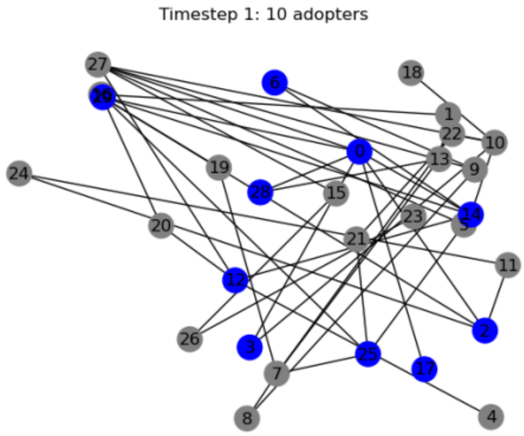
This comparison table illustrates that traditional energy system models rely on unrealistic assumptions that significantly limit their predictive power [39]. While these models excel at system-level optimisation by identifying the most cost-efficient network, they typically treat firms as isolated entities and overlook interdependent decision-making. As a result, they may predict hydrogen network development based solely on cost-benefit analysis, but fail to capture the ”chicken and egg” dynamics and the influence of ammonia-related investments on hydrogen infrastructure evolution. In contrast, threshold-based models are better suited to represent real-world dynamics, including tipping points, investment cascades, and the effects of policy interventions. The comparison by Ridha et al. [39] suggests that a successful energy transition requires moving beyond traditional optimisation models towards approaches that explicitly account for the strategic behaviour of firms in industrial clusters.

2.7 Threshold Models and Cascading Behavior in Networks

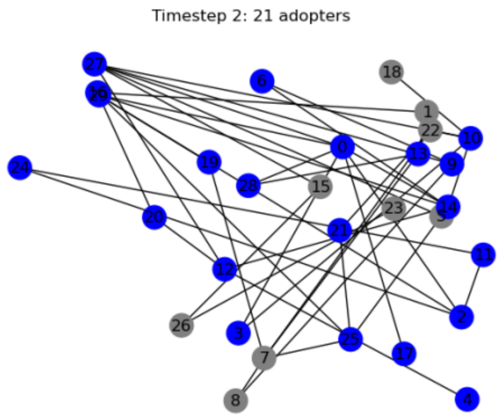
While traditional models fail to capture the strategic, interdependent behavior of firms, this gap is well suited to be addressed with a threshold model [41]. Threshold models are already widely used to simulate system changes characterized by peer influence and non-linear change that occurs when reaching a critical point, or so-called tipping point [50]. Such tipping points indicate that a small change in a part of the network, such as a company reaching its threshold, can trigger large cascading dynamics within the system [41]. These cascading dynamics refer to the rapid, widespread changes that unfold throughout the system once a critical threshold is crossed. This is illustrated in the figures below.



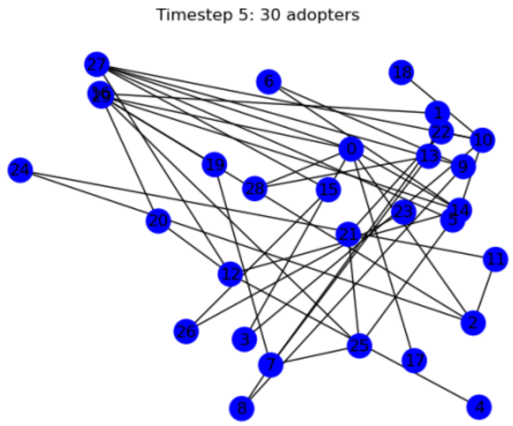
(a) Timestep 0



(b) Timestep 1



(c) Timestep 2



(d) Timestep 4

Figure 2.2: Tipping Point and Cascade Dynamics in a Threshold-Based Adoption Model

The figures represent the development of a threshold model over time. Note that this figure represents a random graph with randomly assigned edges between the nodes. At timestep 0, the model includes two early adopters, highlighted in blue. These early adopters influence the nodes they are directly connected to, referred to as their neighbors [41]. A node's decision to adopt is based on the proportion of neighbors that have already adopted. As more nodes reach their individual thresholds, the network can approach a tipping point [33]. The tipping point represents the moment when a critical mass of adopters is reached, triggering a full transition across the network. In the figure, the tipping point occurs at timestep 2, when a large amount of nodes adopt in a single timestep. Once this point is crossed, adoption accelerates rapidly, producing large cascading dynamics. This pattern of initial slow adoption by early adopters, followed by rapid adoption after the tipping point, is typically recognized as the S-shaped curve of diffusion, shown in the figure below.

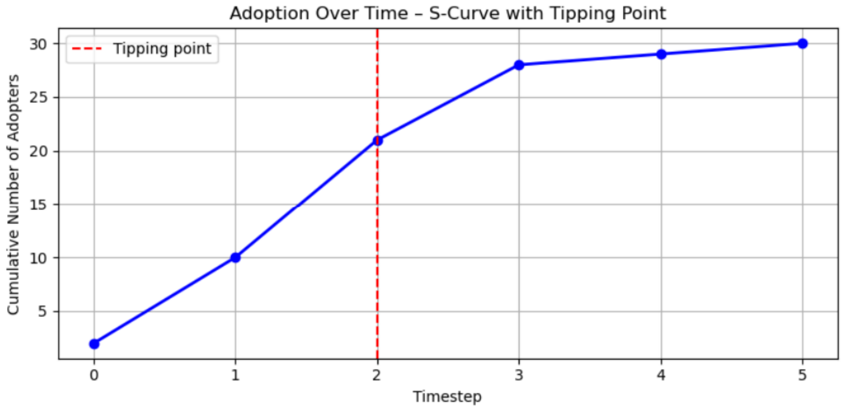


Figure 2.3: S-Curve of Adoption: Illustrating Tipping Point Dynamics in Threshold Models

A key concept in threshold models is the individual threshold, which represents the minimum level of external influence required for an individual to adopt a behavior or transition to a new state [54]. These individuals can have varying thresholds, leading to different times of transition, and resulting in gradual diffusion processes [54].

In the context of innovation diffusion in networks, threshold models are particularly useful for understanding how behaviors or technologies spread based on the interdependencies of individuals [54]. Valente et al. [54] introduced a social network perspective to explain how the diffusion of innovations evolves over time. They argue that individuals engage in new behaviors based on the proportion of others in their network already doing so. This framework allows for predicting diffusion patterns and identifying roles such as opinion leaders and followers.

Such models are particularly relevant in shared infrastructure settings, such as industrial clusters where the development of pipelines or terminals depends on coordinated investment [54]. When early adopters commit to infrastructure, they increase the influence on neighbouring firms by signalling reduced risk or improved viability. As adoption spreads, the cumulative influence on remaining firms grows, increasing the likelihood that others will exceed their predefined thresholds and decide to invest. This process can lead to a cascade of further adoption [54].

Dreyer and Roberts [14] and Valente [54] applied the threshold model to analyze the adoption and development of technologies across firms in a network. Their studies illustrate how peer influence determines both the speed and scope of adoption. However, these models are not yet integrated with network optimization tools that simulate how adoption dynamics affect the evolving spatial configuration and costs of shared infrastructure systems.

This research applies a threshold model to simulate how firms in industrial clusters make investment decisions that shape the development of a hydrogen pipeline network. Rather than modelling the adoption of ammonia infrastructure directly, the model focuses on strategic decisions, such as committing to hydrogen use through infrastructure investments, which collectively determine the network's spatial configuration. By incorporating firm-specific thresholds and interdependencies, the model captures critical tipping points and cascading dynamics. This approach addresses a key gap by integrating threshold-based diffusion modelling with spatial network optimisation, offering a novel framework for analysing how infrastructure co-evolves with firm behaviour in shared energy systems.

2.8 Integration of Graph Theory in Network Planning

Analyzing different networks and their characteristics poses various socio-technical and scientific challenges [18]. These challenges arise in both physical and non-physical networks. Network optimization models provide a structured approach to analyze these challenges. This structured approach should enable the model to address so-called multi-source, multi-sink network problems. These problems refer to networks with multiple 'consumers' and multiple 'producers' [19].

In physical networks, these models typically aim to minimize network design costs. They account for factors such as pipeline length, capacity, and topology [1]. Within these models, uncertainties in supply, demand, and node connections are addressed, while multiple stakeholders (such as companies within industrial clusters) are involved in the decision-making process.

Heijnen et al. (2019) reviewed several of these network optimization approaches and identified three distinct methodologies:

1. Geometric Graph Theory
2. Mixed Integer (Non-)Linear Programming
3. Agent Based Modelling

2.8.1 ABM

Agent-based models (ABMs) are identified as one of the three main approaches for tackling network systems design problems [17]. Compared to MILP and graph theory, ABM is also used to assess the interaction of individuals and groups within networks [17].

According to Heijnen et al. [17], agent-based modeling is a bottom-up approach in which intelligent agents interact within an environment of other agents. Rather than using a centralized design, system behavior and structure emerge from interactions among individual agents. These individual components are referred to as agents.

The foundation of agent-based models lies in Ant Colony Optimization (ACO) algorithms. ACO is an optimization approach where digital "ants" move across a network in search of food, relying only on local information from their immediate surroundings. These ants have no direct knowledge of the best or worst paths. The algorithm conceptualizes the problem as a graph, with the overall objective being to find optimal solutions from a set of candidate solutions, where a candidate solution is a selection of edges that meet the identified constraints.

ABMs are well-suited to modeling both technical subsystems (e.g., energy networks, infrastructure) and social subsystems (e.g., investment strategies, policy choices, technology uptake) in broader energy systems.

2.8.2 MILP

A second category of approach mentioned by Heijnen et al. [17] is Mixed Integer (non-) Linear Programming (MILP). MILP is mainly used to model network design problems mathematically by defining the system as a set of linear constraints and integer decision variables [18].

The primary goal of MILP is cost minimization while ensuring that all sources in a network are connected to nodes [18]. Furthermore, the network must satisfy its demand and supply constraints to arrive at a (near-)optimal solution. A key advantage of MILP is its structured formulation using an objective function and constraint set, such as demand and supply. This makes MILP particularly suitable for handling highly complex optimization problems. Furthermore, MILP includes decision variables which represent choices such as pipeline routing, connection options, and capacity assignment.

2.8.3 Graph Theory

Geometric Graph Theory is one of the most common modeling techniques for designing networks in graph theory. Heijnen et al. (2019) highlight it as a foundational tool for optimizing network design, particularly for minimizing costs in systems with multiple sources and sinks. This approach is also applicable to hydrogen and hydrogen carrier infrastructure research, where most studies rely on graph-theoretical approaches.

Within geometric graph theory, a wide range of heuristics and algorithms have been developed to analyze networks and their characteristics. It is a combination of geometric and graph theory, where the graph $G(n, e)$ is represented as a set of nodes (n) [1]. These nodes typically represent producers or consumers. Edges (e) represent the connections between nodes [1]. These edges can represent physical connections ($e = (n_i, n_j)$), such as pipelines, or non-physical connections, such as interdependencies between nodes.

Graph theory is extensively utilized in the modeling and optimization of various energy network, enabling research to represent interconnections, optimize flow and facilitate efficient energy management [58]. This appraoch is particularly valuable for optimizing dispatching and planning infrastructure in evolving energy systems [58]. Energy networks, regardles of their specific type or layout, can be effectively described as graphs [48, 9].

For example, graph theory has been applied to Regional Integrated Energy Systems (RIES) to support overall planning, with a focus on integrating different energy types to meet economic and environmental objectives [9]. An RIES can be represented as an undirected weighted graph, where nodes correspond to energy stations and sources, and edges represent city roads along which pipelines may be routed [9]. One example is the planning of an integrated energy system for a mixed-use industrial and residential district with diverse energy demands [9]. In such cases, nodes may represent energy sources such as natural gas stations, solar farms, or wind turbines, while edges correspond to major roadways suitable for pipeline construction. Graph-theoretic approaches can then be used to connect these nodes based on specific optimisation objectives, such as minimising total pipeline length.

Modelling the evolution of infrastructure networks while incorporating strategic firm behaviour requires the selection of appropriate analytical tools. This study demands a methodology that balances the structural rigidity of Mixed Integer Linear Programming (MILP) with the flexibility of agent-based models (ABM) to capture complex dynamics relevant to network analysis. Given the objective of simulating infrastructure development based on firm interdependencies, graph theory is identified as the most suitable approach.

Graph theory offers several advantages for modelling infrastructure networks, particularly in the context of network analysis. It provides a well-established set of algorithms, including Dijkstra's algorithm for shortest paths, Prim's and Kruskal's algorithms for spanning trees, and the Ford-Fulkerson method for maximum flow [17, 12, 28]. Its structural simplicity allows for the flexible incorporation of edge weights, constraints, and supply-demand relationships. This makes it particularly well suited for analysing evolving systems such as hydrogen pipeline networks.

The use of graph theory is consistent with academic findings, including those by Heijnen et al.(2019), who identified it as the most appropriate methodology for analysing infrastructure networks.

In this study, the focus is not solely on perfect optimization, but on modeling how infrastructure evolves in practice, step by step under uncertainty. Graph theory is specifically chosen as it supports this focus on infrastructure emergence.

3

Methodology and Simulation Design

3.1 Research Approach

This methodology introduces a novel approach to deriving a social influence network from firm-level attributes and using it as input for a threshold-based adoption model. The output of this model is then translated into a spatial infrastructure design using the Optimal Network Layout Tool (ONLT). Together, these components constitute a dynamic modelling framework that captures how strategic firm behaviour shapes the development of hydrogen infrastructure in industrial clusters. By simulating infrastructure evolution across a structured set of scenarios, this approach provides a foundation for infrastructure planning in a multi-actor context and illustrates how network topology emerges over time.

3.2 Modeling Framework Overview

To structure the modeling approach, a conceptual framework was developed to guide the research. The framework captures the sequential logic of the study and reflects the dynamic nature of investment behavior in industrial clusters, where decisions are influenced not only by costs but also by the behavior of peer firms.

Figure 3.1 presents the four-stage modelling flow that structures this research. The framework links firm-level investment behaviour to spatial infrastructure design through an integrated simulation approach.

The first stage focuses on identifying relevant firm attributes and assigning normalised scores to each firm's attribute values and their interdependencies. Firms within the industrial cluster are assigned attribute values, which are then used to calculate individual investment thresholds. This step addresses Subquestion 1 by establishing which firm characteristics influence investment behaviour. Section 3.3 provides further detail on the attribute selection process.

The second stage focuses on the adoption process simulated through the threshold model. This model captures how firms adopt over time by incorporating interdependencies and simulating how investment decisions unfold through cascading dynamics.

The third stage focuses on the integration of the threshold model with the Optimal

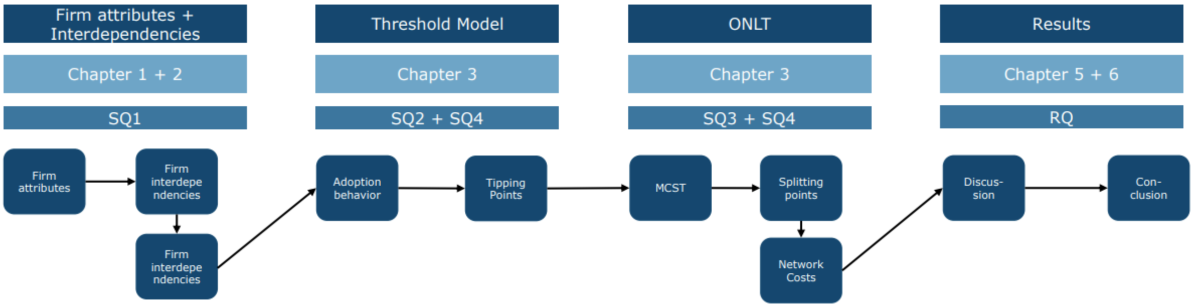


Figure 3.1: Research flow diagram

Network Layout Tool (ONLT). The ONLT constructs a cost-efficient hydrogen pipeline network based on the firms that have adopted in each timestep, using graph theoretical techniques to determine the optimal spatial layout.

The final stage conducts a scenario analysis to evaluate how the hydrogen network evolves under varying demand and import conditions. This analysis identifies which pipelines appear consistently across multiple scenarios and can therefore be considered robust.

To operationalise the threshold adoption model, the first step involves identifying which firm-level characteristics influence both adoption decisions and inter-firm influence within industrial clusters. The following section outlines the selection and justification of these attributes.

3.3 Graph Theory

Designing energy infrastructure such as hydrogen pipeline networks involves navigating trade-offs between cost efficiency, spatial constraints, and long-term scalability. These systems involve high capital investments and extended operational lifespans, making initial design decisions critical, particularly in hydrogen networks, where investment timing and adoption dynamics are uncertain.

Graph theory offers a formalized method to represent such infrastructure. In this framework, the network is modeled as a graph $G = (N, E)$, where the node set $\{n_i\}$ corresponds to firms and the edge set $\{e_{i,j}\}$ represents potential pipeline connections or firm interdependencies [57].

Edges may be weighted to reflect relevant metrics. For example, the weights can represent the physical length of a pipeline, the cost of construction and installation, or the capacity of a specific pipeline [17]. This abstraction facilitates a structured and scalable approach to infrastructure modeling and enables the application of optimization techniques.

Figure 3.2 illustrates a basic graph comprising four nodes and four edges. This simple representation serves as a foundation for more complex network analyses.

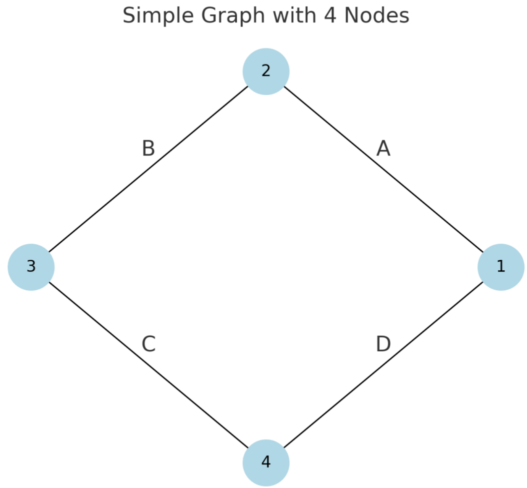


Figure 3.2: Simple graph with four nodes and four edges representing an infrastructure network

Graph theory includes several substructures useful for network design, one of which is the spanning tree. A spanning tree is a subgraph that connects all nodes in the network without forming any cycles [16]. This structure is particularly relevant in infrastructure planning, as it guarantees full network connectivity using the minimal number of links.

Of the many possible spanning trees, the minimum weight spanning tree (MWST) is the one with the lowest total edge weight. In infrastructure applications, edge weights typically represent construction costs, physical distances, or capacity-adjusted costs. Identifying the MWST is a fundamental problem in graph theory and frequently underpins the design of cost-efficient infrastructure systems [16].

Several algorithms can be used to determine the MWST. Two widely applied methods are Kruskal's algorithm and Prim's algorithm [3]. Kruskal's algorithm sorts all edges in ascending order of weight and adds them sequentially, skipping any edge that would create a cycle. Such a cycle is shown in Figure 3.2. This process continues until all nodes are connected. In contrast, Prim's algorithm begins at a selected node and grows the spanning tree by repeatedly adding the lowest-weight edge that connects a new node to the tree. Both algorithms yield the same optimal solution, though they differ in procedural logic and computational efficiency depending on graph structure.

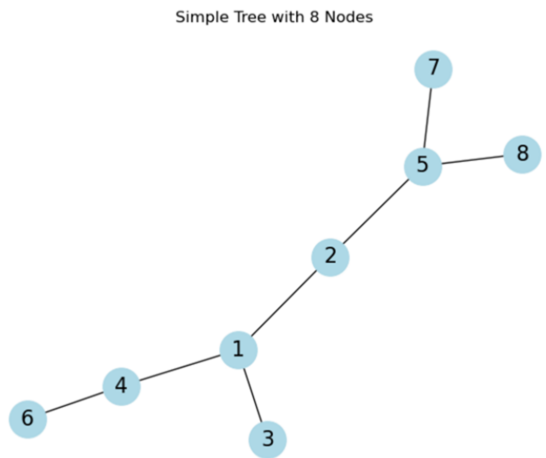


Figure 3.3: Simple tree graph with no cycles, illustrating a minimal path network

Infrastructure development is modeled as a dynamic process. Firm adoption occurs incrementally, determined by each firm's threshold and adoption timing. At each timestep, newly active firms are added to the network, and the optimal pipeline configuration is recomputed to incorporate these additions.

A key assumption in this formulation is that infrastructure constructed in earlier periods remains in place and is reused. This cumulative approach is embedded within the Optimal Network Layout Tool (ONLT), which iteratively adapts the network layout in response to expanding firm participation and evolving flow demands. To determine the most cost effective infrastructure layout over time, this study uses the Optimal Network Layout Tool, which will be introduced in Section 3.7.

In conclusion, this study applies graph theory as a central framework to model both interdependencies among firms and the development of hydrogen infrastructure. Graph-theoretical concepts are operationalized in two core components of the analysis: the threshold model and the Optimal Network Layout Tool (ONLT). In the threshold model, graph theory is used to represent the network of inter-firm interdependencies, where edges capture the social influence between firms. In the ONLT, graph structures are applied to optimize the physical layout of the hydrogen pipeline network, with the objective of minimizing total infrastructure costs.

3.4 Selection of Firm Attributes

The selection of firm-specific attributes is a foundational step in the threshold model, as these attributes determines how firms make infrastructure investment decisions and how these decisions affect both their adoption thresholds and inter-firm influence [61]. This section outlines the attribute selection process and supports *Subquestion 1: What firm-level attributes influence adoption decisions and interdependencies in shared hydrogen infrastructure?*

The attributes were identified through a review of relevant literature and data provided by Power2X. A targeted set of criteria was applied to select attributes for model inclusion, prioritizing clarity, data availability, and decision relevance for infrastructure investment, as shown in Table 3.1.

Table 3.1: Criteria for Selecting Firm-Level Attributes

Criterion	**Guiding Question**
Relevance to Adoption Decisions	Does the attribute directly influence a firm's likelihood to invest in shared hydrogen infrastructure?
Strategic Importance in Infrastructure Planning	Is the attribute often used in real-world infrastructure development or investment decisions?
Availability and Quality of Data	Is reliable, company-level data for this attribute available (e.g., via Power2X or public sources)?
Heterogeneity Across Firms	Does the attribute vary meaningfully between firms, allowing for behavioral differentiation?
Interpretability	Is the attribute easy to explain and interpret by both stakeholders and model users?
Measurability	Can the attribute be quantified in a consistent and scalable way across firms?
Representation of Firm Role or Function	Does the attribute represent the firm's structural role in the cluster (e.g., producer vs. consumer)?

In the model, these attributes serve tree key functions. First, they determine the individual adoption threshold for each firm. Second, they contribute to the edge scores in the influence network, reflecting the strength of inter-firm influence. Third, these attributes were also used to identify the set of firms included in the RIC case, as described in Section 3.4. This approach ensures consistency in firm selection and guarantees that each firm has relevant data available for the specified attributes.

3.5 Attribute Categories

The threshold model applied in this study includes firm specific attributes to capture each firm's individual investment threshold. Each attribute is interpreted as a factor potentially affecting a company's willingness to invest. To determine firm specific thresholds, the attribute data must be transformed to allow consistent comparison across firms. Because the raw attribute values differ in scale, a classification step is applied within each attribute to standardize the data for integration into the threshold calculation. For numerical attributes, values are classified into three categories: low, medium, and high, based on the range and distribution of observed values. This approach aligns with the work of Valente et al. (1996) and Dreyer and Roberts (2009), who use categorical differentiation to reflect varying levels of readiness to adopt. While these studies focus on social models and network degree, this study extends their logic by linking firm specific attributes directly to individual adoption thresholds. This acknowledges that firms with more favourable characteristics are likely to adopt earlier. To ensure comparability across attributes, the assigned category scores are normalized to a scale between 0 and 1.

For each numerical attribute, the collected data is visualised using a histogram. A visual inspection of this histogram enables the identification of natural clusters and boundary values. These values are used to define the limits of the low, medium, and high categories for each attribute. An example of one such a histogram is shown below. The boundary values for the *low*, *medium*, and *high* categories were selected based on the following criteria:

- Visible gaps in the histogram,
- Cluster centres or local density peaks,
- Round values near points of distribution change.

To ensure consistency, each category must include at least 20% of the firms, and no category may contain more than 60%. These constraints are introduced to prevent extreme imbalances that would limit the model's ability to meaningfully differentiate between firms. In addition, these boundaries ensure that all attribute categories contribute to the variation in firm specific thresholds. This is essential for generating realistic adoption patterns within the threshold model. This approach is in line with the equal frequency binning method [60, 23], which is commonly used to categorize attributes with continuous domains. In this method, the range of attribute values is divided into a specified number of bins, denoted as N. For each attribute, the data are sorted and partitioned into N bins such that each bin contains approximately the same number of observations.

The main difference between the standard equal frequency method and the approach applied here is the treatment of the data distribution. In this study, attribute values are classified according to a normal distribution. As a result, the middle category contains the majority of observations, which better reflects the expected distribution in practice, where most firms exhibit average characteristics.

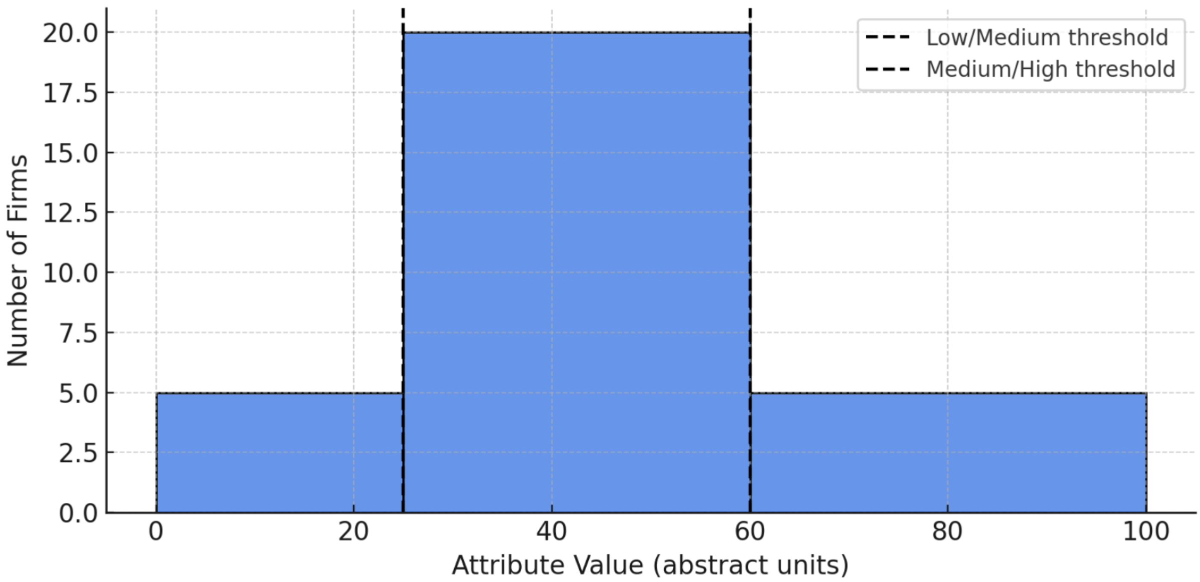


Figure 3.4: Example Histogram Used for Attribute Categorization

This approach typically reveals the following pattern:

- A clear concentration of low values, which provides a logical lower bound for the *low* category;

- A middle segment where most observations are concentrated, which is defined as the *medium* category;
- A limited number of high values, which justifies the definition of a *high* category.

The boundary values for the categories within each attribute were derived with the aim of creating a meaningful differentiation between firms. An example of such a categorization is: $x \leq x_1$, $x_1 < x \leq x_2$, and $x > x_2$, where x_1 and x_2 represent the boundaries determined based on the data distribution.

Example of an abstract category classification:

- **Low:** Values less than or equal to x_1
- **Medium:** Values between x_1 and equal to x_2
- **High:** Values greater than x_2

This method is applied to each numerical attribute in the threshold model to ensure consistency in the categorization of attribute values. A structured method for scoring the different attribute categories is essential for the model to produce meaningful variation in adoption behaviour. The adoption process in the threshold model depends on clear differences in the readiness of firms to adopt. Without a well structured procedure, raw attribute values that are extremely high or low could dominate the threshold calculation. These extreme values often result from future oriented project data or highly ambitious project announcements. A detailed explanation of the category scoring process is provided in Section 3.5.1.

3.5.1 Category Scoring Method

In this study, the term score refers to a normalised score that translates the values of firm attributes into relevant indicators of adoption likelihood. The primary reason for applying the scoring method is that the attributes are measured on different scales. The scoring process ensures that these values can be meaningfully compared and combined into a single threshold score. To achieve this, attribute values are first classified into categories and then translated into normalized category scores. The category boundaries reflect relative differences in scale between firms and their likelihood to adopt. For example, a high value for an attribute such as hydrogen demand may indicate a lower investment threshold, reflecting favourable conditions for adoption. Firms in this category are typically major players and are assigned a score of 0.8. Conversely, firms with a low attribute value are assumed to face a higher threshold and are assigned a score of 0.2. The medium category represents intermediate cases and is assigned a score of 0.5. By assigning an intermediate scores to the medium category the model allows for sufficient variation in threshold values between firms. The selected categories were chosen because they reflect meaningful and distinguishable levels of adoption readiness. These values strike a balance by being sufficiently distributed to produce differentiated adoption patterns in the model, while remaining within a range that avoids unrealistic outcomes.

The scores that are assigned to the *low*, *medium*, and *high* categories are not directly derived from scientific literature. They were determined through an interpretative approach, aiming to translate numerical firm level data into behavioral components.

Several alternative score sets were tested in the threshold model to evaluate the validity of the low, medium, and high values (0.2, 0.5, and 0.8). For instance, the scores 0.1, 0.4, and 0.9 were tested. These increased the differences between firms, which substantially raised the model's run time, while producing nearly identical results. Conversely, the scores 0.4, 0.5, and 0.6 were used to analyse a scenario where differences between firms were minimal. Nevertheless, this configuration produced no adoption dynamics, as the thresholds were too high and too closely clustered. In this study, all firm level attributes are assumed to contribute equally to a firm's threshold score. However, differences within each attribute are reflected in the varying importance of their categories, as determined by the normalised scores assigned to each.

3.5.2 Scoring of Categorical Attributes

In contrast to numerical attributes, categorical attributes are assigned normalized scores using a different approach. To determine these scores, expert interviews were conducted with a panel of ten professionals experienced in the energy transition. These experts are all currently involved or have previously participated in hydrogen and decarbonisation projects across various industrial clusters. They were selected based on their experience with infrastructure development, firm engagement, strategic planning, and advisory roles in multiple industrial settings. Their involvement across a wide range of projects, companies, and cluster contexts provided a robust basis for evaluating the relevance of specific firm attributes. Each expert was asked to evaluate ten pairs of hypothetical firms, with each pair differing across multiple attributes. This type of approach is referred to as a pairwise comparison method [4]. It can be clearly illustrated through the example of optimal passenger car selection. In this case, the pairwise comparison method is used to evaluate different vehicles based on both quantitative and qualitative attributes [27]. Expert judgments are collected by comparing cars across a defined set of criteria, such as price, engine power, and subjective characteristics like safety and design. Even for qualitative attributes, expert reasoning is translated into normative scores, which enables the integration of diverse judgments into a single normalized priority ranking.

The process begins by identifying the alternatives (e.g., Skoda, Ford, VW Golf) and the criteria on which they are evaluated [27]. These include quantitative criteria such as price, engine power, and fuel consumption, and qualitative criteria such as driving safety and design. Experts use the pairwise comparison method to evaluate each car with respect to each criterion. The results are then organized into a matrix, where each entry represents the preference ratio of one alternative over another. These scores are aggregated and normalized, converting the inputs into comparable numerical values suitable for further analysis.

In this study, the pairwise comparison approach involved asking the following question for each pair:

Which entity is more likely to adopt the innovation first, and why?

Adoption was explicitly defined as committing to investment decisions in new infrastructure, such as storage systems, ammonia crackers, or pipeline connections. In addition, it was clarified that hydrogen volumes were expressed in hydrogen equivalents, including both green hydrogen and green ammonia.

The responses were analysed using a simple scoring method [54][4]. This method was used to reduce subjectivity and improve comparability. By focusing solely on the frequency with which a category was mentioned, the method ensures consistent interpretation across experts. For each comparison, any attribute mentioned in the expert's reasoning was assigned a score of 1, while all other attributes received a score of 0. In the case of categorical attributes, specific categories mentioned by the experts were also counted. This allowed for the quantification of the relative importance of each attribute and its categories across all comparisons.

To derive the normalized scores for the categorical attributes, the frequency with which each category was mentioned was normalised to obtain a relative ranking. These scores were summed across all interviews and then divided by the total number of mentions per attribute, as shown in Table 3.2. This table presents results only for the categorical attribute "company type." Other attributes, which are numerical, are excluded here because their scores were defined directly from available data. Nonetheless, the normalized values shown are based on the total mention counts across all attributes.

The first column in the table presents the attribute name, in this case "Company Type," followed by the specific attribute categories in the second column. The third column, "Mention Count," indicates how often each category was selected during the pairwise comparison exercise. The fourth column displays the normalized score, and the final column, "Defined Score," shows the values ultimately used in the model. These defined scores were selected to maintain sufficient differentiation between attribute categories. This was necessary to ensure the threshold model produced distinguishable adoption patterns, which may not occur if the scores are too close to each other.

Table 3.2: Expert Scores for Company Type Attributes

Attribute name	Attribute category	Mention count	Normalized Score	Defined Score
Company Type	Importer	39	0.099	0.90
Company Type	Storage provider	36	0.092	0.80
Company Type	Hydrogen supplier	18	0.046	0.60
Company Type	Hydrogen consumer	15	0.038	0.50

3.5.3 Edge Score Calculation

In addition to the scores assigned to firm level attributes, the connections between firms are also assigned scores to represent the degree of influence one firm may exert on another. To calculate the final influence between two firms, the model first computes a separate edge score for each attribute. This is done by taking the average of the attribute scores assigned to the two connected firms. For example, if Firm X has a low hydrogen demand (score = 0.2) and Firm Y has a medium hydrogen demand (score = 0.5), the resulting edge score for that attribute would be 0.35, as shown in the formula below. This procedure is repeated for each attribute. The final edge score between two firms is then calculated as the simple average of the individual attribute scores. This reflects the assumption that all attributes contribute equally to the overall influence strength between firms.

$$w_{XY}^{a_1} = \frac{0.2 + 0.5}{2} = 0.35$$

The model assumes that adoption influence is strictly positive. In practice, however, negative connections may also occur, or stronger positive connections may arise between firms that differ significantly, for example when they benefit from each other within the supply chain. The effect of these edge scores on the influence between firms will be explained in the threshold model section.

3.5.4 Calculating Firm-Specific Thresholds

The final part of the threshold model focuses on determining each firm's specific threshold. This section explains the rule by which a firm decides to adopt.

Each firm's threshold is derived from its attribute profile. The underlying assumption is that firms with more favourable characteristics, reflected in higher attribute scores, have lower thresholds to adopt. This is captured by the following formula:

$$T_i = 1 - \frac{1}{n} \sum_{a=1}^{n} w_i^a$$

where:

- T_j is the threshold value of firm j
- n is the number of attributes considered
- w_i^a is the score assigned to firm i's value on attribute a

The pseudocode outlining the threshold calculation logic is provided in Algorithm 1 in appendix C.

3.6 Threshold Model Design

In this study, the threshold model represents the behavioural logic underlying firm-level infrastructure adoption. It forms the core of the modelling approach by simulating how strategic adoption behaviour evolves over time and influences the spatial layout of infrastructure. The model captures how firms respond to peer influence and interdependencies, allowing for the identification of cascading effects within industrial clusters [59].

3.6.1 Threshold Model

Before introducing the dynamic and mathematical formulation of the threshold model, this section highlights several important aspects that require explicit explanation.

Timestep

A timestep represents one unit of simulated time in the model. It does not correspond to real-world time (days or years), but they represent discrete moment in which firms update their decisions. In each timestep, firms evaluate whether to invest based on the current state of the network and the level of influence from neighbouring firms. This iterative procedure represents infrastructure development as a sequence of decision rounds, each corresponding to a discrete timestep. At each step, adoption decisions are updated based on the current system state. The process continues until no additional adoption occurs, capturing how adoption unfolds over time within the industrial cluster.

Complete Graph Structure Threshold Model

In graph theory, various types of graphs can be employed depending on the modelling objective. Within the threshold model used in this study, a complete graph (G) is constructed in which every node is potentially connected to every other node in the network. This structure implies that each firm can, in principle, be influenced by all others. However, the strength of these connections varies based on firm-specific attributes, meaning some links carry greater influence than others. This approach enables the construction of a fully connected graph in which edge scores represent the degree of influence. As a result, the model captures the interdependent nature of firms within an industrial cluster in a nuanced and flexible manner.

Threshold Model Dynamics

Within the threshold model, firms are represented as nodes in a social network, which means their connections represent the interdependencies and not physical conneciton [54]. Each firm is assigned a threshold T_i. Firms with more favorable attributes tend to have lower thresholds making them more likely to adopt early, while those with a higher threshold likely postpone their investments [61].

After computing a specific threshold for each firm within the industrial cluster, influence propagates through the network via the scored connections. The model assumes that firms that have already adopted exert a positive influence on their neighbours, thereby increasing the likelihood of adoption.

At each time step, the model calculates the influence a firm receives from its adopted neighbours, expressed as a proportion of the total influence from all of its connections [14]. This proportion is referred to as the *influence ratio* (IR_i) , which is then compared to the firm's specific threshold.

Consider a simple graph containing three nodes (1, 2, and 3). For each node, the total received influence is calculated as the sum of all connection scores with neighbouring firms. The adopted influence is then calculated as the sum of scores from neighbours that have already adopted. A firm will adopt if its influence ratio exceeds its own specific threshold. This process is formalised in the following formula:

For all $i \in \mathcal{F}$, the influence ratio IR_i is defined as:

$$IR_i = \frac{\sum_{j \in A_i} w_{ij}}{\sum_{j \in \mathcal{F} \setminus \{i\}} w_{ij}}$$

Adoption Rule:

$$\text{If } IR_i \geq T_i, \text{ then firm } i \text{ adopts.}$$

- $\mathcal{F}$ is the set of all firms (nodes) in the network
- $A_i \subseteq \mathcal{F} \setminus \{i\}$ is the set of firms that have already adopted and are connected to firm i
- w_{ij} is the score of the connection from firm j to firm i, defined for all $(i, j) \in E(G)$
- T_i is the threshold value of firm i

This formulation is consistent with the study by Valente et al. (1996), which defines an individual's threshold as the proportion of adopters within their social system required for them to adopt an innovation [54]. More specifically, it reflects the share of others in their network who must have already adopted before the individual decides to do so. In addition, this threshold adoption formula also correspond with Dreyer et al. (2008) irreversible k-threshold proces, where a node changes from "uninfected"(state 0) to infected (state 1), if at least k of its neighbors are in state 1 [14]. Here, k is the fixed threshold for a state change. Furthermore, Yuxin Ye et al. (2022) analyse the Linear Threshold Model (LTM), a widely used diffusion framework in which each node is assigned an influence threshold (T_v). In their study, T_v is drawn from a uniform distribution between 0 and 1 and remains constant once determined. This value is generated using a random number generator algorithm. However, the authors acknowledge that threshold values can vary substantially and are often related to observable characteristics such as node attributes, economic willingness, or firm-specific preferences. For example, Yuxin Ye et al. (2022) note that in a majority threshold model, a node's specific influence threshold can be directly derived from its structural position in the network, measured by its degree centrality $D(v)$. Degree centrality quantifies the number of direct connections a node v has to other nodes. In their formulation, the threshold is calculated using the expression $T_v = \frac{1}{2 \cdot D(v)}$ [61]. This implies that higher degree centrality, indicating a more connected node, corresponds to a lower adoption threshold and reflects greater susceptibility to peer influence. In this study, a similar principle is applied, but extended to include a combination of multiple firm-specific characteristics. These attributes are used to compute a normalized threshold for each firm within the cluster.

In contrast, this study derives threshold values from firm-specific attribute data, using a structured scoring method to generate a normalized threshold for each firm. In addition, the influence of edge scores is explicitly incorporated into the adoption logic, consistent with the threshold-based approach. As in Ye et al. (2022), this model assumes that firms that have already adopted exert a positive influence on their neighbours, thereby increasing the likelihood of adoption through accumulated peer influence [61].

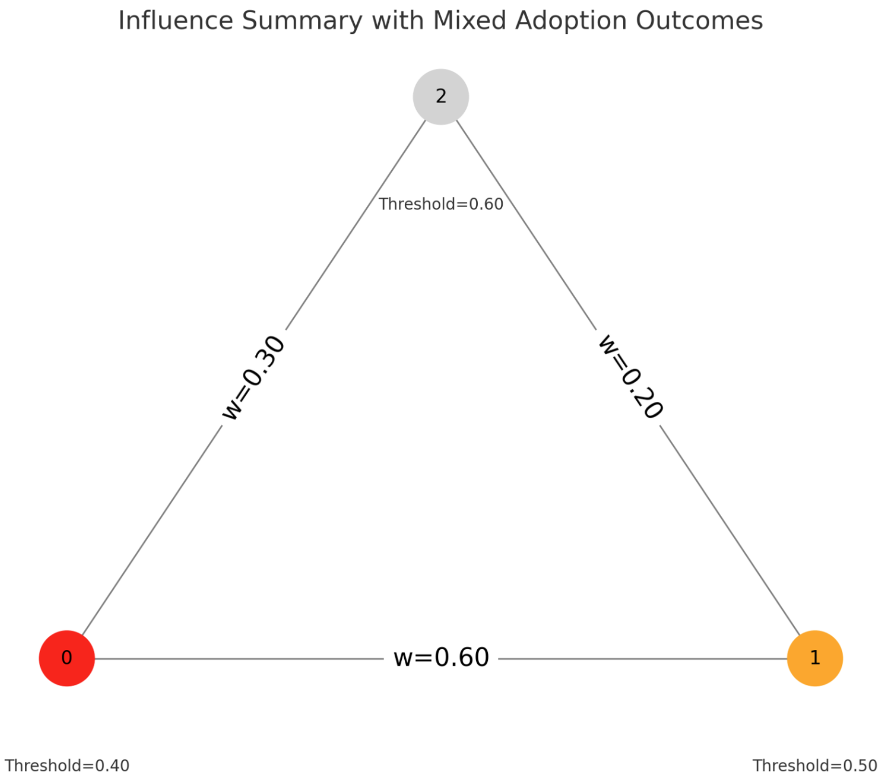


Figure 3.5: Edge scores graph

Looking at the example of the graph in Figure 3.5, which contains three nodes, we see that node 1 has two neighbors: node 0 and node 2. Node 0 has already adopted and shares an edge with node 1 with a normalized score of 0.60. Node 2 has not adopted and is connected to node 1 with a score of 0.20.

To calculate the total influence on node 1, we sum the scores of all its incoming edges, resulting in a total influence of

$$0.60 + 0.20 = 0.80.$$

The infected influence (the cumulative influence from already adopted neighbors) is 0.60. This gives an influence ratio of

$$\frac{0.60}{0.80} = 0.75.$$

Since node 1 has a threshold of 0.50, it will adopt because the influence ratio exceeds its threshold. Node 2 does not adopt at this stage, due to its higher threshold relative to node 1 and its lower edge score with node 0.

In the second time step, the focus shifts to node 2's perspective. Node 2 is connected to both node 0 and node 1, with edge scores of 0.30 and 0.20, respectively. Both of these neighbors have adopted, so the infected influence for node 2 is

$$0.30 + 0.20 = 0.50.$$

However, because node 2 has a higher threshold of 0.60, the influence ratio of

$$\frac{0.50}{0.50} = 1.00$$

is sufficient. In contrast, in an alternative where one of the neighbouring firms had not adopted, or where the influence scores were lower, the node would not adopt.

This example illustrates how both threshold values and the strength of interdependencies (edge scores) together determine adoption decisions.

By incorporating this mechanism into the model, stronger interdependencies, reflected by higher edge scores, are shown to accelerate adoption in the network. This approach captures strategic relationships among firms more realistically.

Summarized

To present a final overview of the threshold model methodology, the model consists of three key elements. First, each node is defined by a distinct set of attributes, which identify the characteristics of each node. All these attributes are assigned scores, where a higher attribute score reflects greater importance in shaping a node's threshold. These attribute scores contribute directly to the individual node's threshold. Nodes with many highly scored attributes tend to have lower thresholds.

Second, there are edge scores, which represent the strength of interdependencies between nodes. These are based on attribute pairs, where each attribute has multiple categories. Each pair of categories (for example, *high* with *high* or *medium* with *low*) is assigned a specific score that reflects the level of influence between firms for that attribute. This calculation is performed for every attribute across all firm pairs and is then combined to construct the complete social network.

Third, each possible category combination between the same attribute of two companies is assigned a score. For every attribute, a graph is constructed showing only connections based on that attribute. These individual attribute graphs are later merged into a single graph that includes all edge scores.

In conclusion, these three elements, the node attributes and their scores, the edge scores, and the individual thresholds, collectively determine the dynamics within the threshold model. The output, which is the adoption pattern among firms in an industrial cluster, is then used as input for the Optimal Network Layout Tool.

3.7 Optimal Network Layout Tool

The Optimal Network Layout Tool (ONLT) is a graph-theoretical tool used to design cost-efficient infrastructure networks based on evolving demand patterns [19]. It is primarily applied to derive cost-optimal layouts for energy transition systems [18]. The ONLT computes the most efficient pipeline configuration that connects all relevant nodes. In this study, these nodes represent firms that adopt hydrogen infrastructure at different timesteps. The tool is particularly well-suited for solving multi-source, multi-sink network problems [18].

At each timestep, the ONLT analyses the set of firms that have adopted and constructs a pipeline network to connect them. The tool uses minimum-cost spanning trees as a core element of its optimisation process [18]. Within the model, it is assumed that the total supply from all supply nodes must equal the total demand from all demand nodes in the base case. The details of the base case are further elaborated in Chapter 5. This assumption is introduced to enable the assignment of a supply or demand value to storage providers, as no reliable data on their inflow or offtake volumes is available. The ONLT model begins by generating a minimum spanning tree (MST), which identifies the shortest possible network that connects all adopted nodes. After constructing the MST, the ONLT further refines the layout to derive a minimum-cost spanning tree that accounts for cost factors beyond distance alone. Within the ONLT, several key assumptions are made. First, it is assumed that total hydrogen supply exactly matches total demand during the optimisation process. Second, the cost function incorporates a capacity cost exponent (β) to reflect economies of scale, meaning that larger-capacity pipelines are relatively more cost-efficient per unit transported.

The cost function $C(G)$ for a network G is defined by the following formula:

$$C(G) = \sum_{e \in E_n(G)} l_e q_e^\beta + s_{pc} \cdot s(G) + \sum_{e \in E_o(G)} l_e \left(u_{pc} \cdot \min(q_e, r_{qe})^\beta + c_{pc} \cdot \max(0, q_e - r_{qe})^\beta \right) \tag{3.1}$$

- $E_n(G)$: The set of all new edges (pipeline connections) in the network G.
- $E_o(G)$: The set of all existing edges that can be reused or extended in the network G.
- l_e: The length of edge e, typically the Euclidean distance between the edge's endpoints.
- q_e: The required capacity for edge e in the final network.
- r_{qe}: The reusable capacity already present on edge e.
- β: The capacity-cost exponent, with a value between 0 and 1. It reflects economies of scale in pipeline construction.
  - If $\beta = 0$, capacity has no influence on the cost.
  - If $\beta = 1$, doubling the capacity doubles the cost (linear cost function).
  - If $0 < \beta < 1$, larger pipelines are more cost-effective per unit transported.
- s_{pc}: The unit cost for creating a splitting point in the network.
- $s(G)$: The total number of splitting points added to the network G.
- u_{pc}: The unit cost factor for using existing pipeline capacity.
- c_{pc}: The unit cost factor for extending existing pipeline capacity.

Table 3.3 provides an overview of the parameter values used in the cost function, along with their explanations and roles within the Optimal Network Layout Tool (ONLT).

Table 3.3: Parameter Settings in the Cost Function [19]

Parameter	**Value**	**Assumption**	**Interpretation**
Splitting Point Cost (spc)	0	No splitting points are used in the model	This parameter is inactive in the simulation
Use of Existing Capacity Cost (upc)	0	Existing edges can be reused without additional cost if constructed in earlier timesteps	Encourages reusing existing infrastructure
Capacity Extension Cost (cpc)	1	Extending the capacity of existing edges is as costly as building new capacity	Reflects realistic capital investment assumptions

The resulting cost function used in this study is presented in Equation 3.2, where $\max(0, q_e - r_{qe})^\beta$ represents a key component that calculates the additional capacity required beyond the reusable capacity already present on a given connection. The cost is computed for the final network layout at the end of the simulation. Consequently, if an edge is initially constructed with a capacity of q_1 and later expanded to accommodate $q_1 + q_2$, the model does not accumulate costs over time steps. Instead, the total cost for that edge is calculated as $l_e \cdot (q_1 + q_2)^\beta$, rather than the sum $l_e \cdot q_1^\beta + l_e \cdot q_2^\beta$.

$$C(G) = \sum_{e \in E_n(G)} l_e q_e^\beta + \sum_{e \in E_o(G)} l_e \cdot \max(0, q_e - r_{qe})^\beta \tag{3.2}$$

However, these values are not actual costs, as the ONLT produces dimensionless outputs in the unit:

$$\text{km} \cdot (\text{ktpa})^{0.6}.$$

To convert these values into estimated costs in euros, a conversion factor is applied. This factor is based on a common industry assumption that constructing one kilometre of hydrogen pipeline costs approximately one million euros [44].

- **Pipeline cost:** €1,000,000 per kilometer
- **Pipeline capacity:** 100 kilotonnes per annum (ktpa)

The ONLT cost function is defined as:

$$\text{ONLT cost} = l \cdot q^\beta$$

Where:

- $l = 1\,\text{km}$
- $q = 100\,\text{ktpa}$
- $\beta = 0.6$

Substituting these values:

$$\text{ONLT cost} = 1 \cdot (100)^{0.6} \approx 15.85$$

To convert this to euros, the real pipeline cost are devided by the ONLT costs:

$$\text{Conversion factor} = \frac{£1,000,000}{15.85} \approx £63,100 \text{ per unit of km} \cdot (\text{ktpa})^{0.6}$$

3.7.1 Justification for Stopping at the Minimum Cost Spanning Tree

While the ONLT model could be extended beyond the minimum-cost spanning tree to include Steiner nodes, this study deliberately limits the analysis to the minimum-cost spanning tree stage. A Steiner node refers to an additional point introduced in the network to further reduce total infrastructure cost, even though it is not itself a supply or demand node. It serves as a splitting point that enables more efficient connections between firms. The figure below illustrates the effect of incorporating a Steiner node (S) in a network with three nodes (A, B, and C).

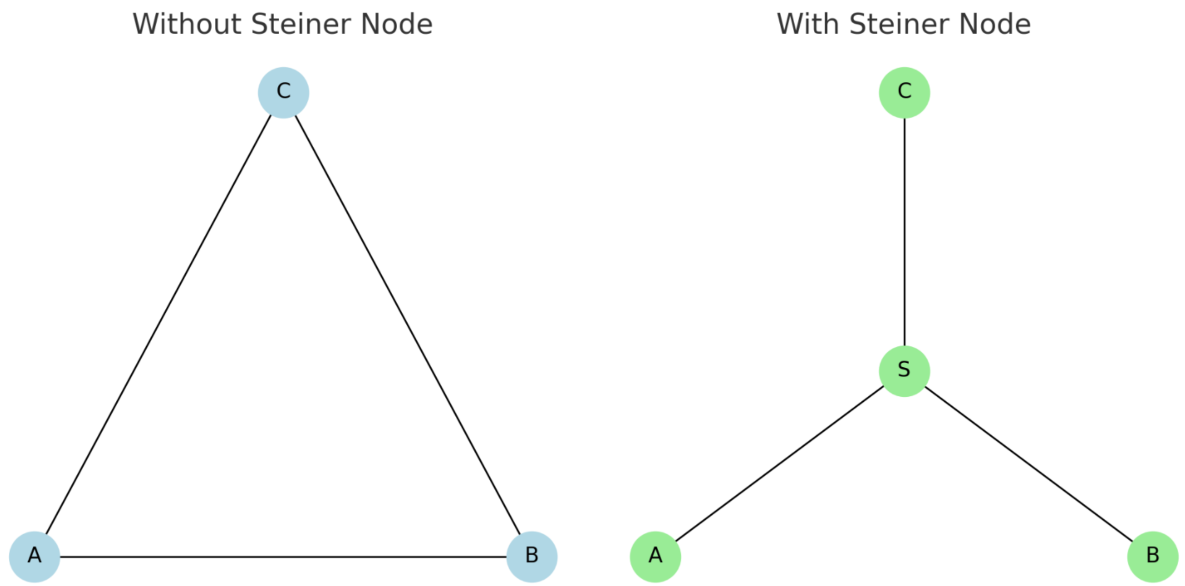


Figure 3.6: Example of a Steiner Node

The decision to stop at the minimum-cost spanning tree (MCST) stage is motivated by the need to effectively assess network robustness. Robustness in this context is evaluated by counting the occurrence of specific edges across multiple scenarios, as detailed in the following section. Although Steiner trees may provide additional cost savings, they complicate the interpretation of results by introducing intermediate nodes that do not correspond to actual firms. As a result, it becomes more difficult to identify which firm-to-firm connections are consistently maintained. By limiting the analysis to MCSTs, each edge represents a direct and interpretable link between active supply and demand nodes, thereby supporting a more meaningful robustness evaluation.

3.8 Scenario and Sensitivity Analysis

To evaluate robustness, the model was tested under multiple plausible future scenarios. Twenty distinct network development paths were generated, based on a combination of four early adopter types and five future configurations: a base case, high and low hydrogen demand, and high and low ammonia import volumes. For each scenario, the ONLT computed a cost optimal network layout based on the simulated firm adoption process, resulting in a diverse set of infrastructure topologies.

As explained in Section 1.7.2, robustness is considered as a key evaluation criterion for networks. In this study, the robustness of a network edge is defined as the proportion of scenarios in which that edge appears in the optimal network layout. This is referred to as edge occurrence. Edges that appear more frequently across scenarios are considered more robust under uncertainty, as they represent low regret infrastructure. These are connections that are likely to remain valuable regardless of future demand or import patterns. To identify robust network topologies, a maximum occurrence heuristic is applied. This approach builds on Heijnen et al. (2014), though their focus lies on the occurrence of specific configurations rather than individual edges [17].

This heuristic assigns a robustness score to each edge based on how often it appears across the different scenarios. An empty graph is then constructed, containing all nodes but no edges. Edges are added iteratively, ranked by their robustness scores, while ensuring that no cycles are formed. This process mimics Kruskal's algorithm, but instead of minimizing edge cost, it maximizes edge occurrence to construct a spanning tree. In Chapter 4, Scenario Design, this method will be applied to all scenario-generated networks and discussed in detail. The pseudocode below presents the procedure for the maximum occurrence heuristic:

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
    - Pick edge with highest occurrence score.
    - **IF** addition of selected edge creates a cycle **THEN**
        - Remove edge from list.
    - **ELSE**
        - Add edge to network.
    - **END IF**
4. **END WHILE**

3.9 Scenario-Based Robustness Analysis

Although this study refers to the analysis across scenarios as a robustness analysis, it is important to acknowledge its limitations. The set of 20 scenarios considered does not constitute an exhaustive or extreme stress test. Rather, the analysis examines the consistency of adoption dynamics and resulting network configurations within a bounded set of plausible future conditions. This scope enables the identification of infrastructure components that appear consistently across scenarios and can therefore be interpreted as robust within this subset. However, it does not amount to a full robustness assessment, which would require a broader scenario space including more extreme parameter values.

3.10 Assumptions and Limitations

In order to ensure transparency within this study, this section outlines the key modeling assumptions and discusses their potetnail implimications for the interpretation and future research.

- **Positive Influence Based on Similarity:** The model assumes that firms only have a positive influence on each other, and that this influence becomes stronger when firms are more similar. Negative effects, such as competition or differences between firms, are not included. This makes it easier to focus on how adoption can spread through the network, but it may miss some real-world behaviours where firms hold back or compete instead of reinforcing each other. Additionally, the model does not account for the possibility that firms may actively avoid adoption if nearby investments are observed to be unprofitable or excessively costly. Such exclusion simplifies the dynamics under study but risks overlooking critical barriers to diffusion.
- **Static Firm Attributes:** Firm-specific characteristics, including size, demand, and spatial parameters, are held constant throughout the simulation period.
- **Cumulative Infrastructure:** Once a pipeline connection is established, it remains in place for the remainder of the simulation. Decommissioning or repurposing of infrastructure is not included.
- **No External Disruptions:** Broader system-level disruptions, such as policy shifts, regulatory changes, or technological breakthroughs, are not explicitly modelled. Scenario variation is limited to differences in firm behaviour and hydrogen demand.
- **Homogeneous Adoption within Firm Types:** The model assumes that only firms of the same type adopt in each simulation. In reality, adoption can occur across mixed types simultaneously. This assumption allows for a clearer comparison of early adopter strategies by isolating the impact of each firm type on the development of the hydrogen network.
- **Unconstrained Edge Construction:** The network layout assumes that pipelines can be built as straight-line connections between firms, without accounting for real-world spatial, regulatory, or permitting constraints.
- **Simplified Decision Criteria:** Firms base investment decisions on a limited set of non-economic attributes. Detailed financial assessments or market-based criteria are not incorporated.

- **Terminal Availability Assumed:** The model assumes that ammonia import terminals will be operational. In reality, these terminals are still in early planning or construction phases, which introduces uncertainty into infrastructure feasibility.
- **Ammonia as Sole Carrier:** Ammonia is assumed to serve only as a hydrogen carrier. Other potential applications or uses of ammonia are not modelled.
- **No Investment Timing Lags:** The time required to complete infrastructure investments is not included. All adoption and construction occur instantaneously within each timestep.
- **Positive influence based on similarity:** The model assumed only a positive influence based on their similarity, whilst this might not be realistic
- **Simplified Investment Logic:** One of the main limitations of the model concerns the simplified representation of investment decision-making among firms. In reality, infrastructure investments are shaped by a complex interplay of financial, regulatory, strategic, and institutional factors, many of which are dynamic and context-specific. The model abstracts from this complexity by reducing investment behaviour to a threshold-based adoption mechanism driven by interdependencies, peer influence, and static firm attributes. As a result, it does not capture the full range of economic, technical, and strategic considerations that influence whether and when firms commit to infrastructure investments. This simplification may lead to an overestimation of both the adoption rate and the speed of network development.

3.11 Data Sources and Parameterization

The input data used in the model is derived from real-world sources, primarily provided by Power2X. This dataset focuses on the Rotterdam Industrial Cluster (RIC) and includes internal estimates of hydrogen and ammonia demand developed by Power2X. It is important to note that these figures represent one possible method of estimating hydrogen demand and do not necessarily reflect the official perspective of Power2X. Demand is expressed in hydrogen-equivalent units and estimated using firm-level CO_2 emissions as a proxy. Hydrogen-equivalent demand refers to the combined demand for green hydrogen and ammonia. This demand data serves as the basis for assigning firm-specific attributes related to hydrogen trade volume. Hydrogen trade volume represents the demand and supply patterns of firms. All demand and supply values refer to projected hydrogen-equivalent demand in 2030.

The model also incorporates firm-specific characteristics, including plot size and spatial location. These values were derived from Power2X's data in collaboration with the Port of Rotterdam on industrial land use and firm siting.

3.12 Model Verification

To ensure consistency and correctness across both the threshold-based adoption model and the ONTL optimization module, several verification steps were conducted. For the adoption model, each firm was assigned a set of attributes with corresponding normalised scores, reflecting differences in importance within each attribute. These attributes were used to derive a firm specific adoption threshold. Firms were modeled as nodes in a graph, with edge scores representing inter-firm influence. Adoption was triggered only when the cumulative influence from neighboring nodes exceeded a firm's threshold, thereby preserving the core logic of the threshold model. Additionally, early adopters were predefined and activated at the initial timestep to initiate the diffusion process. When a specific firm decided to adopt, its threshold was visually checked and compared to the level of influence from its active neighbours to ensure that the adoption resulted from the threshold being exceeded.

Verification of the ONTL component confirmed its capacity to compute cost minimal pipeline networks under dynamic supply and demand conditions. Each simulation run validated that the network generated was a minimum cost spanning tree, subject to the presence of supply and demand nodes. The model also incorporated existing connections across timesteps, ensuring continuity in infrastructure development. This means that once a connection was established in an earlier timestep, it remained in place and was used in subsequent timesteps in the ONLT.

To validate the accuracy of the cost and flow computations, constructed edges and their lengths were manually reviewed for each final network configuration. Edge capacities were cross-checked to confirm they were correctly used in cost calculations. For each edge, total cost was computed as the product of its Euclidean length and its capacity raised to a cost exponent, reflecting scale economies.

Finally, visual inspection supported the overall validation process. Time series plots were generated to track adoption patterns and network growth, confirming model behavior aligned with expectations across all tested scenarios.

4

Case Context and Firm Selection: The Port of Rotterdam Industrial Cluster

This chapter explains the rationale behind the selected case study. The Rotterdam Industrial Cluster (RIC) was chosen as the central case due to its strategic importance and unique characteristics in the context of the Dutch and broader European energy transitions [43]. As the largest seaport in Europe, it serves as a major industrial hub with significant activity in the energy, chemical, and manufacturing sectors. It hosts a high concentration of energy intensive industries, making it a substantial source of greenhouse gas emissions and a key focus area for decarbonisation efforts [45].

The dense spatial configuration of the RIC supports the development of shared infrastructure, such as pipelines and storage facilities, thereby offering opportunities for economies of scale. Moreover, the RIC functions as a primary entry point for hydrogen and potential green ammonia imports, and it is home to several strategic infrastructure projects aimed at accelerating hydrogen value chain development [43]. Finally, the Port of Rotterdam has previously been used in Power2X modelling studies, which allows for continuity in data, stakeholder engagement, and model validation.

4.1 Company Selection Criteria

In this study, companies were selected for inclusion in the model based on a set of predefined criteria to ensure their relevance to the hydrogen transition within the Port of Rotterdam. The primary criterion was that a firm must operate, or plan to operate, on an industrial plot within the Port of Rotterdam. This could include an industrial site, facility, or import terminal.

Second, the firm must demonstrate a significant hydrogen related trade volume, either through hydrogen itself or via green ammonia as a hydrogen carrier. Third, firms were included only if they fulfil a key function in the hydrogen supply chain, such as production, import, storage, or large-scale consumption. Finally, firms were included if they had previously featured in Power2X models focused on hydrogen or ammonia developments in the Port of Rotterdam. The table below provides an overview of the companies selected for this study, based on the defined criteria. Some firms may function as both hydrogen consumers and suppliers. In this model, their classification is determined by the availability of data on either their hydrogen demand or supply. Future research could further investigate the dual roles that some firms may occupy, and how these differing roles influence the adoption process within the Rotterdam Industrial Cluster.

ID	**Company**	**Short Description**
0	LyondellBasell	Major chemical company and hydrogen consumer.
1	Uniper	Hydrogen consumers which uses hydrogen to decarbonise their energy intensive production facilities and industrial processes.
2	HES	Storage provider with port infrastructure.
3	BP	International energy company and hydrogen consumer.
4	Eneco	Renewable energy firm developing green hydrogen projects for hydrogen supply.
5	OCI	Importer focused on ammonia and hydrogen derivatives.
6	Gunvor	Energy trading firm, active in hydrogen supply.
7	ExxonMobil	Global oil and gas company with hydrogen use (consumer) potential.
8	Vopak	Storage company with terminal infrastructure.
9	Huntsman	Chemical manufacturer and hydrogen user.
10	Air Products	Hydrogen supplier and technology provider.
11	Advario	Storage operator active in energy logistics.
12	Chane	Terminal operator focused on bulk storage (storage provider).
13	Air Liquide	Industrial gas producer and hydrogen supplier.
14	ACE Terminal	Planned ammonia import terminal in the port.
15	Air Product and Gunvor Terminal	Joint import terminal project for hydrogen and ammonia imports.
16	VTTI Storage Terminal	Infrastructure for storage of energy carriers.
17	Chane Import Terminal	Planned import terminal for green ammonia.
18	Nobian	Chemical firm producing hydrogen.
19	Shell	Integrated energy company investing in hydrogen and hydrogen supply.

Table 4.1: Overview of firms included in the simulation model

To connect the threshold model to the real-world context of the Rotterdam Industrial Cluster (RIC), Figure 4.1 presents a concrete example of firm locations within the Port of Rotterdam,with each firm represented by its node ID as listed in Table 4.1. In this example, company types are distinguished by node colour, allowing visual differentiation of the various firm types represented in the model.

Figure 4.1: Example of firm locations in the Port of Rotterdam

The specific colour assigned to each company type is detailed in Figure 4.2. Table 4.1 also lists the identification number assigned to each firm, as shown in the corresponding figure.

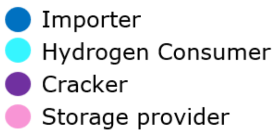


Figure 4.2: Legend of company types and their corresponding node colours.

In conclusion, the Rotterdam Industrial Cluster is an ideal case study for applying threshold and network modelling due to its complexity and diverse industrial landscape. Its high concentration of energy intensive industries positions it as a pivotal hub for hydrogen and ammonia trade, as well as for the development of shared infrastructure. The presence of a wide range of actors allows the model to capture varying adoption thresholds and strategic behaviours. This combination of industrial heterogeneity, strategic relevance, and data availability makes the RIC particularly well suited for analysing hydrogen infrastructure development.

5

Scenario Design

5.1 Scenario Matrix and Adoption Strategy Analysis

To examine how varying future conditions and early adoption behaviors influence the development of hydrogen infrastructure in industrial clusters, this study applies a structured scenario design approach. Given the high level of uncertainty in the energy transition, this analysis does not rely on just one possible future outcome. Two scenario dimensions are distinguished: hydrogen demand and ammonia import volumes. Changes in hydrogen demand affect hydrogen consumers, while shifts in ammonia import volumes primarily influence import terminal operations. These dimensions are systematically combined with four early adopter profiles, resulting in twenty unique simulation cases.

The hydrogen demand scenarios reflect uncertainty in the pace and scale of the energy transition, which are influenced by factors such as technological adoption, policy incentives, and firm-level commitments [6]. These varying demand levels directly affect hydrogen consumers. Their willingness to invest depends on their anticipated future demand, which in turn determines whether their individual investment thresholds are met.

Secondly, the hydrogen import scenarios capture uncertainty in future import volumes, global energy flows, and the strategic role of the Port of Rotterdam. These scenarios primarily affect the import terminals, for which the exact future volumes remain uncertain and are still under development.

For both scenario dimensions, three levels are considered: low, medium (serving as the base case), and high. Since the data from Power2X provides hydrogen-equivalent values, the medium hydrogen demand and medium ammonia import scenarios are combined to define the base case.

To systematically explore how different early adoption configurations affect the development of hydrogen infrastructure in industrial clusters, the model defines four distinct early adopter configurations based on company type. These configurations reflect varying assumptions about which firms adopt hydrogen in the initial time step. The selection of early adopters is critical, as their position in the value chain and their interdependencies determine how influence propagates through the network and which infrastructure segments are prioritized during the early stages of development.

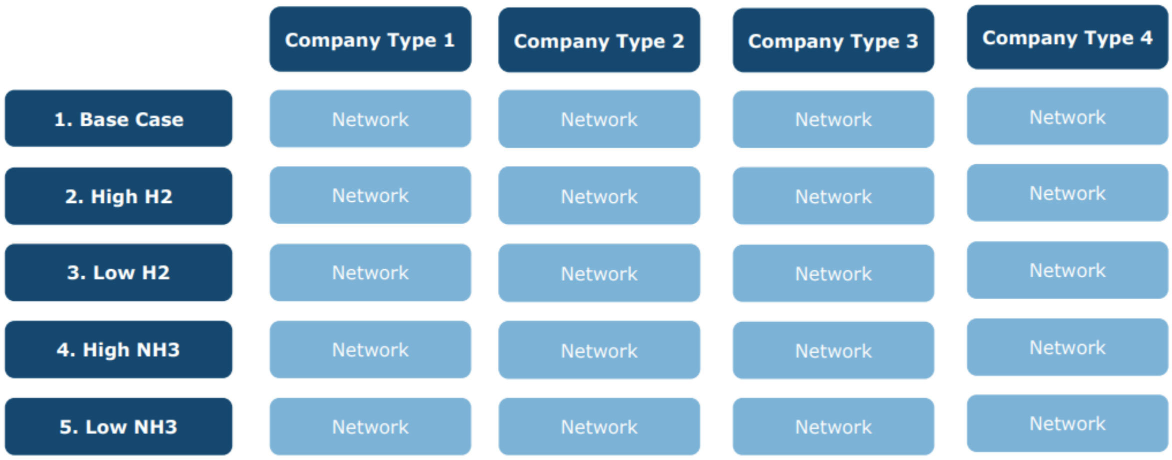


Figure 5.1: Overview of scenario and early adopter combinations used in the simulation.

The full experimental design consists of 20 distinct network configurations, created by combining five future scenarios with four early adopter configurations, as shown in Figure 5.1. For each scenario–adopter combination, the simulation proceeds in two steps. First, the threshold model simulates how adoption spreads through the network, based on the specified early adopter configuration. Second, the ONLT model generates a cost-efficient infrastructure layout at each time step, translating behavioral dynamics into spatial outcomes. This approach enables dynamic modeling of both behavioral diffusion and physical infrastructure development under varying future conditions.

The scenarios serve two distinct analytical purposes in this study. First, the robustness analysis identifies infrastructure segments that consistently emerge across multiple scenario–adopter combinations. Based on this analysis, one robust infrastructure layout is derived from the full set of simulations. Second, the early adopter configurations were analysed to evaluate the performance of different adoption strategies, presented in Figure 5.2. By comparing total infrastructure costs across these strategies, this analysis informs strategic decision-making regarding where to prioritize incentives and which adopters to target for early investment.

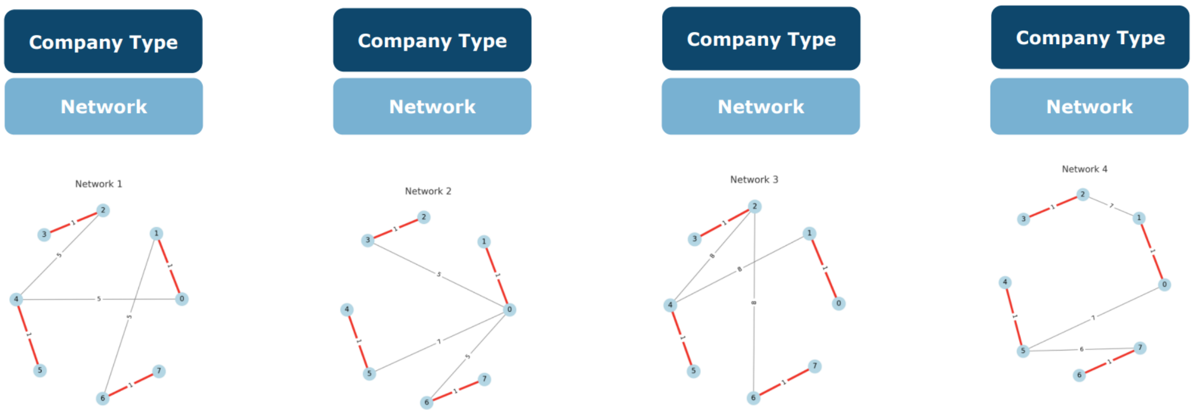


Figure 5.2: Highlighted robust segments across three sample networks

5.2 Conclusion and Use Case

Having outlined the two analytical approaches, it is important to clarify their respective contributions to infrastructure planning under uncertainty. This model applies two distinct approaches to analyse the adoption process. Option 1 assumes no influence over future scenarios or adopter behavior. It supports low-regret, robust planning by identifying infrastructure segments that consistently contribute to network value across a wide range of plausible futures. This means that the robust network is evaluated across all sixteen scenario runs.

Option 2 assumes that early adoption patterns can be partially influenced. This approach supports strategic coordination and the design of targeted incentives by evaluating which early adoption configurations yield the most effective infrastructure outcomes. The comparison is based on the final networks developed under each early adopter configuration, assessed in terms of total cost and pipeline capacity (ktpa).

This framework provides a practical decision-support tool for infrastructure developers, the Port of Rotterdam authorities, government agencies, and project developers such as Power2x. As an active stakeholder in green molecule development, Power2x can apply these insights to prioritise investment and spatial planning decisions, thereby reducing exposure to uncertainty-related risks. Option 2, in particular, offers a basis for evaluating early adopter strategies, enabling informed adjustments to the choice of configurations that may lower infrastructure costs or associated risks. These insights can support the targeting of specific early adopters to facilitate an efficient and coordinated infrastructure rollout.

6

Simulation Results and Network Development

This section presents the findings from applying the dynamic modelling framework to analyze hydrogen network development within the Rotterdam Industrial Cluster. The analysis covers 20 simulations runs, each representing a unique combination of future scenarios and early adopter configurations. The results are structured in three parts. First, the findings from the literature review are discussed to identify which firm attributes may influence investment dynamics within an industrial cluster. Second, all simulations are examined to identify robust pipeline segments that appear consistently across multiple futures, addressing subquestions two and three. Third, the analysis focuses on company type configurations to evaluate the most cost-efficient network associated with each early adopter strategy. This part addresses subquestion four.

6.1 Attribute Identification and Categorisation

This section presents the initial inputs to the dynamic modeling framework, specifically addressing the first sub-question:

> What threshold values and interdependencies exist between companies within the RIC?

The purpose of this section is to explain how firm-specific threshold values and interdependencies were derived. To address this, four attributes were identified based on the predefined selection criteria. These attributes form the foundation of the model and were selected based on data from Power2X, supplemented by insights from the literature and expert knowledge, As described in Section 3.11.

The first attribute incorporated in the model is hydrogen trade volume. This attribute represents each firm's hydrogen demand or supply, measured in kilotonnes per annum (ktpa) of hydrogen equivalent, including both hydrogen and green ammonia. It serves as a proxy for the firm's operational scale and strategic involvement in the energy transition. Firms with higher hydrogen trade volumes are assumed to have a stronger incentive to invest early, as they are more deeply involved in hydrogen value chains [10]. Furthermore, the capacity of the pipeline is directly influenced by the hydrogen trade volumes of different companies [40].

A second attribute is plot size, measured in hectares (ha). This attribute indicates the physical space a firm occupies within an industrial cluster and serves as a proxy for the capacity to accommodate new infrastructure, such as on-site cracking facilities or a large electrolyser. Larger plots are assumed to facilitate easier integration of such infrastructure and reduce spatial constraints, thereby making adoption more feasible. In the model, plot size is incorporated into the threshold calculation based on the assumption that it contributes to a firm's logistical readiness to invest.

Third, the attribute grid connection is incorporated into the threshold model. This attribute quantifies the estimated electrical capacity (in megawatts, MW) available to each firm. Due to the unavailability of direct grid connection data, estimates were derived from each firm's current industrial activity and publicly announced future projects. This attribute is relevant because a higher estimated electrical capacity indicates that a firm is better positioned to implement energy-intensive infrastructure on its site, such as an ammonia cracker. These installations require a stable and robust grid connection [52]. In the threshold model, stronger grid connections lower a firm's threshold, thereby increasing its likelihood to invest.

The fourth attribute included in the model is company type, which reflects the strategic role a firm plays within the hydrogen and ammonia value chains. These roles include hydrogen consumers, hydrogen suppliers, storage providers, and import terminals. The relevance of this categorisation lies in the differentiated strategic significance of these roles and the extent to which firms are willing to engage in the energy transition. For example, import terminals may carry substantial strategic weight due to their infrastructural positioning, while hydrogen consumers may also hold strategic relevance through their influence on offtake certainty. Both categories, despite differing operational functions, are instrumental for the efficient rollout of infrastructure and a coordinated transition. Their relevance further suggests a higher probability of early adoption behaviour.

In conclusion, the selection of these specific attributes was guided by their direct relevance to investment decision-making within industrial clusters, as well as by their objectivity and measurability. Each attribute reflects a key dimension of operational readiness in the context of the emerging hydrogen and ammonia value chains. As these attributes are primarily based on objective data or structurally derived estimations, they enhance the transparency and reproducibility of the modelling process.

Table 6.1: Overview of firm-level attributes used in the threshold model

Attribute	Description and Rationale
Hydrogen Trade Volume	Represents each firm's hydrogen demand or supply (in ktpa). Serves as a proxy for operational scale and involvement in hydrogen value chains. Higher volumes indicate greater likelihood of early investment.
Plot Size	Measured in hectares (ha). Reflects the physical footprint of a firm and its capacity to integrate new infrastructure. Larger plots suggest fewer spatial constraints and higher readiness.
Grid Connection	Estimated electrical capacity (in MW). Derived from current activities and planned projects. Indicates whether a firm can support energy-intensive infrastructure such as ammonia crackers.
Company Type	Categorical role in the value chain (e.g., consumer, supplier, storage, import). Reflects strategic importance and engagement level in the energy transition. Different roles imply different adoption thresholds.

6.1.1 Hydrogen Trade Volume: Category Boundaries

Based on the hydrogen trade volume data and the boundary selection method described in the methodology, the following categories were defined. The low category includes firms with volumes below 30 ktpa, typically smaller actors with limited involvement in hydrogen trade. The medium category ranges from 30 to 150 ktpa and represents the majority of industrial firms. The high category consists of firms with volumes above 150 ktpa, which are strongly embedded in the hydrogen supply chain. The histogram below is cropped to enhance the visibility of the low and medium categories and to clearly illustrate the defined thresholds.

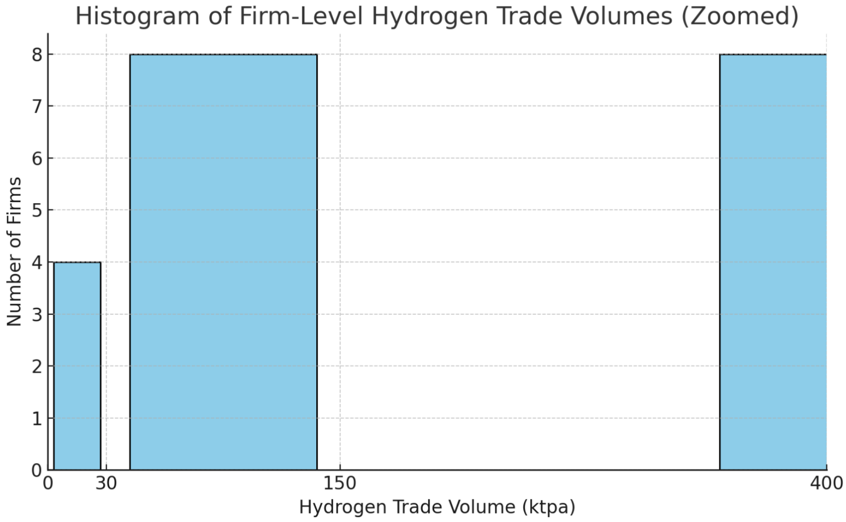


Figure 6.1: Categorisation of Firms by Hydrogen Trade Volume (ktpa)

6.1.2 Grid Connection: Category Boundaries

Based on the bar chart in Figure 6.2, the following boundaries were established. The low category includes firms with relatively limited electrical capacity, defined as 50 MW or less. This group consists of five companies, three of which are storage firms. Their operations require less grid capacity. The mid range includes the majority of firms and is assumed to represent sufficient grid capacity to support moderate infrastructure investments. This category is defined by grid capacities between 50 MW and 250 MW. The high category contains firms with significantly larger grid capacity, showing an increase relative to the medium group. For example, Eneco falls within this category, with a grid connection of 800 MW. This is linked to their planned large scale green hydrogen project, which is expected to become operational in 2029 with a capacity of 800 MW [38]. An overview of the estimated grid capacities is provided in Appendix A. Due to limited data availability, the estimation relied on the known total annual electricity demand of 602.5 MW for a cluster that includes Nobian, Huntsman, Air Liquide, and Shin-Etsu. This total was evenly divided among the four companies, resulting in an estimated grid connection capacity of 150.63 MW per company. This estimate aligns with the scale of other approximations based on the observed activities on their respective plots.

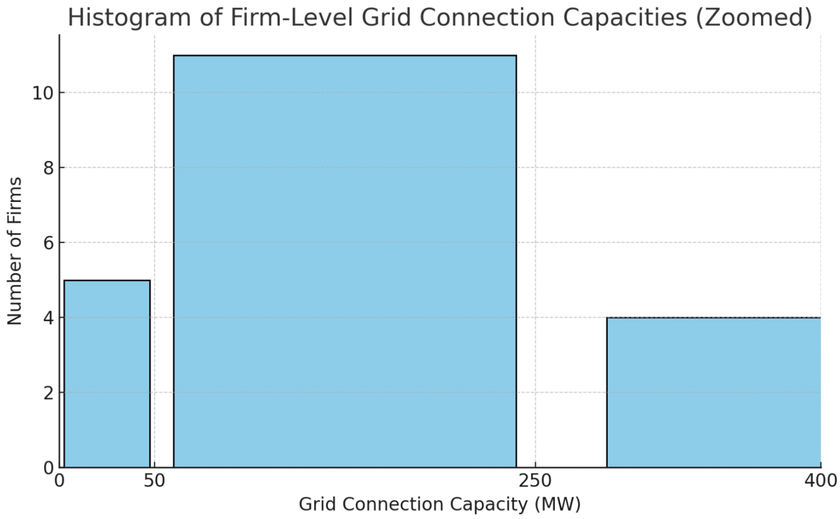


Figure 6.2: Categorisation of Firms by Grid Connection Capacity (MW)

6.1.3 Plot Size: Category Boundaries

Based on the histogram in Figure 6.3, the final numerical attribute was divided using the following boundaries. The low category, defined as 30 hectares or less, includes firms with limited spatial capacity, which may constrain on site infrastructure investments. The medium category represents the majority of firms, with moderate space availability ranging from 30 to 100 hectares. The high category comprises large scale firms with high logistical readiness. This distribution satisfies the requirement that no category includes more than 60 percent of firms, and each category contains at least 20 percent.

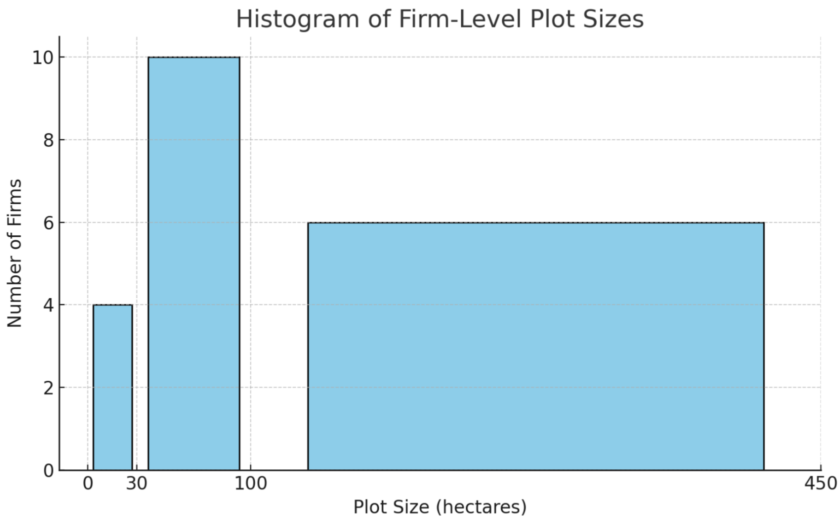


Figure 6.3: Categorisation of Firms by Plot Size (hectares)

6.1.4 Company Type: Category Boundaries

The final attribute, company type, is categorical. Scores for this attribute were assigned based on expert interviews, as described in the methodology chapter. Experts were asked to evaluate hypothetical firm comparisons and indicate which firm was more likely to adopt first. The frequency with which each company type was cited was normalised to obtain a relative score. These outcomes are presented in Table 6.2. The complete results are provided in the appendix (Table A.4).

Company Type	**Assigned Score**
Import Terminal	0.9
Storage Provider	0.8
Hydrogen Supplier	0.6
Hydrogen Consumer	0.5

Table 6.2: Assigned scores for company types in the threshold model

6.2 Firm Thresholds and Edge Scores in the Influence Network

This section presents the firm specific threshold values and the inter firm connection scores that define the degree of influence between nodes in the threshold model. Each firm is assigned a threshold that reflects its readiness to invest, based on a weighted combination of attribute scores. The model assumes a fully connected graph in which each firm has the potential to influence all others. However, the strength of this influence varies and is determined by attribute similarity, as described in Section 3.5.3.

Together, these two components form the core mechanism of the threshold model. Threshold values govern the timing and likelihood of individual firm adoption, while edge scores determine how adoption spreads through the network. An overview of the firms in the RIC case and their corresponding threshold values is provided in Table 6.3.

Node	Company	Company Type	Threshold
0	LyondellBasell	Hydrogen consumer	0.5
1	Uniper	Hydrogen consumer	0.325
2	HES	Storage provider	0.2
3	BP	Hydrogen consumer	0.375
4	Eneco	Hydrogen supplier	0.4
5	OCI	Importer	0.4
6	Gunvor	Hydrogen supplier	0.475
7	ExxonMobil	Hydrogen consumer	0.25
8	Vopak	Storage provider	0.375
9	Huntsman	Hydrogen consumer	0.45
10	Air Products	Hydrogen supplier	0.625
11	Advario	Storage provider	0.5
12	Chane	Storage provider	0.375
13	Air Liquide	Hydrogen supplier	0.4
14	ACE Terminal	Importer	0.325
15	Air Product and Gunvor Terminal	Importer	0.375
16	VTTI Storage Terminal	Storage provider	0.375
17	Chane Import Terminal	Importer	0.3
18	Nobian	Hydrogen supplier	0.475
19	Shell	Hydrogen supplier	0.325

Table 6.3: Overview of companies with their node numbers, company types, and thresholds

From Table 6.3, it can be observed that firms such as ExxonMobil (0.25), Uniper (0.325), and BP (0.375) have relatively low threshold values. This suggests that these hydrogen consumers are more likely to adopt early, once a small proportion of other firms have already adopted. Their low thresholds may indicate that they are operationally prepared to transition to hydrogen quickly, potentially due to pressing decarbonization requirements.

Furthermore, storage providers exhibit more moderate threshold values, such as HES (0.20), Chane (0.375), and Advario (0.50). These firms may adopt more reactively, requiring a higher level of surrounding adoption before committing. This is likely due to their reliance on both upstream hydrogen supply and downstream demand, which makes their investment decisions more dependent on developments elsewhere in the network. In addition, importers also cluster around mid range threshold values, typically between 0.3 and 0.4.

Hydrogen supplier show both end of the spectrum. For example, Air Products has a relatively high threshold (0.625), while Shell displays a more moderate value (0.325). This variation reflects that some suppliers may only commit to investment once a substantial network and stable demand are in place, whereas others may be more likely to adopt earlier under less certain conditions.

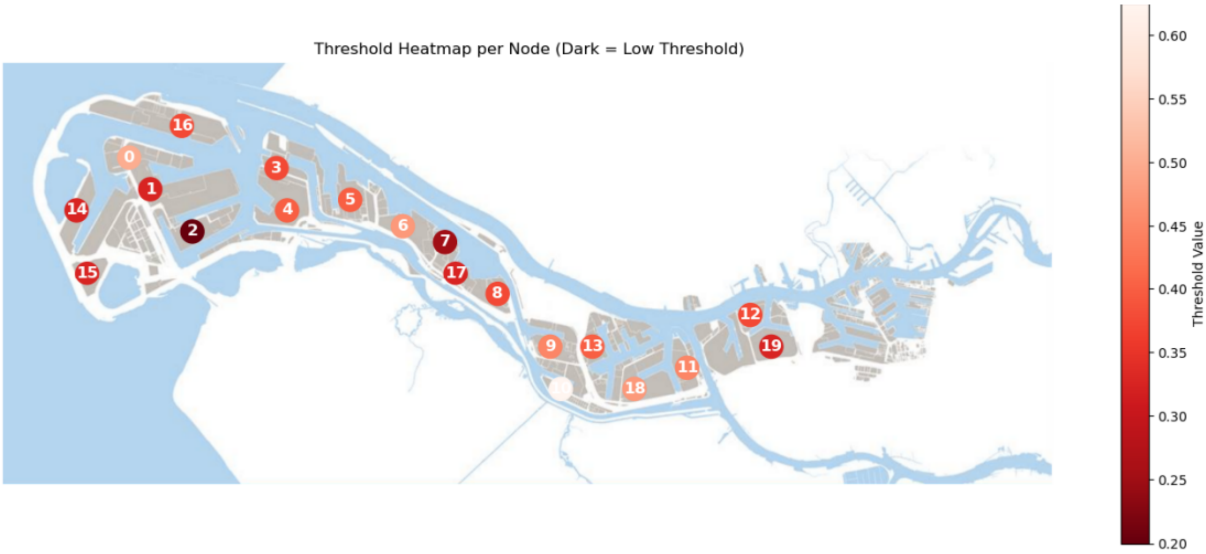


Figure 6.4: Threshold Heatmap

Figure 6.4 presents a heatmap visualisation of the distribution of threshold values, where high thresholds are shown in dark red and lighter colours indicate lower thresholds. Overall, the threshold values appear to be evenly distributed across the cluster. However, a distinct grouping of firms with low thresholds can be observed, including Huntsman (9), Advario (11), Air Liquide (13), and Nobian (18). This suggests that these firms are likely to participate early in the adoption process.

In addition to firm specific thresholds, the edges and their associated scores determine how influence propagates through the network. Figure 6.5 displays the five most influential edges between firms, indicating the strongest channels of influence. As shown in Table 6.4, both OCI (5), an import terminal, and HES (2), a storage provider, are involved in three of the top five edges. This suggests that these firms hold central positions in the network and can be considered highly influential in the adoption process.

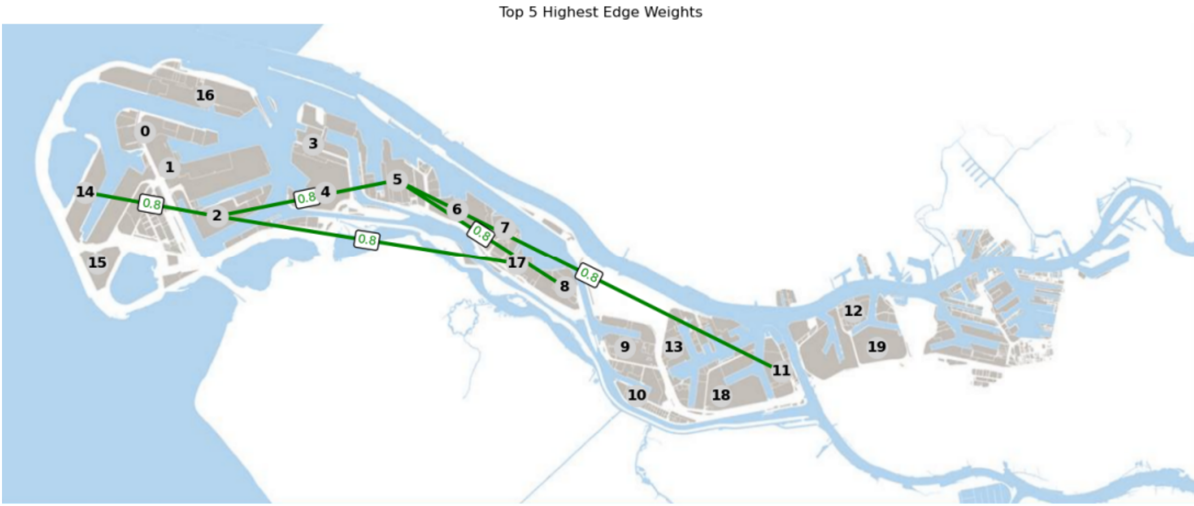


Figure 6.5: Important Edges

Rank	Edge (Node1, Node2)	Score
1	(2, 5)	0.8
2	(2, 14)	0.8
3	(2, 17)	0.8
4	(5, 8)	0.8
5	(5, 11)	0.8

Table 6.4: Top 5 Highest Edge Scores in the Network

In contrast, Figure 6.6 presents the five edges with the lowest influence values within the threshold model. Notably, Lyondell (0) is involved in three of these edges, indicating that the firm has limited influence on the adoption behaviour of others in the network. This can be attributed to Lyondell's low attribute similarity with other firms in the network. As a result, its adoption decisions are unlikely to trigger cascading investments among neighbouring firms.

Figure 6.6: Important Edges

Rank	Edge (Node1, Node2)	Score
1	(0, 6)	0.300
2	(0, 18)	0.300
3	(0, 10)	0.325
4	(3, 6)	0.350
5	(3, 18)	0.350

Table 6.5: Top 5 Lowest Edge Scores in the Network

6.3 Adoption and Network Development: Overview and Approach

This section presents the simulation results related to adoption patterns and infrastructure network development. A total of 20 simulations were conducted, covering all combinations of five scenario settings and four early adopter configurations. Due to the scope and the level of detail of the results, this section focuses on the most relevant and analytically insightful outcomes.

To clarify the underlying logic of the dynamic modelling approach applied to adoption and infrastructure development, one illustrative example is explained in detail. This example reflects the base case scenario, defined by a medium hydrogen demand and medium hydrogen supply configuration. The analysis focuses specifically on the hydrogen supplier configuration. This case illustrates how firm-specific adoption thresholds are translated into observed adoption patterns and how the ONLT algorithm generates a cost-optimised pipeline layout at each time step.

Following this walkthrough, a synthesis of the key findings across all simulations is presented, with particular attention to shifts in adoption timing, the emergence of strategic nodes, and recurring patterns in infrastructure development. The section concludes with a visual summary of the final robust network layout and the associated infrastructure costs.

6.3.1 Illustrative Case: Base Case Scenario from the Hydrogen Supplier Configuration

This section initiates the analysis of the simulation results on adoption patterns and infrastructure development. The selected case combines the base case scenario, which reflects medium hydrogen demand and medium ammonia import, with the hydrogen supplier configuration.

Threshold Adoption Process

The figure below shows the initial time step of the threshold model, with hydrogen suppliers marked in red. Figure 4.2 in the methodology section provides the legend, including the colour scheme for all company types. The red nodes represent the firms identified as early adopters in this configuration, specifically the hydrogen suppliers. The hydrogen suppliers included in this configuration are:

- Eneco (4)
- Gunvor (6)
- Air Products (10)
- Air Liquide (13)
- Nobian (18)
- Shell (19)

Figure 6.7: Hydrogen Suppliers Location

As shown in the figure 6.7, hydrogen supplier represent a substantial proportion of the firms included in the model, accounting for approximately 36 percent. Since the influence on adoption is determined by the share of already-adopting firms, this relatively high initial uptake increases the likelihood of further adoption in subsequent time steps. The hydrogen suppliers are geographically well distributed across the cluster, suggesting that their influence is also spatially well distributed.

Figure 6.8: Threshold-Based Adoption Status at Timestep 1

Figure 6.8 presents the next time step in the adoption process. In this step, two additional nodes are observed to adopt: HES (2), a storage provider, and ExxonMobil (7), a hydrogen consumer. Their adoption follows the initial decisions made by the hydrogen suppliers. As shown in Table 6.3, HES has a threshold of 0.20 and ExxonMobil a threshold of 0.25, both of which are relatively low compared to the remaining firms in the model. This low threshold indicates a higher readiness to adopt when neighbouring firms have already done so. These low thresholds explain their early adoption. For HES, the low threshold results from favourable infrastructure characteristics, including strong grid connectivity (251 MW) and a large plot size (125 hectares). ExxonMobil has a similar profile in terms of these attributes, but its threshold is noticeably higher. This difference results from the variation in company type scores between HES and ExxonMobil. According to expert interviews, storage providers are considered to have greater strategic importance than hydrogen consumers, which is reflected in their lower threshold values.

Figure 6.9: Threshold-Based Adoption Status at Timestep 2

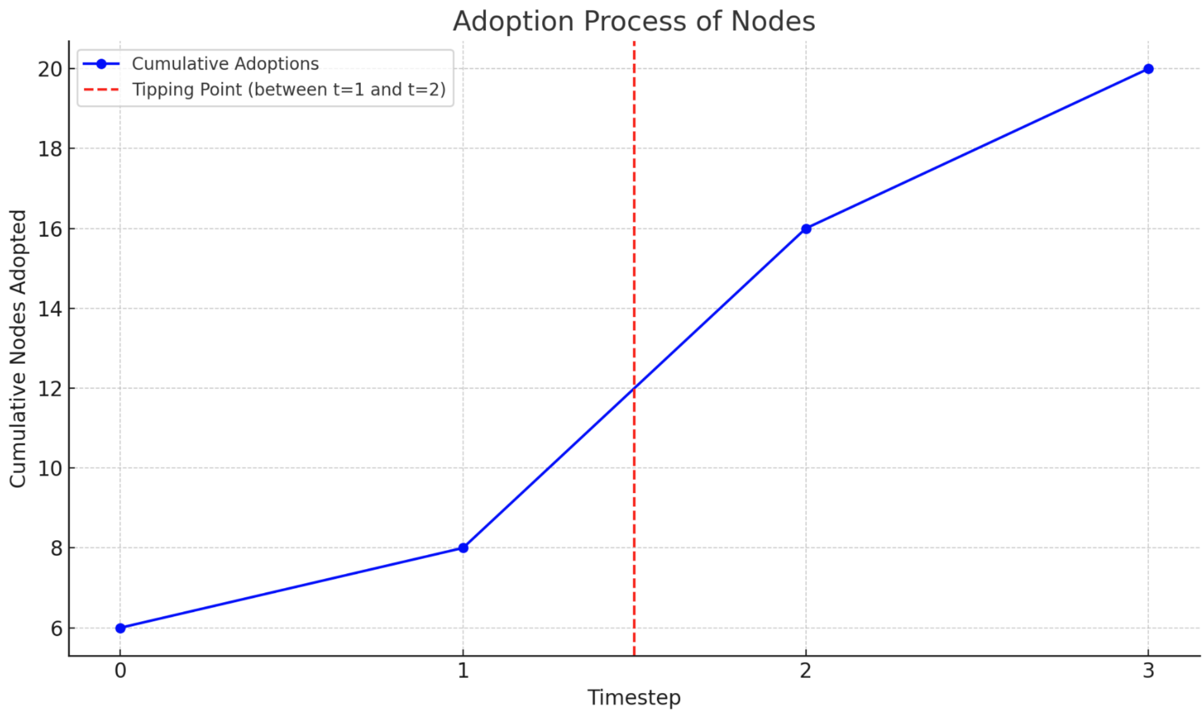


Figure 6.10: Hydrogen Suppliers Location

In the transition from timestep 1 to timestep 2, the model reaches a tipping point in the adoption process, as illustrated in Figure 6.10. At this stage, a significant number of firms adopt, leading to a cascading effect across the network. Whereas only eight firms had adopted in the first time step, the number increases to sixteen in the second. The red dashed line is placed between timestep 1 and timestep 2 to indicate that the tipping point is initiated at timestep 1 but becomes visible in timestep 2. The newly adopting firms are:

Firm	Threshold Value
Uniper	0.325
OCI Import Terminal	0.4
Vopak	0.375
Chane Storage Terminal	0.375
ACE Import Terminal	0.325
Gunvor Import Terminal	0.325
VTTI Storage Terminal	0.375
Chane Import Terminal	0.325

Table 6.6: Threshold values for newly adopting firms at time step two

Among the newly adopting firms, four are storage providers. With HES having adopted in the previous time step, nearly all storage providers have now adopted, except for Advario. Advario's relatively limited grid connection capacity (50 MW) and small plot size (26 hectares) contribute to a higher threshold value. All of these firms exhibit higher thresholds compared to both HES and ExxonMobil, which aligns with their later adoption timing.

At this point in the simulation, only three firms have not yet adopted: BP, Huntsman, and Advario. Apart from Advario, a storage provider, the remaining firms are hydrogen consumers. BP presents an interesting case. Although its threshold is equal to that of Vopak, VTTI Storage Terminal, and Chane Storage Terminal (all 0.375), it has not yet adopted. This difference results from the lower level of influence BP receives in the previous time step. The strength of social ties and the selection of firm attributes determine the level of influence. Despite BP having more favourable attribute values than Vopak, as shown in the table below, it remains less influenced due to its classification as a hydrogen consumer.

Storage providers are considered to have greater strategic importance than hydrogen consumers, which results in a higher influence they receive within the model. This attribute makes them more likely to respond to nearby adopters, which increases their chances of adopting early.

Table 6.7: Comparison of firm characteristics: BP and Vopak

Attribute	BP	Vopak
Company Type	Hydrogen Consumer	Storage provider
H_2 Trade Volume	108 ktpa	75 ktpa
Grid Connection	250	50
Plot Size	250	100

Figure 6.11: Threshold-Based Adoption Status at Timestep 3

ONLT Network Development

The results from the threshold model form the basis for simulating the development of the hydrogen network. The ONLT algorithm generates a cost-optimised network layout by matching the demand and supply of the nodes that are active at a given time step. A network connection is only established when both demand and supply nodes are present. For example, if only supply nodes are active, no pipeline construction occurs. In this illustrative case, the first time step includes only supply nodes, as shown in Figure 6.12.

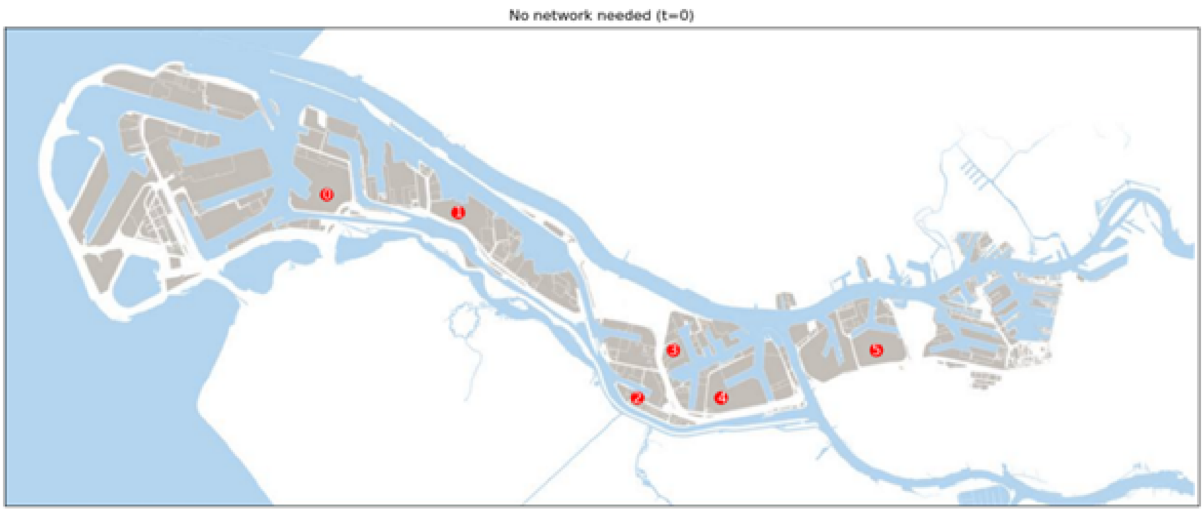


Figure 6.12: Network state at timestep 0 in the Hydrogen Supplier First configuration

In the next time step, new firms are added based on the adoption outcomes from the threshold model. These include HES, a storage provider, and ExxonMobil, a hydrogen consumer. Because the assumption is made that supply and demand must be balanced before the network can be constructed within the ONLT framework, storage providers are assigned sufficient demand to absorb any excess supply. This keeps the model in balance and makes network construction possible using the 2030 data.

Figure 6.13 displays the resulting network configuration. Three edges are constructed in this time step. One connects HES(0) to Eneco(1). The other two form a longer route, connecting Gunvor(2) to ExxonMobil(3) and then ExxonMobil to Air Liquide(5), as shown in Figure 6.13.

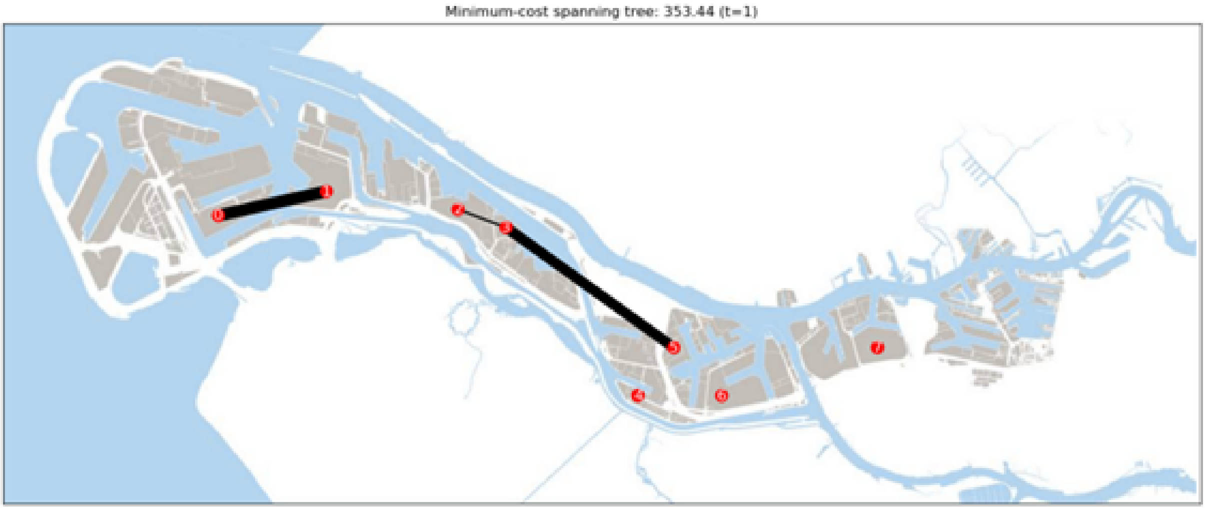


Figure 6.13: Network development at timestep 1

There is one pipeline connection for HES, which is sufficient to meet its full demand. In contrast, ExxonMobil, with a comparable demand level, requires two connections. This is notable because Air Liquide alone could supply 200 units, enough to meet ExxonMobil's demand. Nevertheless, the ONLT selects the two-pipeline solution as cost optimal. This outcome highlights how the algorithm prioritises overall cost efficiency over direct supply capacity, even when a single source appears sufficient. Figure 6.14 provides a simplified overview of the connections established in timestep 1, including the corresponding flows over these pipelines in kilotonnes per annum.

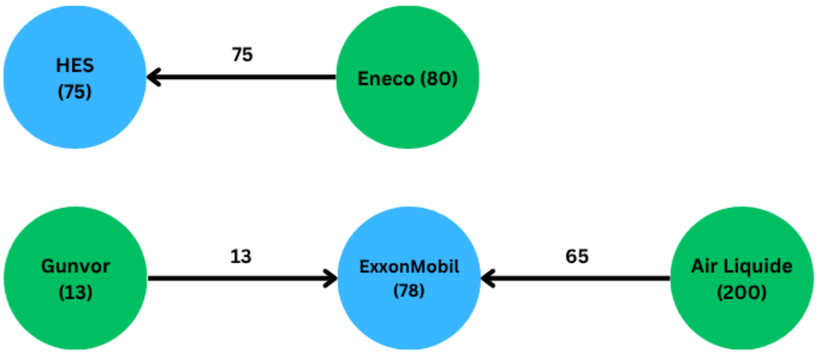


Figure 6.14: Simplified overview of pipeline connections

According to the threshold model, a tipping point occurs in the next time step, resulting in a total of sixteen adopting firms. In the ONLT, connections established in earlier time steps are treated as existing infrastructure in subsequent steps. This is illustrated in Figure 6.15, where existing connections are shown in blue and newly constructed connections are indicated in black. The new connections result from the adoption of firms that add both supply and demand capacity to the network.

A notable observation in this configuration is the isolation of the connection between HES and Eneco. While most other nodes become integrated into the larger network, this link remains disconnected. A similar development is observed on the right side of the port, between Chane Storage Terminal (8) and Shell (19). These isolated connections suggest that nearby firms are more likely to construct separate pipelines to meet their demand. This is primarily due to the limited residual capacity of the existing pipeline. In the case of HES and Eneco, the pipeline has a capacity of 75 units, which is already fully utilised.

By contrast, the other two existing connections are well integrated into the broader network. This can be attributed to the higher residual supply capacity of Air Liquide compared to Eneco. Eneco has a maximum supply of 80 kilotonnes per annum, of which 75 are already allocated to HES. Air Liquide, on the other hand, has a capacity of 200 kilotonnes per annum, with only 65 utilised by ExxonMobil. This makes Air Liquide a more attractive connection point in subsequent optimisation steps due to its remaining supply potential.

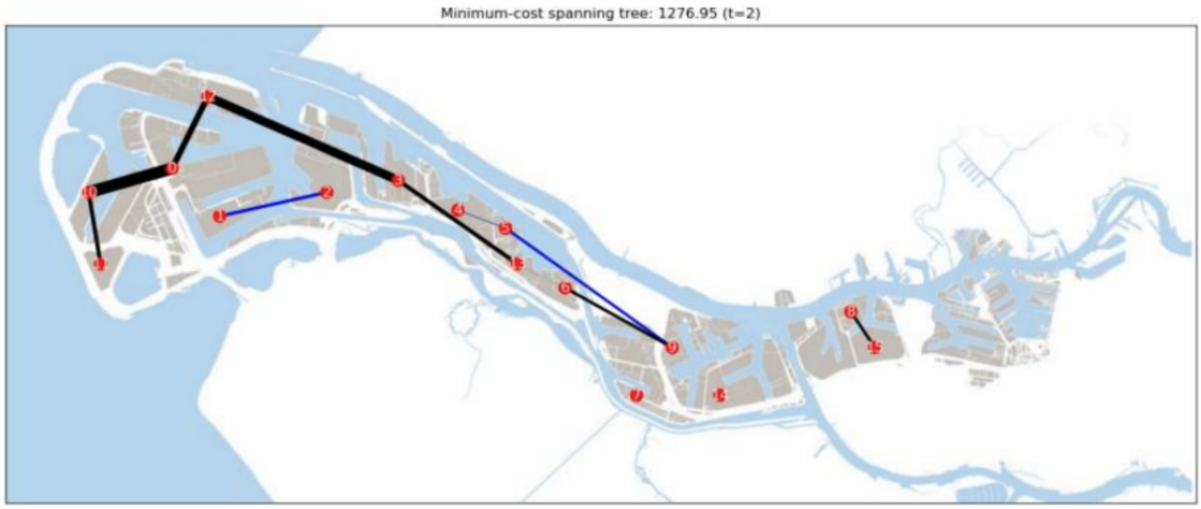


Figure 6.15: Network development at timestep 2

As shown in Figure 6.16, in the later stages of the simulation, the adoption of Lyondell (0), a hydrogen consumer, introduces new infrastructure requirements. To enable hydrogen delivery to this firm, two new pipeline connections are required: one linking HES (2), a storage provider, to Uniper (1), and another connecting Uniper (1) to Lyondell (0). Lyondell's demand places additional pressure on the network, resulting in capacity constraints that necessitate the upgrade of the existing pipeline between HES (2) and Eneco (4), indicated in purple.

In addition, two more connections are established in response to Lyondell's adoption. One pipeline links Eneco (4) to BP (3), a hydrogen consumer, while another connects Eneco (4) to the Chane Import Terminal (17), thereby increasing the available supply. These additions reflect how late-stage adoption by a large consumer can trigger both retrofitting of existing infrastructure and costly expansion of the network.

Ultimately, Lyondell's entry into the network leads to the construction of two new pipelines and the upgrading of one existing connection. This outcome underscores the inefficiencies that can result from uncoordinated early-stage planning, particularly when large-scale demand emerges after the initial network structure has been established.

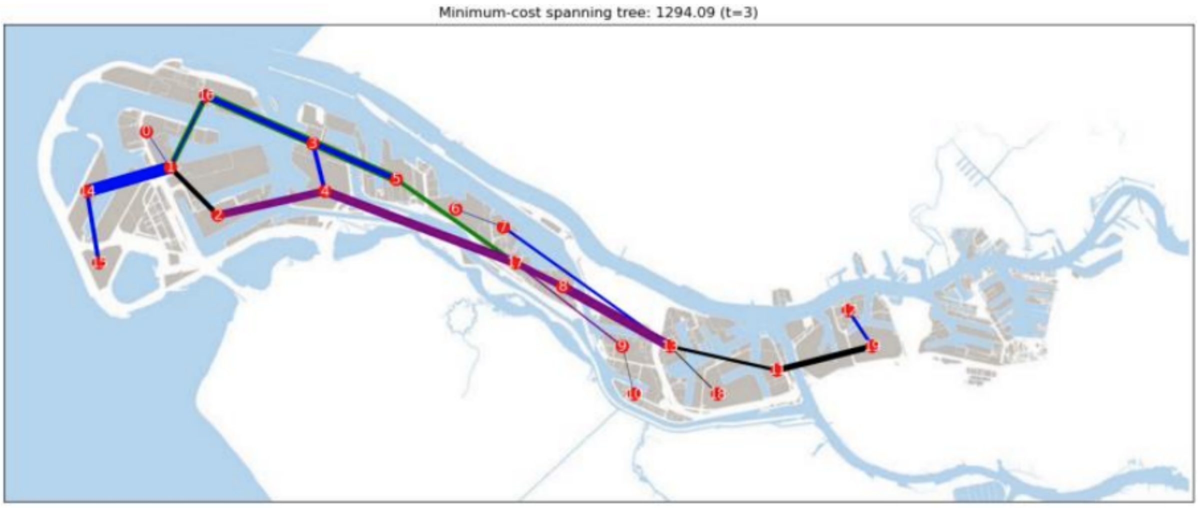


Figure 6.16: Network development at timestep 3

Figure 6.17 presents the final network configuration in the base case scenario, where hydrogen suppliers act as early adopters. Due to inefficiencies and uncertainty in both network development and firm adoption, the resulting network is not cost optimal. As illustrated in figure 6.17, the final layout contains a cycle. The presence of a cycle indicates redundant connections between firms, meaning that multiple pathways exist for hydrogen flow between specific nodes.

While such redundancy may enhance network reliability, it also results in additional infrastructure costs that are not strictly necessary. Given that the ONLT aims to construct cost efficient pipeline systems, it may seem contradictory if the final network does not reflect the most cost optimal layout. This outcome arises from the timestep based construction of the hydrogen network, where the network evolves sequentially as new firms adopt. Each stage builds on the previous one, introducing path dependencies. Once an edge is constructed in an earlier timestep, it remains fixed in the network. If the network were optimised in a single step with complete knowledge of all future adopters, the resulting layout would be more cost efficient. However, by simulating network development over time, the model captures more realistic decision making under conditions of uncertainty.

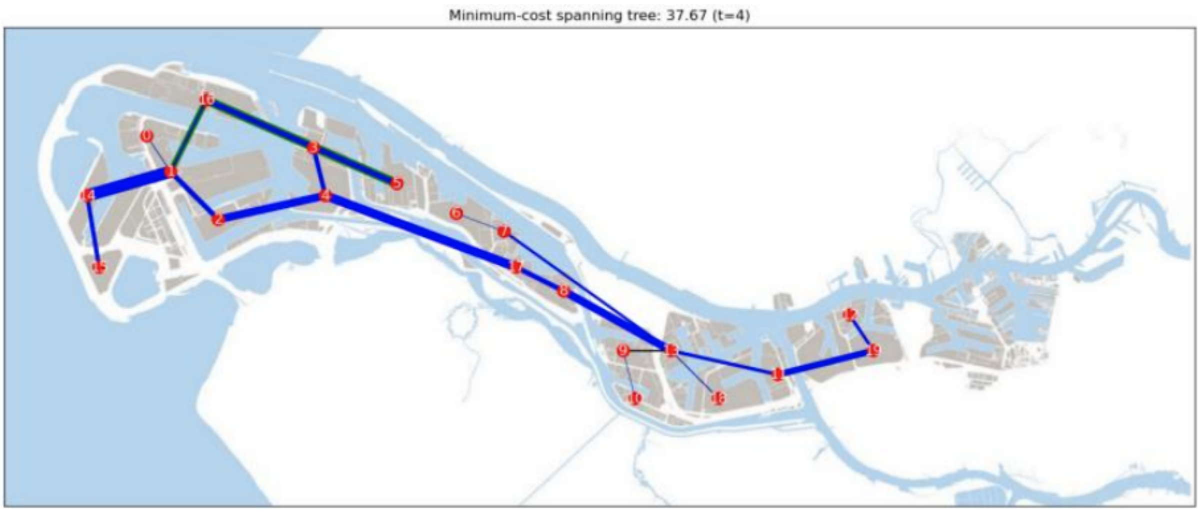


Figure 6.17: Final network configuration at timestep 4

6.4 Comparative Analysis of Adoption and Network Development

This section analyses the key patterns that emerge across sixteen distinct scenario–adopter simulation runs. One adopter configuration, in which hydrogen consumers were selected, did not result in a viable network construction. In this case, the threshold model triggered adoption only on the demand side, leaving no available supply to generate a network within the ONLT. The focus lies on non-redundant and analytically relevant developments that improve understanding of the complex adoption process, rather than on a comprehensive presentation of each individual network layout. The complete network developments are provided in Appendix Chapter D.

The objective of this comparative analysis is to explore how different adoption dynamics and infrastructure trajectories evolve under uncertainty. The analysis is structured around three main analytical lenses. First, it examines how variation in scenario assumptions and early adopter configurations influences firm-level adoption patterns. Second, it identifies which firms are most likely to function as strategic hubs within the developing network. Third, it highlights recurring suboptimal network features, including the formation of long pipeline segments or network cycles that arise due to specific adoption sequences.

This synthesis aims to provide actionable insight for future infrastructure planning in industrial clusters, with particular emphasis on cost efficiency and network robustness.

6.4.1 Adoption Timing and Its Drivers

The first analytical lens focuses on the timing of firm adoption and the factors that influence this process. Firm-level adoption timing varies significantly across scenarios, primarily as a result of changes in either hydrogen demand or ammonia import volumes. These variables directly affect firms' threshold values and thereby influence the likelihood and timing of adoption. Table 6.8 presents an overview of the average adoption timing of the nodes, grouped by early adopter configuration. The hydrogen consumers column remains largely empty, as adoption by these firms does not significantly influence the adoption of others and therefore fails to trigger cascading effects. Furthermore, when storage providers act as early adopters, the adoption process remains consistent across all scenarios, indicating that their early participation does not meaningfully influence the diffusion dynamics. This indicates that storage providers generate highly predictable adoption cascades among firms. Furthermore, aside from a single node that adopts in the hydrogen consumer first configuration, hydrogen suppliers exhibit the fastest average adoption time (2.29), compared to 2.34 for import terminals and 2.53 for storage providers. This reflects the strong influence hydrogen suppliers exert on other firms.

At the individual node level, node 2 (HES) shows an average adoption time of 1, which corresponds to the first timestep in the model. This rapid adoption is the result of a low threshold. In contrast, node 10 (Air Products) displays both a high average adoption time (3.5) and the highest standard deviation (0.71). This indicates that Air Products' adoption timing varies significantly depending on which company type initiates adoption. The standard deviation reflects the variability in adoption timing across scenarios, and the high value suggests that Air Products does not follow a consistent adoption pattern.

Node	Company	AVG Hydrogen Suppliers	AVG Import Terminals	AVG Storage Providers	AVG Hydrogen Consumers
0	LyondellBasell	3.0	2.8	3.0	–
1	Uniper	2.0	1.8	2.0	–
2	HES	1.0	1.0	–	1.0
3	BP	2.6	1.8	3.0	–
4	Eneco	–	2.8	3.0	–
5	OCI	2.6	–	3.0	–
6	Gunvor	–	2.4	3.0	–
7	ExxonMobil	1.2	1.0	1.0	–
8	Vopak	2.2	2.8	–	–
9	Huntsman	3.0	2.8	3.0	–
10	Air Products	–	4.0	3.0	–
11	Advario	3.0	2.8	–	–
12	Chane	2.2	1.8	–	–
13	Air Liquide	–	2.8	3.0	–
14	ACE Terminal	2.2	–	2.0	–
15	Air Product and Gunvor Terminal	2.0	–	2.0	–
16	VTTI Storage Terminal	2.6	2.0	–	–
17	Chane Import Terminal	2.4	–	2.0	–
18	Nobian	–	3.0	3.0	–
19	Shell	–	1.8	2.0	–

Table 6.8: Gemiddelde adoptietijdstappen per node voor vier bedrijfstypen

A clear illustration is the case of ExxonMobil (Hydrogen Consumer), whose adoption moment differs notably across scenarios. In low-demand scenarios, ExxonMobil adopts later than in the base case or high-demand configurations. The reduced demand leads to higher thresholds, making early investment less likely. Conversely, in scenarios characterised by high ammonia imports, BP, a hydrogen consumer, adopts in earlier time steps. This is notable, as a high ammonia import at the import terminals does not affect BP's threshold value directly. However, it influences the scores of the interdependencies between BP and the import terminals, thereby contributing to BP's early adoption. This results from BP's high hydrogen demand and the substantial hydrogen supply from import terminals, leading to a stronger edge connection.

This pattern reflects a common feature in energy transition projects, often referred to as the chicken and egg problem, in which supply and demand developments are mutually dependent. Firms may postpone investments until sufficient supply is secured, while suppliers hesitate in the absence of confirmed demand. The model demonstrates that firms such as BP are particularly sensitive to this dynamic, delaying their investment decisions until an adequate supply, for instance from the ammonia import terminals, is guaranteed.

A critical risk highlighted by the simulation results is the impact of late-stage adoption. Firms that adopt in later time steps, such as Air Products (hydrogen supplier) in the high hydrogen demand scenario, often require the construction of long and costly pipelines to establish a connection with the existing infrastructure. This outcome is partly driven by the modelling assumption that new adopters connect directly to existing firms, rather than to intermediate pipeline segments. While this simplifies network expansion, it may not fully reflect real world infrastructure development practices. In many cases, new connections would logically attach to shared infrastructure rather than specific firms. However, in the model, nearby demand nodes are already satisfied, which often leads to longer connections for new adopters. An example of such late adoption by Air Products is shown in the figure below.

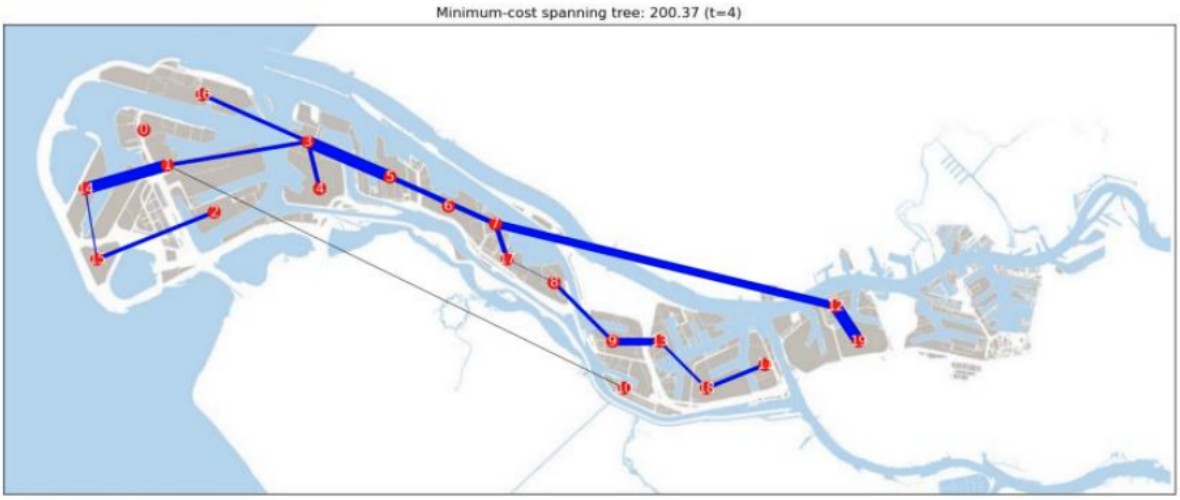


Figure 6.18: High-Cost Connection Resulting from Late Adoption by Air Products

The delayed adoption is primarily a consequence of firm-specific attributes that are relatively low, including limited hydrogen trade volume and a small plot size. These characteristics reduce the firm's investment potential and delay their engagement in the network. The specific attribute values for Air Products are provided in Table 6.9.

Furthermore, the infrastructure close to Air Products, constructed prior to its adoption, may lack the flexibility to accommodate the additional connection. In particular, pipeline capacity in the surrounding area may already be constrained, further increasing the cost and complexity of integration. Therefore, given the high demand and the available supply from Air Products, a connection is established with HES (2), which has the highest unfulfilled demand at that stage.

Table 6.9: Attributes of Air Products

Attribute	**Value**
Company Type	Hydrogen supplier
H_2 Trade Volume	13 ktpa
Plot Size	15 ha
Threshold	0.625

The results further indicate that low-demand scenarios not only lead to slower adoption but also result in more fragmented network development. Instead of forming a single, integrated system, the network divides into several smaller and more localised sub-networks, which prioritise short-distance connections to satisfy the limited demand. A fragmented hydrogen network refers to the development of isolated or poorly connected infrastructure segments rather than a single integrated system. From the perspective of infrastructure developers, port authorities, and policymakers, such fragmentation is considered a suboptimal outcome due to its negative impact on the long term viability and efficiency of the hydrogen economy.

First, fragmentation limits economies of scale, as pipelines serve fewer firms and operate below optimal capacity. It also increases the risk of stranded assets resulting from low utilization [11]. In addition, fragmented networks offer limited resilience and redundancy. In the event of a pipeline failure, alternative routing options are often unavailable. This reduces operational flexibility and increases vulnerability to disruptions [11].

Fragmentation also conflicts with key hydrogen infrastructure design criteria such as cost efficiency and robustness, as outlined in Table 1.3. Disconnected subnetworks require duplicate infrastructure such as pipelines, endpoints, and control systems, thereby increasing overall costs. Finally, a fragmented network lacks system wide connectivity, making it more susceptible to fluctuations in demand and supply. If one subnetwork fails, the absence of interconnections prevents the rerouting of flows, which undermines reliability. An example of such a fragmented network layout is shown below for the low hydrogen demand scenario. These two figures present 2 timesteps of the network development in the low hydrogen demand scenario with the storage providers as early adopters.

This outcome contrasts with high-demand scenarios, where broader connectivity becomes economically attractive, resulting in a more cohesive and interconnected network. In low-demand cases, the ONLT tends to generate compact layouts that favour short, local connections. These findings suggest that low demand does not necessarily have to be interpreted as an unfavourable scenario. However, it does increase the risk of network fragmentation and the loss of early integration opportunities.

Overall, the adoption dynamics are highly sensitive to both localised supply and demand conditions, as well as to the initial early adopter configurations.

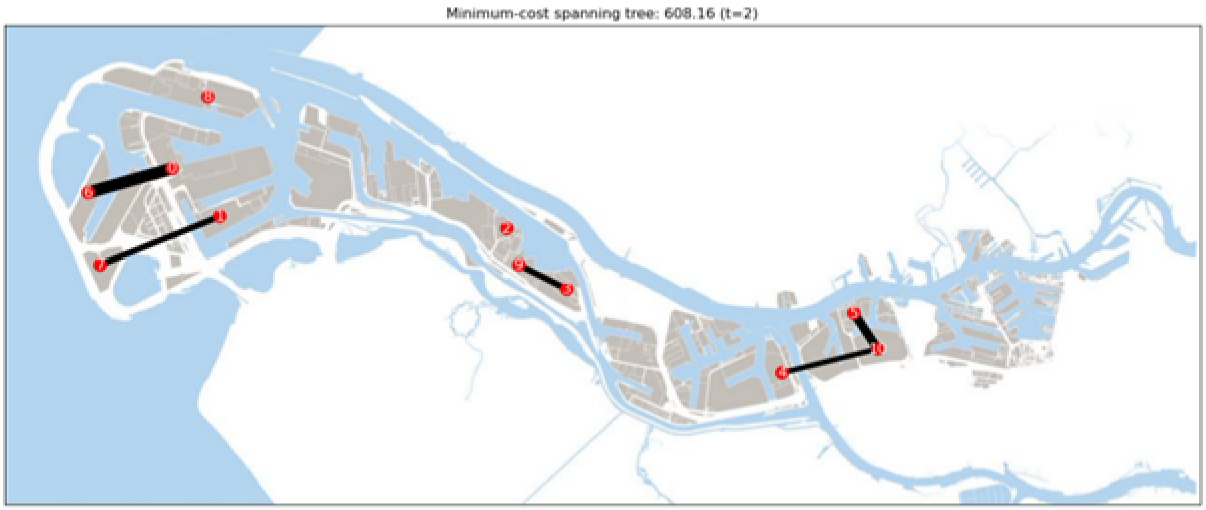


Figure 6.19: Fragmented Network Configuration : Timestep 2, Low-Demand Scenario

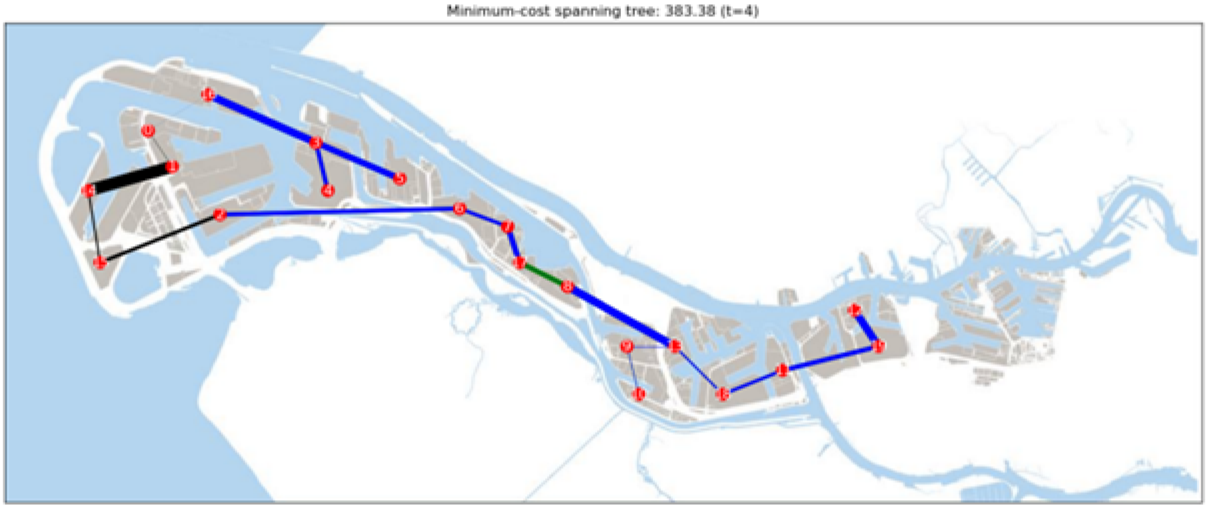


Figure 6.20: Fragmented Network Configuration : Timestep 4, Low-Demand Scenario

6.4.2 Strategic Nodes

The development of hydrogen infrastructure within industrial clusters is not evenly distributed across firms. Instead, certain firms consistently emerge as strategic nodes or hubs across multiple scenarios. A hub is defined as a highly connected node that plays a central role in the hydrogen network. These hubs significantly shape the spatial configuration of the network and are crucial for several reasons. First, they enhance network connectivity by linking multiple firms. Second, they reduce infrastructure redundancy by serving as distribution points. Third, they are often strong candidates for public or shared investment due to their strategic location. This section analyses which firms consistently emerge as hubs across different scenarios and examines their influence on the overall network configuration.

The emergence of strategic hubs is driven by a combination of factors, including geographic location within the cluster, firm-specific attribute values, and the timing of adoption. Their presence can significantly affect network efficiency and resilience by enabling coordinated infrastructure expansion and reducing the risk of fragmented development. This can be measured, for example, by tracking a firm's degree centrality, which refers to the number of connections a firm has within the network. Table 6.10 presents the degree centrality values of the nodes shown in Figure 6.21. It is evident that node 13, representing Air Liquide, has the highest degree centrality.

Nodes 0–10			Nodes 11–19+		
Node	**Company**	**Degree Centrality**	**Node**	**Company**	**Degree Centrality**
0	LyondellBasell	0	11	Advario	1
1	Uniper	2	12	Chane	1
2	HES	1	13	Air Liquide	4
3	BP	3	14	ACE Terminal	2
4	Eneco	2	15	Air Product and Gunvor Term.	1
5	OCI	2	16	VTTI Storage Terminal	0
6	Gunvor	2	17	Chane Import Terminal	2
7	ExxonMobil	2	18	Nobian	2
8	Vopak	2	19	Shell	2
9	Huntsman				
10	Air Products				

Table 6.10: Degree centrality and company names for all nodes in the final edge list

Air Liquide consistently emerges as a significant hub across multiple simulation runs, characterised by high connectivity. Its central location within the industrial cluster, combined with substantial hydrogen supply capacity and moderate threshold values, makes it an attractive node for network integration. As a result, Air Liquide frequently connects to both demand and storage nodes, reinforcing its strategic position within the network.

However, in scenarios with high ammonia imports, its central role diminishes. The additional supply from import terminals reduces the reliance on domestic hydrogen suppliers, thereby shifting Air Liquide to a less central position in the overall network structure. This variation is illustrated in the figures below, where Air Liquide is indicated in green. The first shows Air Liquide in a key strategic role in a high hydrogen demand scenario, while the second depicts its reduced importance in a high ammonia import scenario.

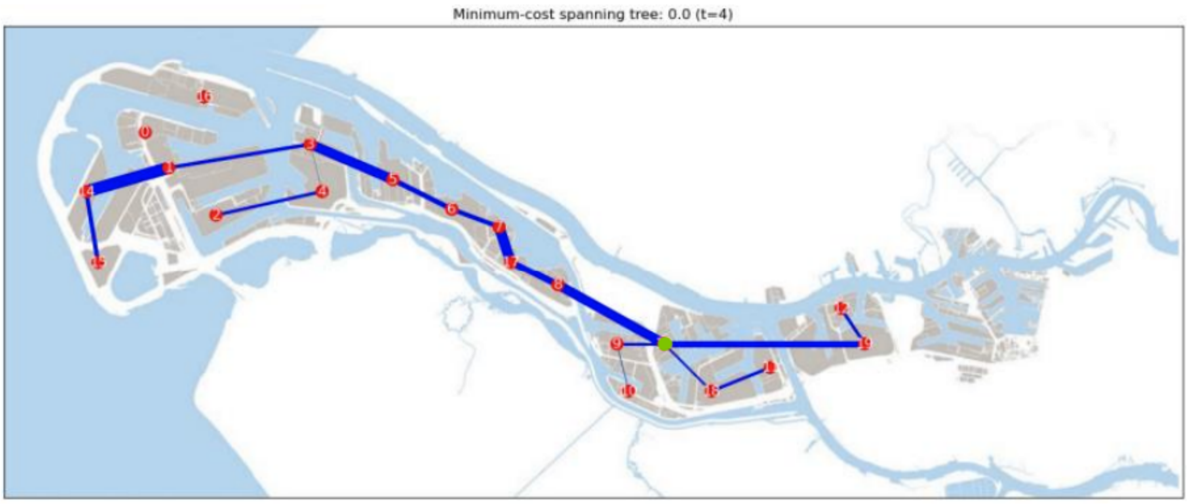


Figure 6.21: Air Liquide as a Strategic Hub – High Hydrogen Demand Scenario

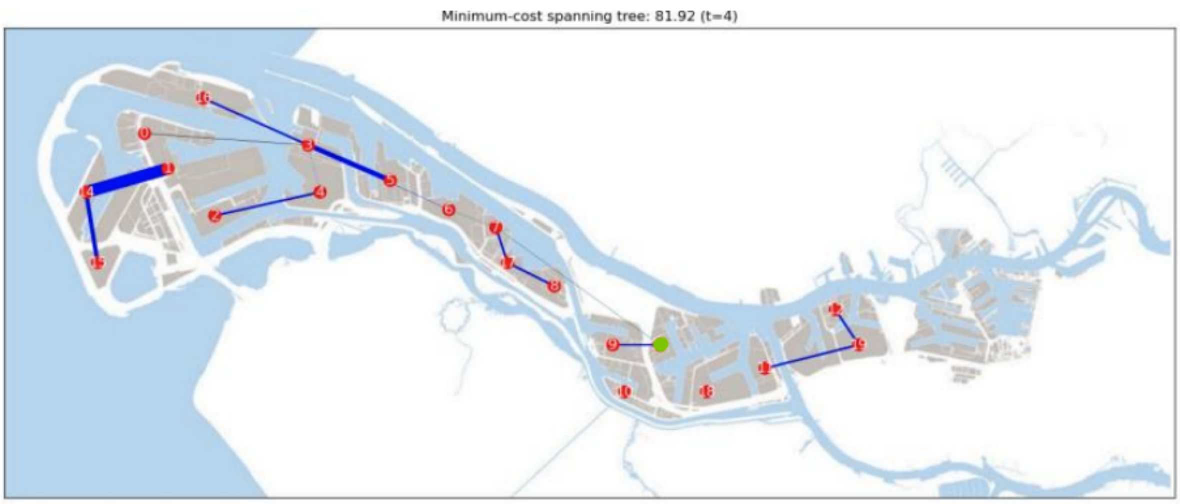


Figure 6.22: Reduced Role of Air Liquide – High Ammonia Import Scenario

Secondly, Eneco can also be identified as an important node, particularly during the early stages of network development. Although Eneco does not consistently emerge as the most connected firm, its early adoption and favourable location within the cluster make it a foundational anchor around which local subnetworks tend to form.

In addition, BP becomes a strategic hub in certain scenarios, especially those characterised by high hydrogen demand or high ammonia imports. In these cases, BP's substantial hydrogen demand results in a lower adoption threshold. Once BP adopts, it frequently establishes multiple connections within the network. This illustrates how demand-side firms can also play a central role in shaping the structure and connectivity of the hydrogen network.

The emergence and influence of strategic hubs reveal that specific firms within an industrial cluster, due to their attributes and locations, can dominate network structures under certain scenarios. Understanding the conditions under which these hubs emerge is essential for infrastructure planners and investment stakeholders. Targeting these firms for early engagement may improve network efficiency, reduce infrastructure costs, and lower the risk of stranded assets.

Moreover, coordinated investment in these hubs can support the realisation of economies of scale, given their high utilisation potential for shared infrastructure. Strategic alignment with these key nodes can therefore enhance both the technical and economic performance of hydrogen networks.

6.4.3 Structural Patterns in Network Formation

The simulation runs reveal distinct structural patterns in the development and formation of hydrogen networks across various scenarios. These patterns highlight both efficient and suboptimal configurations. For instance, in low hydrogen demand scenarios, the resulting networks often become fragmented into smaller, modular components. A notable example is observed in the scenario where storage providers are the initial adopters under low hydrogen demand, leading to a network split into four isolated parts, as shown in Figure 6.19.

This fragmented structure results from a combination of lower adoption thresholds and reduced demand. These conditions encourage firms to form short, local connections rather than invest in longer, more expensive pipelines. While such configurations may minimise costs in the short term, they can limit the long-term scalability of the network. Relying on nearby supply and demand may constrain the development of a more integrated and resilient infrastructure. As more firms adopt in later stages, previously built local connections may require costly retrofitting to support larger-scale integration. Retrofitting refers to upgrading existing infrastructure to support new connections or expanded use [46].

In contrast, high hydrogen demand scenarios typically result in larger and more integrated network structures. A greater number of firms adopt within a shorter time frame, leading to the rapid formation of extensive, connected infrastructures. However, this accelerated development often introduces inefficiencies. Such inefficiencies are illustrated in Figure 6.23. This figure illustrates the inefficiencies that emerge as a result of early adoption driven by low threshold values. In the initial stages of network development, smaller pipeline investments are made that may not have sufficient capacity to accommodate firms adopting at later stages. These early infrastructure choices can constrain flexibility and force late adopters to construct longer and less efficient connections.

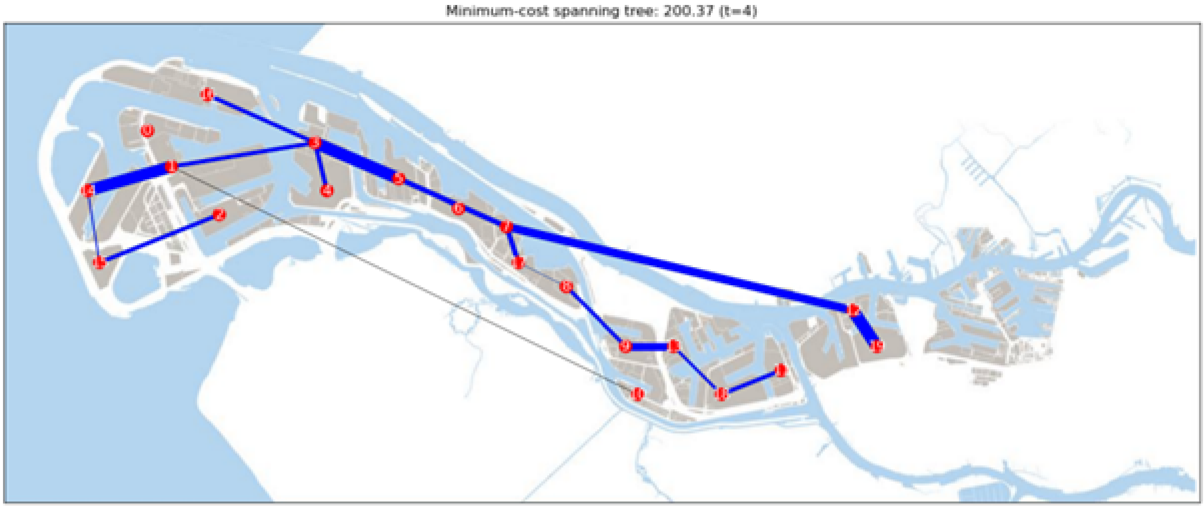


Figure 6.23: Final network configuration at timestep 4

A further example of this inefficiency appears in the high hydrogen demand scenario where storage providers are the initial adopters. From the Chane Import Terminal (17), two parallel network branches develop. This occurs because both Air Liquide (node 13) and Shell (node 19) have large supply capacities. However, the resulting pipelines follow a partially parallel layout, suggesting that a shared pipeline could have been a more efficient alternative. This example is shown in Figure 6.24.

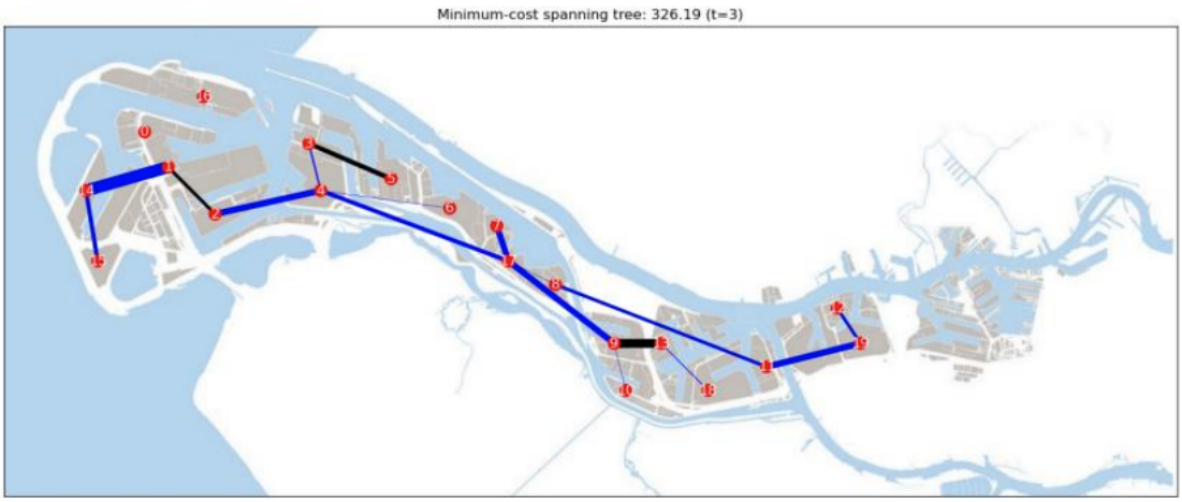


Figure 6.24: Final network configuration at timestep 4

This parallel development arises from timing differences in adoption. Air Liquide (13), along with several nearby demand nodes, adopts later in the process, after a pipeline connection has already been established involving Shell (19). Due to capacity constraints in the existing infrastructure, the ONLT generates new parallel pipelines rather than integrating the additional demand into the earlier connection. This illustrates how early, uncoordinated investments can lock in suboptimal pathways and increase long term infrastructure costs.

However, this outcome is also influenced by two key modelling assumptions. First, connections are made directly between firms rather than to shared pipeline infrastructure.

Second, the cost parameter for capacity expansion (*cpc*) is set to 1, meaning that extending capacity is treated as equally costly as building a new pipeline. A lower value for *cpc* would likely favour the extension of existing connections over the creation of redundant routes.

In this study, a *cpc* value of 1 is used based on the assumption that expanding existing pipeline capacity does not offer a cost advantage over building new infrastructure. This assumption aligns with the study's focus on modelling hydrogen network development as a process driven by sequential firm adoption under conditions of uncertainty.

Furthermore, in scenario where there is a late and slow adoption, for example the low ammonia import scenario, this slow development proces frequently lead to more ineffeciencies. Cycles appear due to oncoordinated and late adoption which leads to redundant paths between already connected nodes.

Finally, a frequently recurring outcome is the exclusion of the VTTI Storage Terminal from the network, except in scenarios where sufficient supply is available nearby. It is important to note that, in this study, storage companies are modelled solely with demand, as no dynamic supply–demand time steps are incorporated. This simplification affects how storage nodes are integrated into the network.

VTTI's suboptimal location at the edge of the port, combined with moderate attribute values, makes its integration highly sensitive to scenario-specific dynamics. In cases where storage terminals are modelled with variable supply or demand profiles, their likelihood of being incorporated into the network is expected to increase. This highlights the importance of spatial positioning and attribute assumptions in determining node relevance within infrastructure development processes.

6.4.4 Robustness Across All Scenarios

This part of the results focuses on the robustness of pipeline connections across all simulated scenarios and early adopter configurations. This section identifies pipeline segments that consistently emerge regardless of hydrogen demand, import volumes, or early adopter types. This is crucial for strategic infrastructure planning during the energy transition, as such investments are capital intensive and long term [40]. Robust pipeline connections can offer valuable guidance for phased rollout strategies [63].

Robust connections can offer significant benefits across uncertain scenarios. Their high performance under various future conditions makes them examples of low-regret infrastructure. This means that robust edges are likely to minimize the negative consequences of choosing a path that turns out to be suboptimal.

Prioritizing robust segments promotes economies of scale and lowers the risk of stranded assets. These connections are likely to form the backbone of the future hydrogen network. Because these segments are identified as robust, they ensure high utilization over their long lifespan and therefore could benefit from economies of scale. An overview of the edges and their occurrence across all scenarios is shown in Figure 6.25. This figure provides additional information on the frequency of edge occurrences in the final network. Figure 6.25 shows a heatmap of edge frequencies in the final network. The heatmap effectively visualizes how often each pipeline segment appears across scenarios.

With this heatmap, nodes with many frequently occurring edges can be identified as key hubs in the network. It also reveals pipeline routes that consistently appear across multiple scenario simulations. These routes are likely to be essential infrastructure backbones. Focusing on these segments reduces the risk of stranded assets. Appendix

Chapter B provides additional information on the frequency of edge occurrence across all scenarios.

By highlighting robust segments under uncertainty, the heatmap supports more effective capital allocation.

Figure 6.25: Heat Map

Note that 20 simulations were run, and 4 of these considered hydrogen consumers as early adopters, which resulted in no network generation. Therefore, a total of 16 networks were generated.

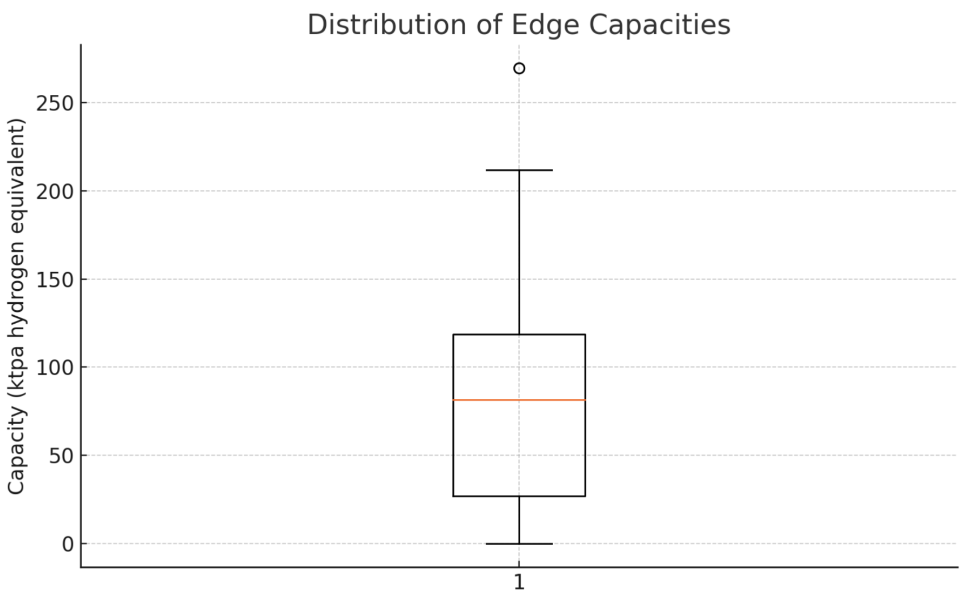


Figure 6.26: Distribution of edge capacities (ktpa hydrogen equivalent)

Figure 6.26 shows the box plot that visualizes the distribution of all capacity values of the edges that occur across the scenarios. The median capacity of all the edges is approximately 80 ktpa of hydrogen equivalent, with a range spanning from 30 to 120 ktpa . This capacity is assigned to the edge by the ONLT based on which supply and demand nodes are active in a given timestep and how they can be connected in a cost-optimal manner to meet the required flows. Only a small number of outliers are observed, with the most extreme value approaching over 260 ktpa. This indicates that a few edges are significantly over-dimensioned relative to the rest of the network. This results from a specific edge carrying a very large flow, likely due to the absence of nearby supply or demand nodes.

The final robust network, shown in Figure 6.27, has a total cost of 1229.67 in relative units. Applying the conversion factor discussed in Section 3.7, this corresponds to an estimated total network cost of €77,592,177. The network is generated using a maximum occurrence heuristic [18]. The process builds on the idea of generating multiple plausible futures. The occurrence of all possible edges is then mapped across this optimal network. In the final network, three connections appear in fourteen different scenarios. These are the connections between Chane Storage Terminal (12) and Shell (19)(supplier), between Huntsman (9)(consumer) and Air Liquide (13)(supplier), and between Uniper (1)(storage) and the ACE import terminal (14). It is important to note that Air Liquide, Shell, and the ACE terminal all have very high supply levels, which leads them to frequently form connections to meet demand. In contrast, Uniper has the highest demand. Its recurring connection to the ACE terminal is explained by the combination of high supply at the terminal and their geographic proximity, which makes this link almost always present in the network.

Figure 6.27: Final Graph subquestion 2 and 3

6.4.5 Early Adopter Strategy Trade-offs

In addition to the observed differences across scenarios, the selection of specific early adopters also influences the development of the hydrogen network. This reveals important trade offs between cost, connectivity, and strategic function. Accordingly, this section addresses the final subquestion:

Sub-question 4: How do external incentives (e.g., subsidies) influence firm behavior and network development?

To address this question, a comparative analysis was conducted across four early adopter strategies, each representing a specific company type. For each configuration (hydrogen suppliers, import terminals, storage providers, and hydrogen consumers), the dynamic model was run across five future scenarios: the base case, high and low hydrogen demand, and high and low ammonia import volumes. The resulting networks were evaluated in terms of total costs and pipeline capacities. Network costs were calculated using the ONLT cost function, while capacities were derived from the simulated supply and demand relationships among active firms. Pipeline capacities reflect the minimum required flow between connected nodes in each timestep.

The analysis was conducted in two stages. First, for each company type, network development was traced across all scenarios to assess how different early adopter strategies influence network evolution. Second, a robust network was identified for each company type configuration by examining outcomes across the five scenarios. The results of the networks are shown in Table 6.11.

Company Type	**Total Cost (approx.)**	**Total Capacity (ktpa)**
Hydrogen Suppliers	€73 million	3000
Import Terminals	€72 million	2300
Storage Providers	€70 million	2600
Hydrogen Consumers	–	–

Table 6.11: Comparison of total costs and capacities by company type

When storage providers are selected as early adopters, the resulting network is the most cost efficient overall compared to configurations where hydrogen suppliers or import terminals are the initial adopters. The total network cost in the storage provider configuration amounts to €70 million, as shown in Figure 6.28 . These firms are spatially well distributed between suppliers and consumers, enabling the formation of an efficient local hydrogen backbone. This supports the development of a locally integrated network. The resulting network tends to exhibit moderate capacity per connection, relatively short pipeline lengths, and balanced connectivity.

Figure 6.28: Storage Provider Configuration

In contrast, the configuration in which hydrogen suppliers adopt first results in the highest total network cost, reaching €73 million, and the highest total capacity, at 3000 ktpa. The high capacity indicates that a large volume of hydrogen is being transported through the network. When hydrogen suppliers adopt early, they inject substantial volumes into the system at an early stage. This encourages the development of a more extensive pipeline infrastructure to accommodate and distribute the available supply. This leads to the formation of a high capacity network, shown in Figure 6.29. These results reflect the suppliers' role as a centralised source of supply, requiring extensive distribution to reach demand nodes across the cluster. The geographic locations of hydrogen suppliers are less dispersed compared to, for example, storage providers. Their spatial clustering leads to longer pipelines and higher associated costs.

Figure 6.29: Hydrogen Supplier Configuration

The final early adopter configuration, which focuses on import terminals, results in a network with moderate total cost (€72 million) and the lowest total capacity (2300 ktpa). However, this strategy frequently leads to isolated subgraphs and long, inefficient pipeline routes, presented in Figure 6.30. This outcome reflects the typical location of import terminals at the edges of the cluster, where they are poorly connected to the rest of the system. Their primary role is to inject supply into the network, but in the absence of nearby early demand, the resulting infrastructure remains underutilised.

Figure 6.30: Import Terminal Configuration

6.4.6 Evaluation Against Design Criteria

Apart from robustness, which is one of the key design criteria for hydrogen infrastructure, Table 1.3 identifies four additional criteria against which network configurations are evaluated. The results from the scenario simulations are assessed according to all four criteria.

Cost efficiency is evaluated using the ONLT model, which calculates the total network cost for the final robust configuration shown in Figure 6.27. Based on this assessment, the storage-provider-first configuration yielded the lowest overall network costs.

Scalability captures the extent to which late adopters can be integrated into the existing network without requiring substantial redesign. A highly scalable configuration allows for flexible expansion. The storage-provider-first configuration demonstrates high scalability by enabling straightforward integration of additional firms.

Utilization and risk sharing refer to how frequently pipeline segments are shared among multiple firms. Networks with well-connected hubs promote shared use of infrastructure and reduce the risk of stranded assets. Networks with well-connected hubs enable multiple firms to share pipeline segments, thereby increasing overall infrastructure utilization. In contrast, the import-terminal-first configuration occasionally results in underutilized and isolated segments. These segments typically serve a single firm or carry low flow volumes, limiting infrastructure sharing and increasing unit costs.

6.4.7 Conclusion and Takeaways

This chapter presented a comparative analysis of sixteen network configurations, based on early adopter types and varying demand and import conditions. The aim was to identify robust network layouts and to examine how different adoption strategies influence both the adoption process and the development of the hydrogen infrastructure. Specifically, the analysis highlighted how firm specific attributes, interfirm influence on investment decisions, and spatial configuration shape infrastructure development. Three main themes emerged across the scenarios: the emergence of strategic nodes, the impact of late adoption, and the trade off between fragmentation and centralisation in network layouts.

Air Liquide, Eneco, and BP emerged as strategic nodes, depending on scenario conditions. Air Liquide frequently functions as a central connectivity hub due to its favourable location and high supply capacity. Eneco, by contrast, typically appears as an early stage node and is therefore likely to form the foundation of the hydrogen backbone. BP, on the other hand, emerges as a demand driven hub, particularly in high demand scenarios, illustrating how demand nodes can also influence network topology.

Furthermore, late adoption, often due to high thresholds or geographic isolation, tends to result in costly and inefficient pipelines, as observed in the case of Air Products. These findings highlight the critical chicken and egg dynamic in infrastructure development and the energy transition: early adopters may benefit from lower connection costs, but they also face higher uncertainty.

The analysis also reveals a fundamental trade off between fragmentation and centralisation, which depends critically on the balance between supply and demand. Low demand scenarios resulted in more fragmented but cost efficient networks. In contrast, high demand scenarios produced more centralised, high capacity layouts with higher total costs.

Finally, the robust network identified through edges appearing across all sixteen simulation runs provides a foundation for low regret investment strategies. The low regret segment, particularly those involving high capacity nodes such as Shell–Chane, Huntsman–Air Products, and Uniper–ACE terminal, demonstrates value across a range of future scenarios. Among the early adopter strategies, storage providers tend to yield the most cost effective networks. In contrast, hydrogen suppliers support higher volume flows but at greater cost, while import terminals often lead to underutilisation due to their typical location at the edges of the industrial cluster.

7 Discussion

This study introduces a dynamic modelling framework to simulate how firm level investment decisions, shaped by interdependencies, firm specific attributes and adoption thresholds, drive the development of hydrogen pipeline networks in industrial clusters. Using a threshold based model combined with a cost optimisation tool, the results demonstrate that hydrogen infrastructure development is highly sensitive to early adoption by specific firms within the hydrogen value chain. The findings reveal complex and nonlinear dynamics that are often overlooked in traditional static energy models.

These simulations reveal that late adoption by firms often results in more costly and inefficient pipeline connections. They also show that strategic firms such as Air Liquide, Eneco, and BP can emerge as critical hubs within the cluster, although the emergence of such nodes varies by scenario.

Furthermore, the analysis indicates that initiating adoption with storage providers tends to result in a robust and cost efficient network. In contrast, starting with hydrogen suppliers produces a high capacity network but at significantly higher costs. Early adoption by import terminals frequently leads to underutilisation due to their peripheral location and limited early demand. Starting with hydrogen consumers never leads to sufficient adoption by supply firms.

These findings support the expectation that firm level attributes such as company type, grid connection, hydrogen trade volume, and plot size play a central role in shaping firm behaviour. The results underscore the importance of incorporating such attributes into infrastructure planning under uncertainty, moving beyond simplified cost minimisation approaches.

7.1 Interpretation of Results

The results also reveal important variations in firm level thresholds based on operational characteristics, highlighting real world barriers to infrastructure adoption. Firms with more favourable attributes such as higher hydrogen trade volume, larger plot size, and stronger grid connection tend to have lower thresholds, making them more likely to invest. In contrast, firms with low hydrogen trade volume, limited grid capacity, or small plot sizes exhibit higher thresholds and lower readiness to invest. Company type also plays a significant role; firms categorised as import terminals or storage providers often display lower thresholds due to their strategic importance.

The model used in this study further highlights the importance of interfirm relationships and demonstrates that interdependencies influence the diffusion of investments. Firms, represented as nodes in a social network, influence one another, with those that have already adopted exerting a positive influence on their neighbours. This peer influence is crucial for addressing the chicken and egg problem in infrastructure development, where many firms hesitate to invest without certainty regarding supply or demand.

Some firms also emerge as strategically important because their high centrality and favourable attributes lead to early stage adoption. These firms can influence adoption dynamics even among firms with higher individual thresholds. This effect results from their strong connectivity, early adoption, and high influence within their local network. Early adopters not only initiate physical infrastructure, but also act as catalysts for behavioural change within an industrial cluster. For example, when hydrogen suppliers or storage providers were selected as early adopters, adoption cascaded more rapidly through the network compared to configurations where adopters with lower scores were chosen. Influence is not distributed evenly, and targeted engagement of specific actors can significantly enhance rollout efficiency.

Furthermore, the scenario differences used in this study highlight the sensitivity of network expansion, costs, and rollout speed to variations in hydrogen demand and ammonia import volumes. Low demand and import scenarios typically resulted in slower adoption among firms and more fragmented network development. This led to smaller, localised sub networks focused on short distance connections, which may constrain long term scalability. Late adoption, often driven by firms with less favourable attributes, frequently required the construction of long and inefficient pipelines, increasing total network costs.

In contrast, scenarios with high demand and import volumes resulted in faster and more continuous network expansion, with lower overall costs. These findings suggest that future infrastructure planning should consider not only firm level readiness but also broader supply configurations. Centralised import capacity, especially when located near strategically positioned firms, proved particularly effective in reducing network fragmentation and enabling cost efficient infrastructure backbones.

Finally, the analysis identifies several firms that consistently emerge as critical infrastructure nodes and serve as keystone players in the transition. Firms such as ACE Terminal, Eneco, and Shell frequently form early connections and play a central role in linking multiple parts of the network. These companies share common characteristics, including high hydrogen trade volumes and either strong grid connections or large plot sizes. These attributes appear to be key indicators for identifying central actors in other industrial clusters that are likely to function as connection hubs. Their consistent involvement suggests that infrastructure planning would benefit from prioritising these firms as hubs for early coordination. Air Liquide also consistently functioned as a central connectivity hub due to its strategic location and high supply capacity. However, its role weakened in scenarios with high ammonia imports and increased reliance on domestic energy supply. BP, driven by its substantial hydrogen demand, emerged as a strategic hub in the high demand and high import scenarios. This underscores that demand side firms can also significantly influence the network topology. When analysing other industrial clusters, a similar approach can be applied to identify important demand side firms with comparable characteristics. These characteristics include a high expected hydrogen demand, sufficient physical space to support infrastructure integration, and a strong planned grid connection. Additionally, a central location within the cluster further enhances a firm's strategic role in network development.

These findings suggest that targeted early engagement of specific firms can improve network efficiency and reduce overall costs, thereby mitigating the risks of stranded assets and supporting the realisation of economies of scale. Across all scenarios, the most cost efficient networks tended to occur when storage providers were the initial adopters, reflecting their effective spatial distribution within the Rotterdam Industrial Cluster. In such cases, companies with high hydrogen demand and strong grid connections, such as Eneco, emerge as strategic hubs and can be identified as priority partners for early stage collaboration.

7.2 Scientific Contribution and Comparison with Existing Literature

This study stands in clear contrast to traditional energy infrastructure models, which often adopt a centralised and static approach focused solely on cost minimisation or the achievement of supply and demand equilibrium under predefined scenarios. As highlighted by Ridha et al. (2022), these models typically neglect interdependencies among firms and assume independent firm behaviour, thereby overlooking the complex strategic decision making that characterises real world infrastructure development. The application of threshold logic builds on the work of Valente et al. (1996), Dreyer and Roberts (2009), and Rossi et al. (2017), and directly captures the chicken and egg problem that is common in shared infrastructure development. These conventional approaches fail to address this dynamic, which can significantly delay progress in the energy transition. By incorporating a dynamic modelling framework, this study makes a meaningful contribution to the existing literature.

The dynamic modelling framework used in this study directly addresses the limitations outlined above by simulating firm level investment decisions that are shaped by interdependencies and uncertainties. The threshold logic is consistent with an agent based approach, modelling firms that interact with others within a social network. Their investment decisions are influenced by the actions of neighbouring firms, capturing nonlinear adoption patterns, tipping points, and cascading effects.

Furthermore, the integration of the threshold model with the Optimal Network Layout Tool (ONLT), based on graph theory, represents a key contribution of this study. It addresses a gap in the literature, where previous threshold models were not combined with spatial network optimisation to simulate evolving infrastructure layouts and their associated costs.

7.3 Strengths and Limitations

This study demonstrates several key strengths by introducing a dynamic modelling framework that integrates a threshold based adoption model with an optimal network layout tool. By incorporating both behavioural dynamics and network cost optimisation, the model captures adoption patterns that are often overlooked in purely techno economic analyses.

Second, the model draws on real world firm level data from Power2X for the Rotterdam Industrial Cluster, including hydrogen trade volume, plot size, and grid connection. This enables the construction of scenarios grounded in realistic spatial and technical configurations.

Third, the inclusion of interfirm influence through a weighted network reflecting observed interdependencies adds a critical layer of behavioural realism. This allows the model to simulate the cascading effects of early adoption across different strategic scenarios.

Despite these strengths, this study also acknowledges several limitations. One of the most significant is the simplification of the investment decision making logic, as discussed in Section 3.10. One of the most significant limitations of this study is the simplification of investment decision-making logic. The model assumes that firm adoption is solely driven by a threshold mechanism based on static firm attributes. In practice, however, decisions related to hydrogen infrastructure investment involve a far more complex set of considerations, including financial modelling, risk–return analysis, regulatory assessments, long-term market projections, and extensive stakeholder negotiations. While such processes are difficult to simulate, they are critical to shaping infrastructure development outcomes. This simplification may lead to an overestimation of adoption rates and the pace of network expansion. Moreover, the abstraction limits the model's predictive accuracy and underscores the need for future validation with stakeholders. It also highlights the potential value of integrating behavioural diffusion models with more economically or policy-oriented investment frameworks. Another important aspect concerns the uncertainty surrounding the expert derived scores for the categorical attribute company type, which were determined through an interpretive approach rather than established scientific literature. While the applied scoring method enhances reproducibility, it may introduce a degree of subjectivity into the firm level adoption thresholds. Similarly, the boundaries used to define the low, medium, and high categories for numerical attributes were based on visual inspection of histograms rather than established literature. These chosen boundaries likely introduce additional subjectivity into the model, which may influence the threshold values and, consequently, the adoption process.

Additionally, the model assumes fixed attribute values over time and does not account for evolving hydrogen demand, changing ammonia import volumes, or shifts in firm strategy. These dynamic factors could significantly influence adoption behaviour in practice. The model also assumes that all interfirm connections exert a positive influence, whereas in reality, adoption by one firm might reduce the willingness of others to invest due to competitive pressures or market displacement. This assumption simplifies the complex competitive dynamics that may emerge in real industrial environments.

Another key assumption in the threshold model is that all firm-level attributes are considered to contribute equally to a firm's threshold. This equality among attributes reduces the risk of overparameterization. While this simplifies the model, it may overlook the possibility that some attributes have a greater influence on adoption decisions than others. Furthermore, the normalized category scores within each attribute are based on interpretative logic rather than empirical validation. Although these values may produce plausible adoption dynamics, they could be further refined through the integration of scientifically grounded data. Additionally, interdependencies between firms are modelled as static. In reality, however, these relationships are likely to evolve over time, which could substantially influence both the adoption process and resulting network development.

Finally, the assumption of unconstrained pipeline construction, where connections are represented as straight lines, does not reflect spatial, regulatory, or permitting constraints. These real world limitations could significantly affect the actual cost and feasibility of infrastructure development.

These limitations suggest that the results should be interpreted as exploratory and illustrative, rather than as direct predictions of future developments. Nonetheless, the model provides a useful framework to examine how firms and their interdependencies may shape infrastructure development pathways in industrial clusters.

7.3.1 Model Assumption and Their Implications

In addition to the general limitations, this study relies on several assumptions that shape the scope and interpretation of the results. These assumptions can be grouped into three categories: behavioural, technical, and scenario related.

From a behavioural perspective, the model assumes that adoption is purely driven by positive peer influence and similarity between firms. It does not account for negative interdependencies such as competition, strategic exclusion, or the possibility that unprofitable investment decisions by neighbouring firms may discourage adoption. In addition, the simplified investment logic reduces complex decision making processes to a threshold based mechanism that relies on static firm attributes. This abstraction may lead to an overestimation of adoption rates and overlooks the possibility that different attributes may carry varying levels of importance in real world decision making.

Technically, the model assumes unconstrained pipeline construction as straigh line connections, thereby ignoring spatial regulatory or permitting constriants that affect the real world infrstructure development. Once constructed, the infratructure is assumed to remain in place indefinitely, with no decomissioning or repurposing. Additionally, pipelines are only built between active firms, and not directly to existing pipelines. This can increase cost estimates and reduce the flexibility.

Finally, the model assumes homogeneous adoption within each firm type, meaning that only firms of the same type act as early adopters in each simulation. Furthermore, adoption occurs in discrete timesteps without delay. While these design choices support clearer comparison between scenario configurations, they limit the diversity and realism of transition pathways observed in real world infrastructure development.

7.4 Scalability, Generalizability, and Robustness

While this study demonstrates the application of the dynamic modelling framework within the Rotterdam industrial cluster, it is not bound to this specific context. This section discusses the potential of the framework for application in other industrial regions and its computational scalability.

The approach is designed to be both generic and transferable. It relies on firm level data such as geographic location, hydrogen trade volume, and grid connection, which are often available in other clusters. The core elements of the model, including the threshold based adoption logic and the network optimisation method, are not limited to hydrogen infrastructure. They can also be applied to other green molecule infrastructure planning challenges.

Successful replication requires only basic firm level data, which is commonly accessible. The attribute scoring logic demonstrated in this study can be adapted to reflect local conditions and industry characteristics in different industrial contexts. However, several key elements would require careful adjustment. For example, geographic conditions and spatial constraints would influence infrastructure costs and technical feasibility. In addition, the industrial composition of clusters varies considerably, with different firm types and value chain relationships. These differences would necessitate tailored attribute definitions and scoring schemes. Finally, local policy environments and regulatory frameworks may influence the timing of adoption and should be reflected through context specific calibration.

Scalability to Larger Systems

The current implementation in this study is tailored to a relatively small scale system. Successful replication and upscaling of the model to simulate hundreds of firms or incorporate a large number of scenarios would introduce several challenges.

First, while the optimal network layout tool performs efficiently for small to medium networks, its performance may degrade as the number of nodes and the size of the graph increase significantly. Second, collecting firm specific attribute data at a large scale can be time consuming and resource intensive. Third, the calculation of influence scores between all firm pairs becomes increasingly intensive as the number of firms grows. Finally, generating and analysing large scenario sets would further increase the overall computational burden.

However, the model also offers potential solutions to these scalability challenges. Hierarchical modelling strategies could be used to partition large systems into smaller, manageable subnetworks, with intercluster connections modelled at a higher level of abstraction. This approach allows for selective application of the most computationally intensive components while preserving the framework's core behavioural insights.

Uncertainty

The current analysis, based on 20 simulation runs across five scenarios and four early adopter configurations, offers a bounded exploration of uncertainty rather than an exhaustive coverage of all possible future states. As such, the findings should be interpreted as a structured examination of plausible outcomes. This bounded approach functions as a structured sensitivity analysis rather than a comprehensive uncertainty quantification. The scenarios capture variation in critical variables that are expected to have a significant influence on network development patterns. However, several sources of uncertainty remain unaddressed, such as regulatory changes and technological developments that could significantly affect adoption dynamics.

Future studies could enhance the robustness of the analysis by increasing the number of simulation runs, applying Monte Carlo methods, or extending the robustness assessment. In addition, scenario design could benefit from stakeholder guided storyline development to ensure that the scenarios reflect industry specific concerns. These enhancements would transform the current analysis into a more comprehensive tool for uncertainty assessment.

Lessons and Insights

In conclusion, this framework yields several insights that are transferable across different contexts. The threshold based adoption logic captures interfirm dependencies that are often observed in infrastructure development. The attribute based scoring methodology enables the inclusion of firm behaviour and structural differences between firms. Finally, the ONLT provides a rigorous method for evaluating spatial infrastructure efficiency in a cost effective manner.

Moreover, the insights generated by this framework reflect fundamental dynamics that are likely to emerge in other industrial clusters facing the challenge of coordinated infrastructure development under uncertainty. While specific conditions may vary, the qualitative understanding of how firm attributes, network effects, and decision making interact to shape infrastructure development offers valuable guidance for planners and policymakers in other contexts.

7.5 Implications

The findings of this study offer important implications for policymakers, industrial advisory firms, and infrastructure developers involved in the hydrogen transition. For industrial project developers such as Power2X, the model provides a practical decision support tool to navigate uncertainties in new infrastructure projects. For example, they can use insights into threshold behaviour to identify firms with lower investment barriers, making them suitable candidates for early engagement or strategic partnerships. The results suggest that strategic firms with strong influence and favourable attributes should be prioritised.

The model can directly inform decisions about which first movers to target. It demonstrates that selecting storage providers as early adopters leads to the most cost efficient network configurations, supporting the development of an effective hydrogen backbone in the industrial cluster. Project developers can use these insights into firm characteristics and readiness to design a phased infrastructure rollout aligned with adoption likelihood and spatial demand patterns.

Furthermore, the identification of critical infrastructure nodes such as Air Liquide and Eneco provides a clear basis for prioritising investments to reduce the risk of underutilised infrastructure. Finally, the analysis of robust pipeline segments that appear consistently across scenarios supports low regret investment strategies and helps minimise the risk of stranded assets.

It is important to note that although this study used the RIC as an illustrative case, its dynamic modeling framework and key insights are broadly applicable to other industrial clusters that face similar coordination and infrastructure challenges in the energy transition.

Although this study does not directly compare outcomes with a fully top down planning approach, the findings indicate that a hybrid strategy, combining behavioral dynamics with spatial optimization, may offer more advantageous results. A purely top down model risks overlooking interfirm adoption behavior, potentially resulting in misaligned investments or stranded assets.

7.6 Future research

Future research should focus on enhancing the model's dynamic capabilities and refining its current assumptions to generate more robust insights. A critical extension would involve moving beyond static firm attributes and incorporating dynamic changes over time to reflect evolving firm strategies, demand growth, or regulatory developments. This could also include modelling real time economic variables and market incentives, such as fluctuating energy prices or competitive dynamics, which are not currently simulated.

In addition, future work should aim to strengthen the methodological basis for attribute scoring by grounding these decisions in established literature. In this study, each attribute was treated as equally important, with normalized scores assigned across low, medium, and high categories. Introducing differentiated attribute scores would allow for a more nuanced analysis of how specific characteristics influence adoption outcomes.

Finally, incorporating expected firm level returns from specific infrastructure investments would introduce a critical economic dimension to the adoption logic. This would align the model more closely with real world investment decision making processes.

7.6.1 Validation of Investment Logic

One of the most critical limitations identified in this study is the abstraction of real-world investment decisions into a simplified threshold logic. While this approach enables the simulation of adoption dynamics, it does not reflect how firms make investment decisions in practice. To improve the realism and reliability of the model, future research should incorporate a structured validation of the investment logic, preferably through empirical engagement with stakeholders or comparison to observed investment behaviour. Therefore, the following step-by-step validation approach is proposed:

Stakeholder Interview or Expert Panels

The first step in the validation process involves conducting structured interviews with a range of relevant stakeholders and experts, including infrastructure developers, project finance specialists, and decision-makers at firms active in the hydrogen value chain. The objective is to identify the key factors that influence investment readiness and commitment in practice. More specifically, these interviews aim to uncover the practical drivers and barriers that influence firms' investment decisions. Key questions may address topics such as:

- What internal criteria (e.g., return on investment, risk tolerance, board approval) must be met before your firm commits to infrastructure investments?
- Can you describe a past hydrogen or energy infrastructure investment made by your firm, and what factors triggered the final decision?

Comparison with Real Investment Cases

Secondly, the modelled adoption sequence should be compared against real-world cases of hydrogen infrastructure development, where available. Relevant examples include existing pipeline projects and industrial decarbonization initiatives. This comparative analysis can help identify systematic deviations between simulated and observed investment behaviour, particularly in terms of investment timing, risk assessment, and the influence of early adopters. Such findings can reveal where model assumptions align with, or diverge from, actual decision-making processes.

Incorporating ROI-Based Decision Rules

Thirdly, the model should be extended to incorporate an economic viability threshold within the adoption logic. This could involve integrating indicators such as a minimum expected return on investment (ROI) or acceptable payback period. Including such criteria would allow the model to reflect how firms weigh financial feasibility against social influence. This addition would offer a more realistic representation of capital allocation decisions within firm-specific investment frameworks.

Scenario Co-Creation with Experts

Furthermore, expert participation can be used to co-develop future scenarios and refine model parameters. This ensures that both the adoption logic and the scoring of firm attributes reflect industry-specific considerations, the regulatory environment, and competitive dynamics that influence investment behaviour.

Sensitivity Analysis on Behavioral Parameters

Lastly, a targeted sensitivity analysis of the behavioural parameters should be conducted to systematically test the model's robustness under varying investment assumption scenarios. By examining how changes in attribute scores and threshold values influence adoption patterns, this analysis can identify which factors most strongly shape network formation and therefore warrant more precise empirical calibration. For each variation, the model is rerun and the resulting adoption sequences and network configurations are compared. By analysing which parameter changes lead to the greatest deviations in network outcomes, the most influential behavioural assumptions can be identified.

By integrating stakeholder insights with systematic parameter testing, future versions of the model could achieve closer alignment with the complexity of real-world investment behaviour and provide more actionable insights for planners and infrastructure developers.

8
Conclusion

This study aimed to understand the adoption of hydrogen infrastructure within industrial clusters by simulating how firm specific characteristics, interdependencies, and investment decisions shape network development. To achieve this, a threshold based adoption model was developed and combined with a network optimisation tool (ONLT), enabling the simulation of adoption behaviour and infrastructure evolution over time. A key contribution of this study is its ability to capture the complex and non linear dynamics between firms and their specific attributes, such as hydrogen demand, grid connection, plot size, and company type, within a modelling framework that supports the evaluation of network robustness under uncertainty. This thesis addressed the following research question:

> *How do firm-level characteristics and interdependencies influence the development of hydrogen infrastructure in industrial clusters?*

To answer the main research question, several subquestions were investigated. These contribute to the overall objective of this thesis. The first subquestion is:

> **Subquestion 1:** *What threshold values and interdependencies exist between companies?*

This study reveals that a combination of firm level attributes, such as hydrogen demand or supply, grid connection, plot size, and company type, is critical in determining both the individual adoption thresholds and the interdependencies between firms. Firms with more favourable attributes are assigned lower thresholds, indicating a greater readiness to adopt. Interdependencies are modelled through assigned edge scores that reflect the similarity of attributes between firms. This allows influence to cascade through the network. Firms with similarly high attribute values exert stronger influence, making them central in driving collective adoption dynamics.

> **Subquestion 2:** *How do threshold values and interdependencies impact firms' investment decisions?*
>
> **Subquestion 3:** *How do threshold model outcomes under different scenarios shape the optimal hydrogen pipeline layout?*

In relation to subquestions 2 and 3, which focus on the threshold model dynamics and network generation, the findings consistently indicate that network development is strongly influenced by investment decisions and firm specific thresholds. The resulting network structure is shaped by the interaction of firm level attributes. These interacting factors lead to complex and non-linear patterns of adoption across the network.

For example, robust infrastructure segments tend to form around early adopters that combine favourable attributes with a strategic central location within the cluster. Storage providers frequently act as key enablers, triggering broader adoption and leading to the formation of integrated and cost efficient backbone networks. Their effectiveness is partly due to their geographic distribution throughout the cluster, which increases their connectivity and influence across different firm types. Firms such as Air Liquide and Eneco consistently acted as central hubs within the network. Eneco, for instance, combines highly favourable attributes, including a strong grid connection and a substantial hydrogen supply, giving it the profile of a foundational early stage node with high connectivity. This makes it strategically attractive for other firms to connect to. A similar pattern is observed for Air Liquide, which also functions as a hydrogen supplier with comparable favourable attributes, although located in a different part of the cluster. Identifying such firms is essential for anticipating where critical hubs are likely to emerge.

In contrast, late adopters such as Air Products often require expensive and inefficient connections, primarily due to the absence of nearby active infrastructure. Although Air Products is also a hydrogen supplier, its relatively low hydrogen volume, limited grid connection, and small plot size result in one of the highest thresholds in the model. As a consequence, Air Products requires a substantial number of neighbouring adopters before it is willing to connect, classifying it as a ”wait and see” actor. However, because its location is close to Air Liquide, it is likely that Air Liquide serves the nearby consumers, further reducing the strategic importance of Air Products in early network formation.

In addition to supply side actors, demand side nodes can also play a strategic role in shaping network development. For example, BP emerged as a demand driven hub, particularly in the high demand scenario. This highlights how macro level conditions can significantly alter network topologies. It is therefore essential not to focus exclusively on supply nodes, as demand nodes can actively influence both the structure of the network and the dynamics of investment. Large and reliable demand nodes, especially those with substantial plot sizes and strong grid connections, serve as strategic targets for ensuring offtake certainty. In high demand scenarios, such firms tend to attract infrastructure investment and can evolve into demand hubs.

> **Subquestion 4:** *How do external incentives (e.g., subsidies) influence firm behavior and network development?*

The final subquestion focuses on specific early adoption configurations and compares the resulting networks to identify which configurations lead to the most optimal outcomes in terms of cost and capacity flow. The adoption behaviour of different company types influenced both the pace and structure of network development. Early adoption by storage providers resulted in the most cost efficient networks, while early adoption by hydrogen suppliers produced networks with higher overall capacity but also significantly higher costs. These findings suggest that targeted subsidies should be aligned with broader strategic objectives, whether the priority is minimising cost or maximising capacity, when supporting early adoption in industrial clusters.

The developed framework offers valuable scalability potential for project developers such as Power2X when evaluating hydrogen infrastructure opportunities across different industrial clusters. In addition to the model's scalability, the findings from this study offer valuable insights into specific firm behaviour, the emergence of strategic hubs, and the identification of robust infrastructure components. These insights can support the analysis of other industrial clusters facing similar infrastructure challenges. Power2X can apply the predefined firm level criteria to identify relevant actors in other clusters and collect the necessary data based on firm specific attributes. Combined with a different cluster layout and the spatial configuration of firms, the model is capable of simulating adoption dynamics in various industrial contexts. This enables developers to determine which clusters present the most favourable conditions for early infrastructure development and to identify firms that are likely to emerge as strategic hubs, as well as infrastructure segments that remain robust across multiple future scenarios.

These findings offer several practical insights for industrial project developers, advisory firms, and policymakers involved in hydrogen infrastructure planning and the decarbonisation of industrial clusters. The model serves as a practical decision support tool, highlighting the importance of identifying firms that can act as strategic early movers to accelerate infrastructure rollout. In particular, encouraging early adoption by specific firms or coordinating investments within a group of interdependent companies can prevent costly delays and inefficient network layouts. By simulating different adoption pathways, the model identifies which configurations are likely to result in integrated rather than fragmented networks, and which specific network segments can be considered robust. By incorporating firm behaviour and peer influence, this approach supports a more coordinated and cost effective strategy for infrastructure planning, reducing the risk of stranded assets and better reflecting the real dynamics within industrial clusters.

Appendix Overview

This appendix provides an overview of the supplementary material that supports the analysis presented in this thesis. It includes supplementary data, a detailed overview of all attribute values, the results of expert interviews and the corresponding scoring method, pseudocode for the threshold calculation, and the full simulation results for all scenario and early adopter configurations. Table A.4 presents the scores for the categorical attribute company type, which were derived from the expert interviews.

A
Attribute Values

This appendix chapter presents the specific values of the firm level attributes used as input in the model. These values were collected using data from Power2X and existing literature, as described in the data sources section. The attribute values form the basis for determining each firm's adoption threshold and influence within the network.

Firm	**Hydrogen Trade Volume (ktpa)**
LyondellBasell	19
Uniper	450
HES	75
BP	108
Eneco	80
OCI Import Terminal	1200
Gunvor	13
ExxonMobil	153
Vopak	75
Huntsman	55
Air Products	13
Advario	75
Chane	75
Air Liquide	200
ACE Terminal	2000
Air Product and Gunvor Terminal	2000
VTTI Storage Terminal	73
Koole Import Terminal	1000
Nobian	25
Shell	232

Table A.1: Firm-level hydrogen trade volumes (ktpa)

Firm	**Plot Size (ha)**
LyondellBasell	75
Uniper	60
HES	125
BP	250
Eneco	21
OCI Import Terminal	20
Gunvor	140
ExxonMobil	101
Vopak	100
Huntsman	80
Air Products	15
Advario	26
Chane	60
Air Liquide	37
ACE Terminal	70
Air Product and Gunvor Terminal	60
VTTI Storage Terminal	90
Koole Import Terminal	40
Nobian	30
Shell	400

Table A.2: Firm-level plot sizes (hectares)

Firm	Grid Connection (MW)
LyondellBasell	81.6
Uniper	500
HES	251
BP	250
Eneco	800
OCI Import Terminal	150
Gunvor	30
ExxonMobil	251
Vopak	50
Huntsman	150.63
Air Products	42.4
Advario	50
Chane	50
Air Liquide	150.63
ACE Terminal	150
Air Product and Gunvor Terminal	150
VTTI Storage Terminal	150
Koole Import Terminal	100
Nobian	150.63
Shell	200

Table A.3: Firm-level grid connection capacities (MW)

Company Type	Assigned Scores
Import Terminal	0.9
Storage Provider	0.8
Hydrogen Supplier	0.6
Hydrogen Consumer	0.5

Table A.4: Assigned Scores for company types in the threshold model

B

Edge Counts

The table below forms the basis for generating the robust network across all scenario and early adopter configurations. It provides an overview of the top connections that appear most frequently across the 14 simulation runs. The focus is limited to edges with a count of five or more, although many other edges appear less frequently. The first two columns represent the two nodes that constitute each edge.

Table B.1: Top 20 Most Frequent Edges Across Scenarios

Node A	**Node B**	**Count**
1	14	14
12	19	14
9	13	14
3	5	13
3	4	13
7	17	13
8	17	12
14	15	12
2	4	11
13	18	11
11	19	10
4	17	9
9	10	9
6	7	8
1	3	7
11	18	7
3	16	7
0	1	6
1	2	6
2	15	5

C

Pseudocode Threshold Calculations

The pseudocode below outlines the procedure used to calculate each firm's specific threshold value, based on its individual attribute scores. This pseudocode offers a clear representation of the underlying calculations and reflects the logic implemented in the Python code used within the model.

Algorithm 1 Firm-Specific Threshold Calculation

Require: Firm f with attributes $A = \{a_1, a_2, \ldots, a_n\}$
Require: For each attribute a_i: predefined category ranges (*low*, *medium*, *high*) and corresponding scores (w^i_{low}, w^i_{med}, w^i_{high})
Ensure: Threshold value T_f for firm f

Initialize empty list $W \leftarrow [\,]$
for each attribute a_i in A **do**
    Determine value v_i of attribute a_i for firm f
    Identify category c_i into which v_i falls (*low*, *medium*, or *high*)
    Assign corresponding scores w_i based on c_i
    Append w_i to list W
end for
Compute average score: $\text{avg\_score} \leftarrow \frac{1}{n}\sum_{i=1}^{n} w_i$
Compute threshold: $T_f \leftarrow 1 - \text{avg\_score}$
return T_f

D

Simulation Outputs

The final chapter of the appendix presents the intermediate results from all simulation runs included in the analysis. Each run consists of multiple timesteps that indicate which firms are active in a given timestep and which connections are established. In the visualisations, new connections appear in black during the timestep they are created. In subsequent timesteps, these previously established connections are shown in blue. If an edge appears in purple, it represents an existing connection whose capacity has been extended. The appearance of nodes over time reflects the dynamic outcomes generated by the threshold model.

D.1 Base Case Scenario

D.1.1 Hydrogen Supplier First

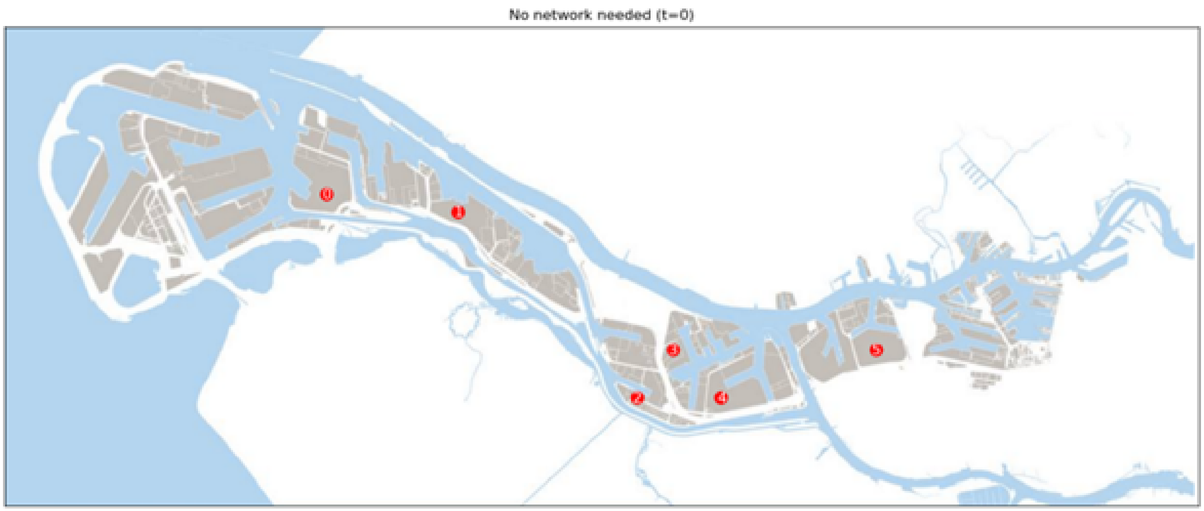


Figure D.1: Simulation Results

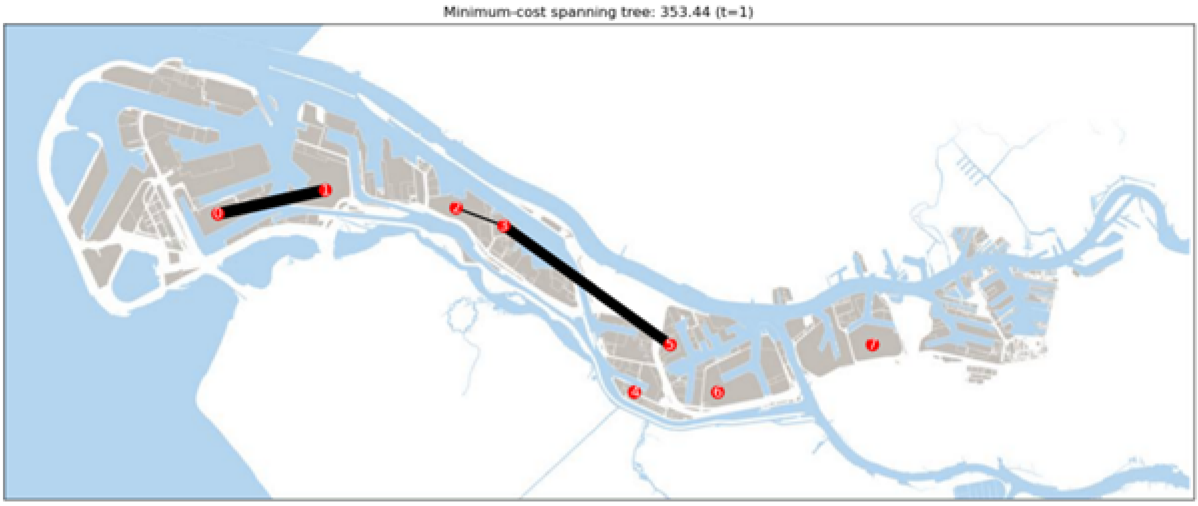


Figure D.2: Simulation Results

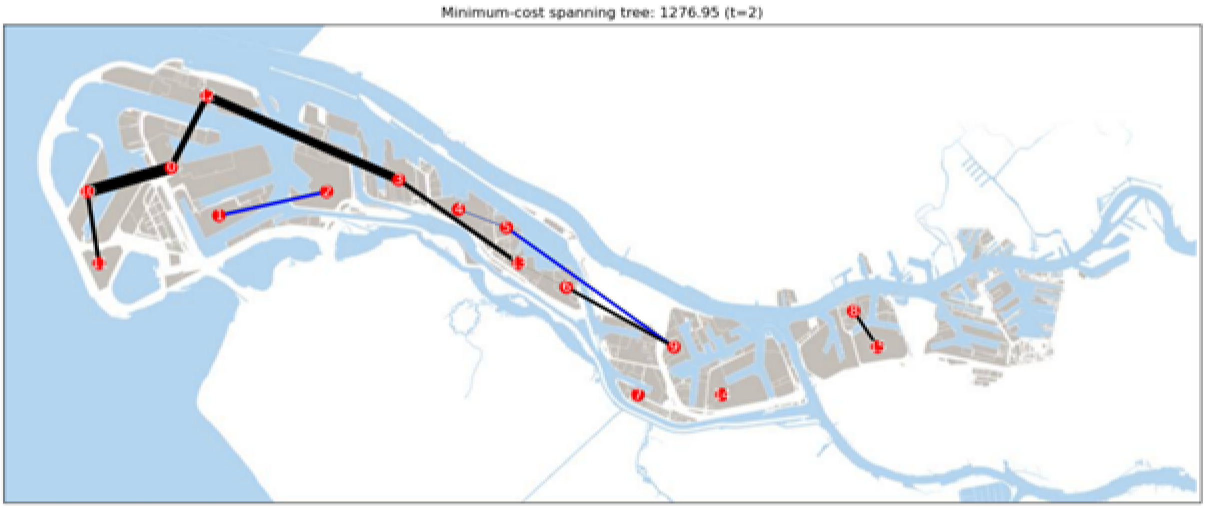


Figure D.3: Simulation Results

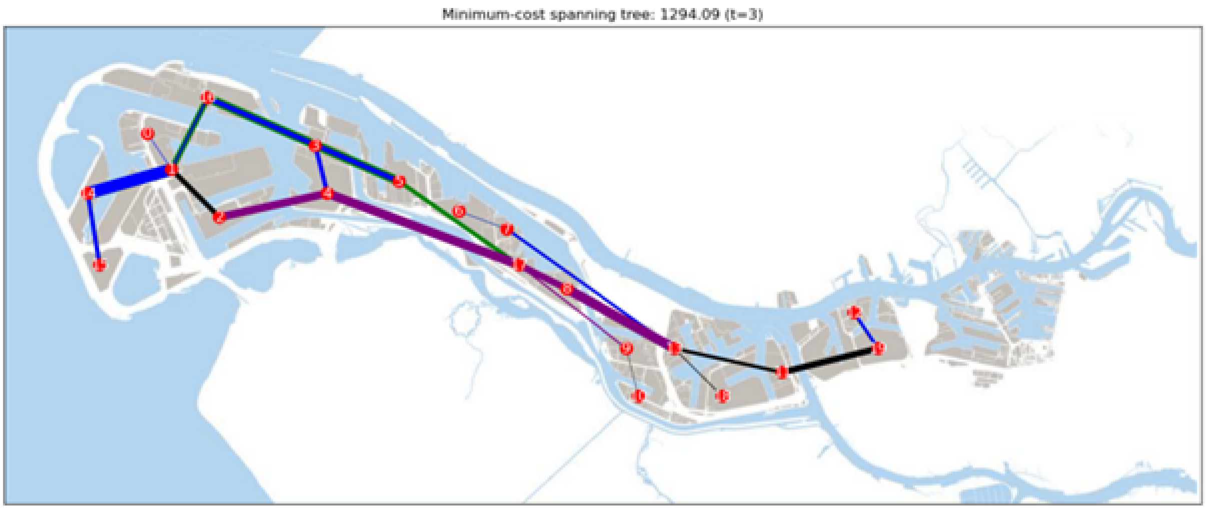


Figure D.4: Simulation Results

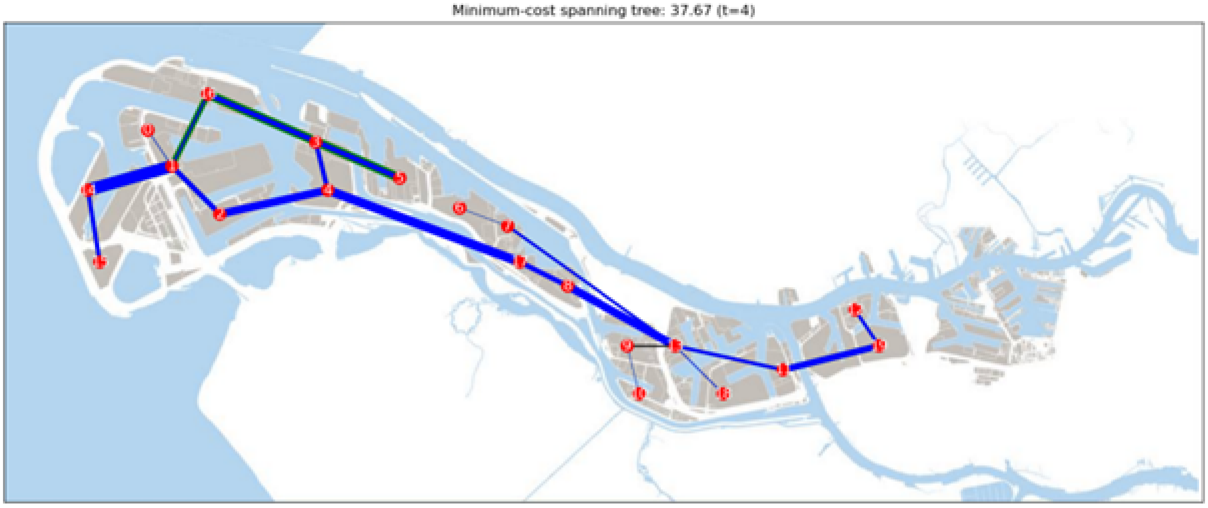


Figure D.5: Simulation Results

D.1.2 Hydrogen Consumer First

Figure D.6: Simulation Results

Figure D.7: Simulation Results

D.1.3 Import Terminals First

Figure D.8: Simulation Results

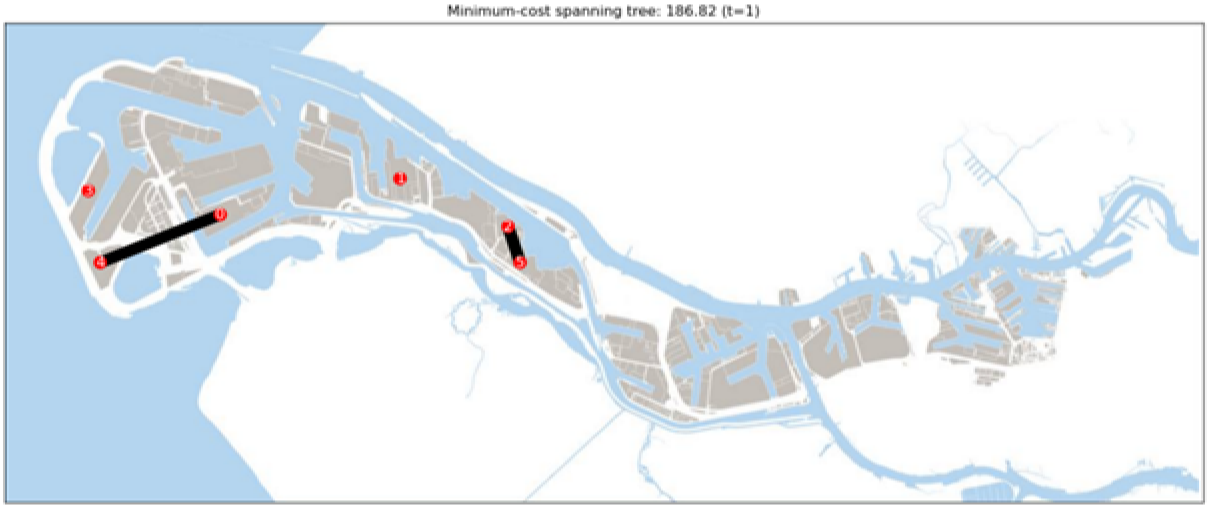


Figure D.9: Simulation Results

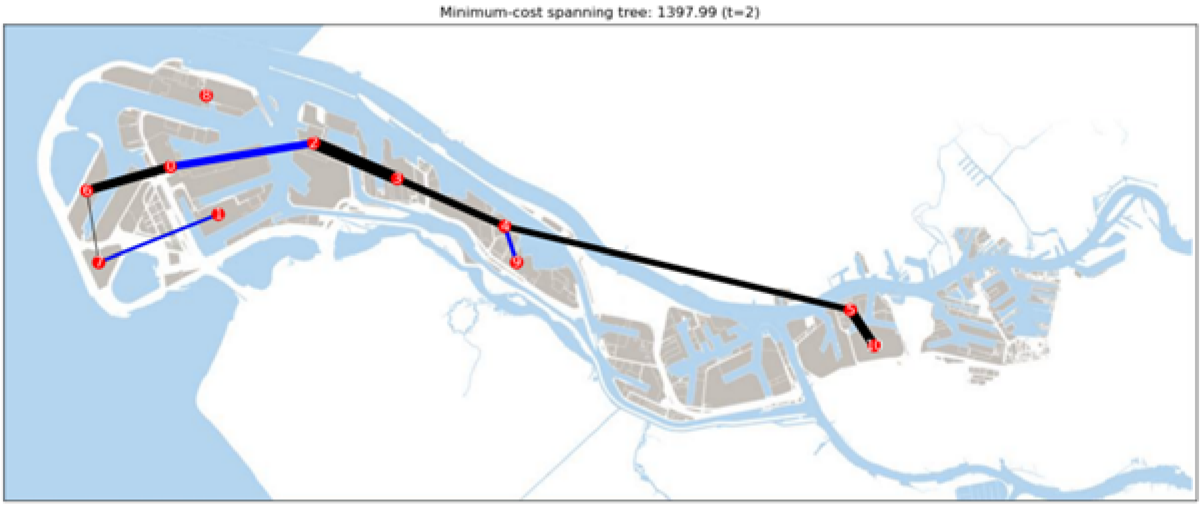


Figure D.10: Simulation Results

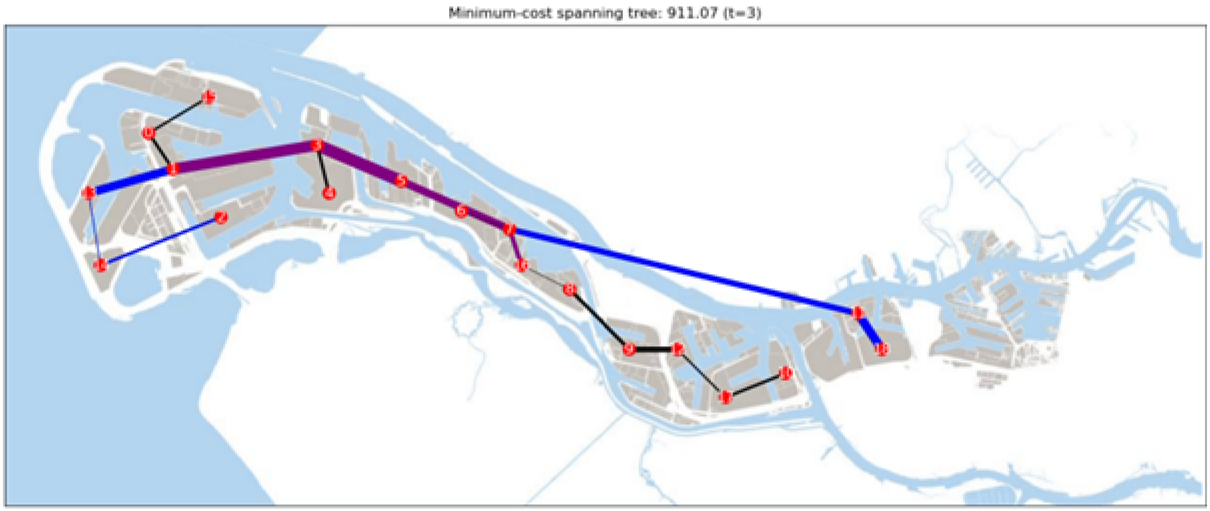


Figure D.11: Simulation Results

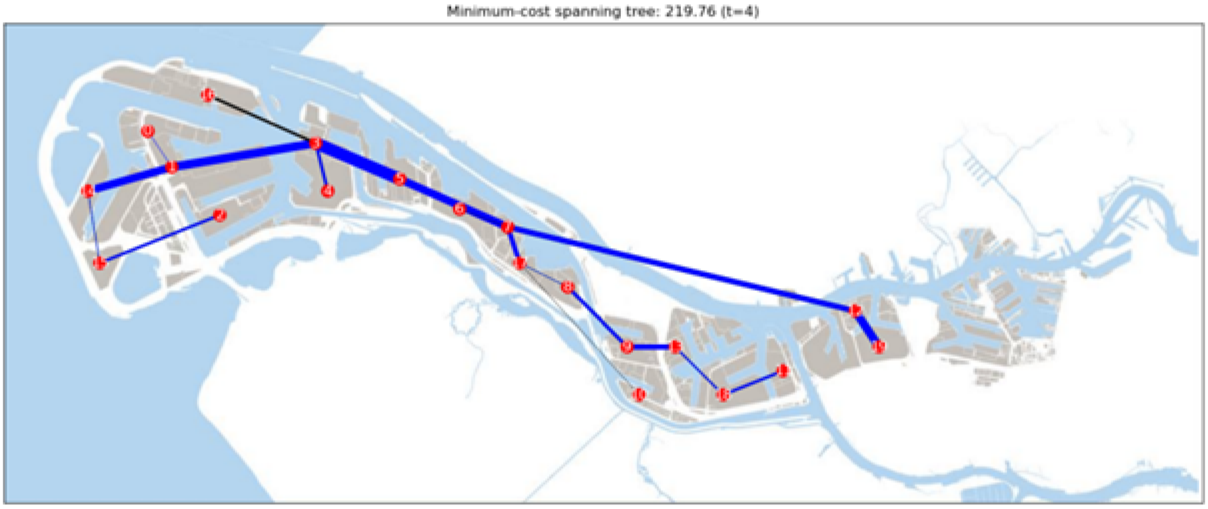


Figure D.12: Simulation Results

D.1.4 Storage Providers First

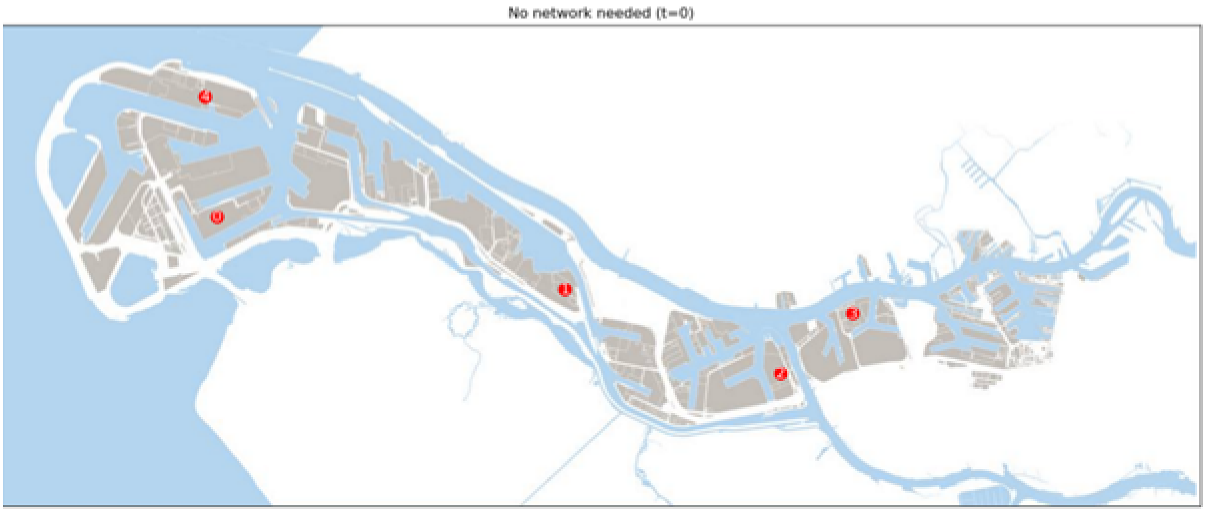
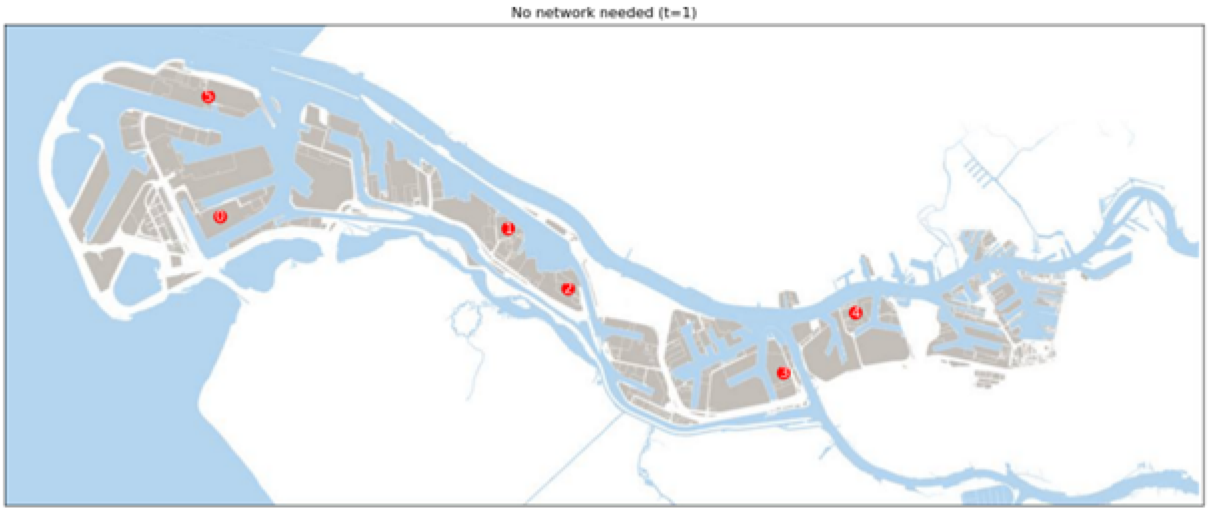


Figure D.13: Simulation Results



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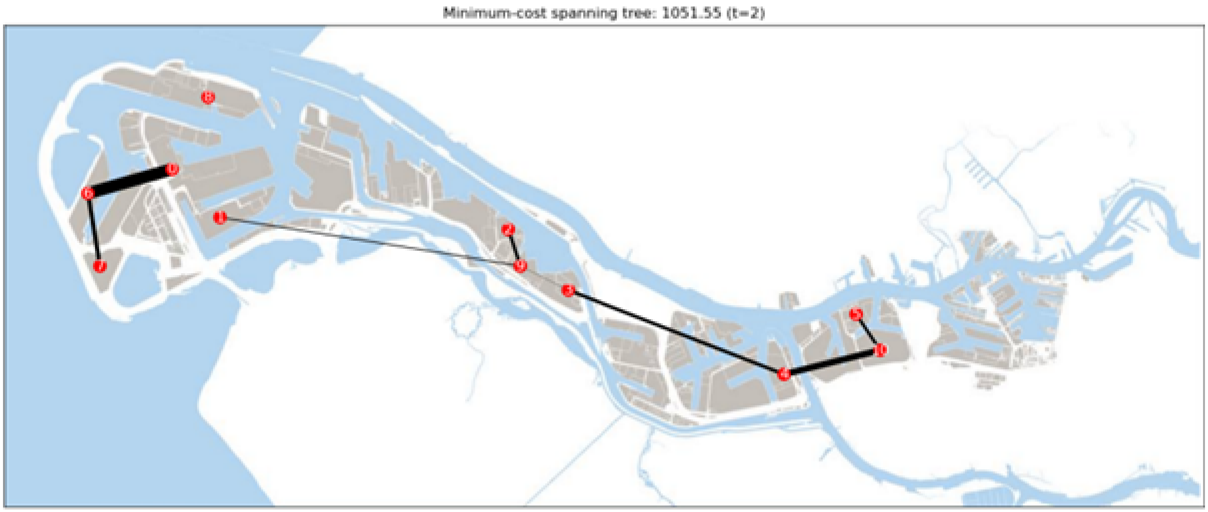


Figure D.15: Simulation Results

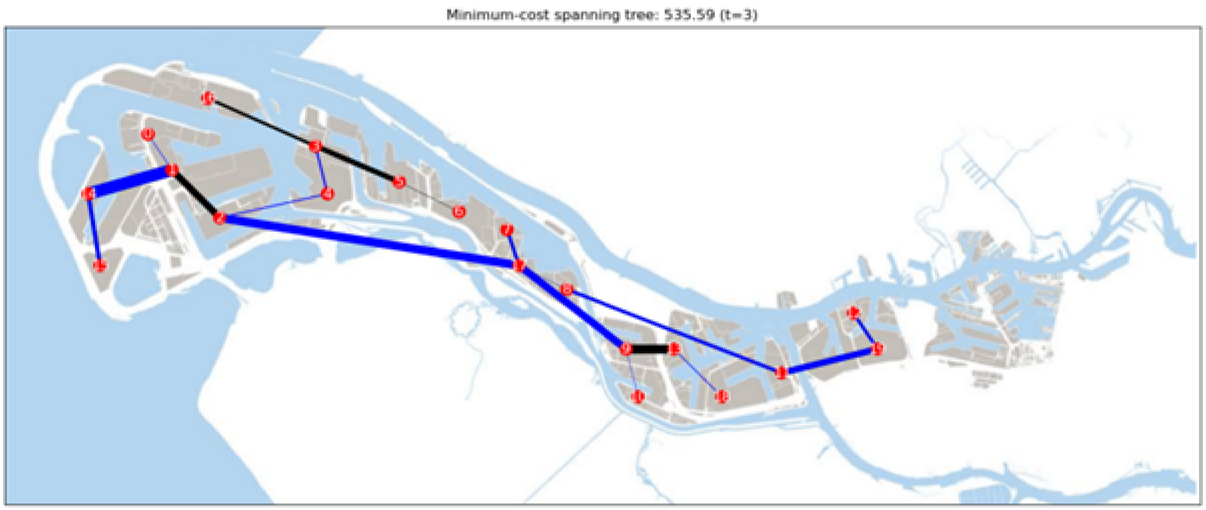


Figure D.16: Simulation Results

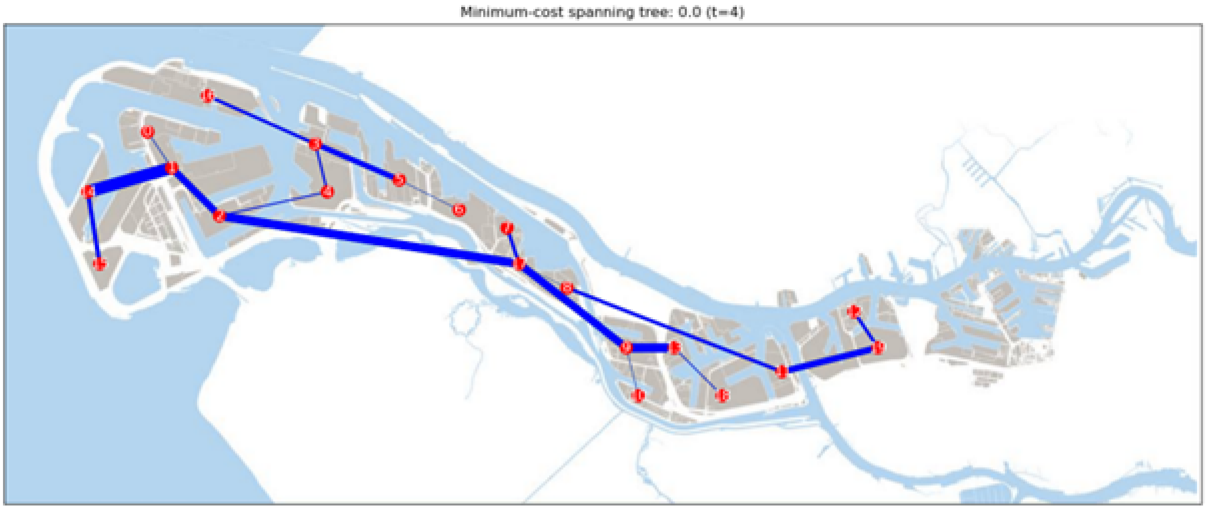


Figure D.17: Simulation Results

D.2 Low Hydrogen Demand Scenario

D.2.1 Hydrogen Supplier First

Figure D.18: Simulation Results

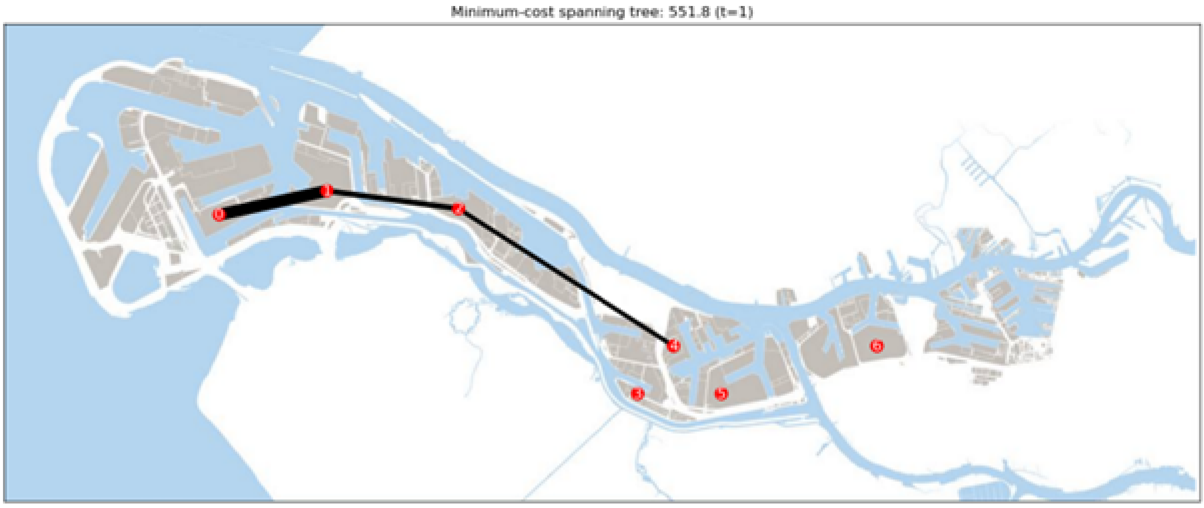


Figure D.19: Simulation Results

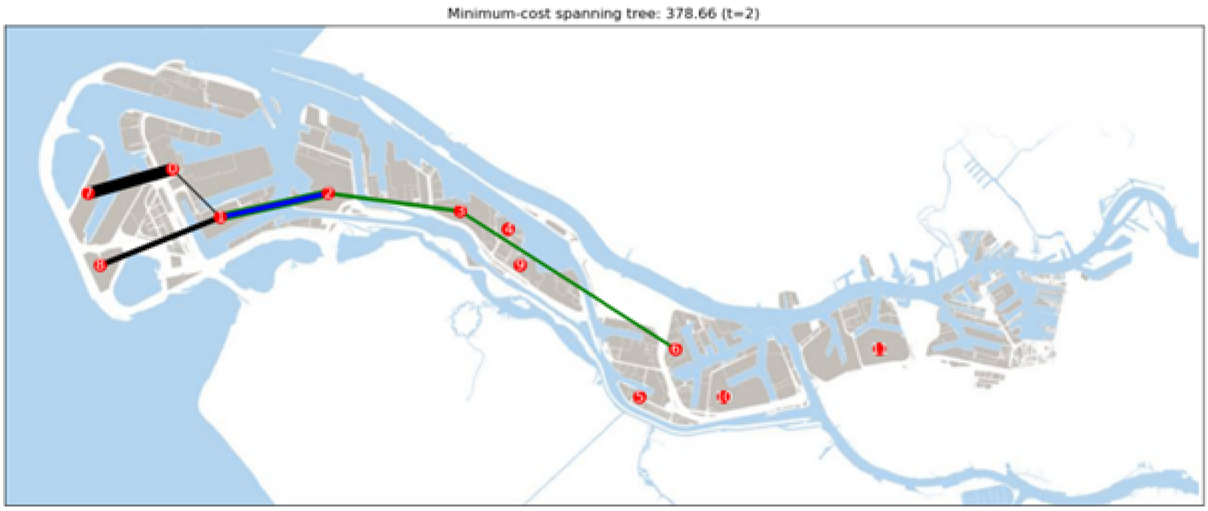


Figure D.20: Simulation Results

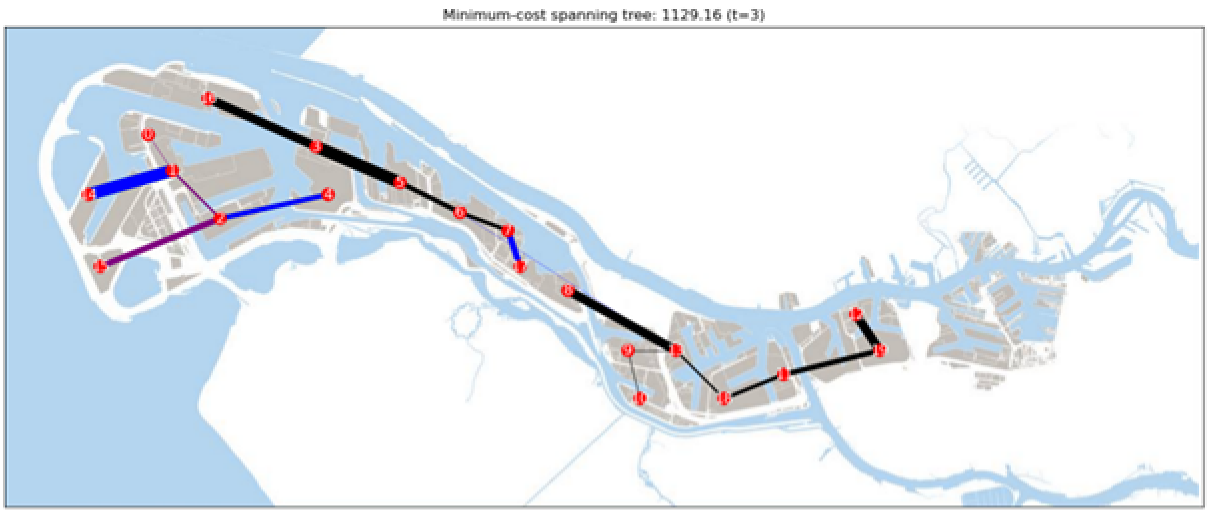


Figure D.21: Simulation Results

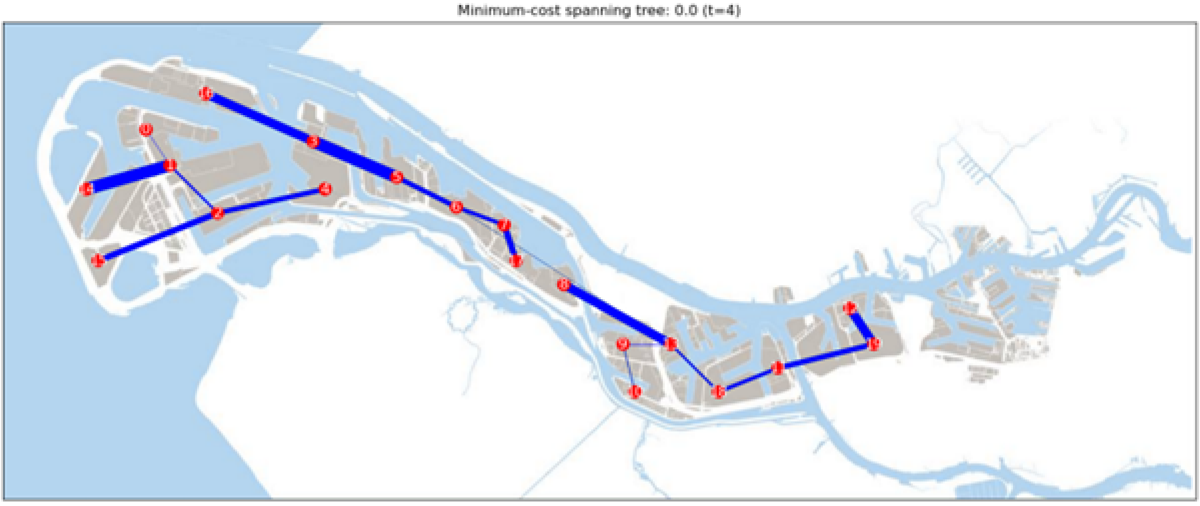
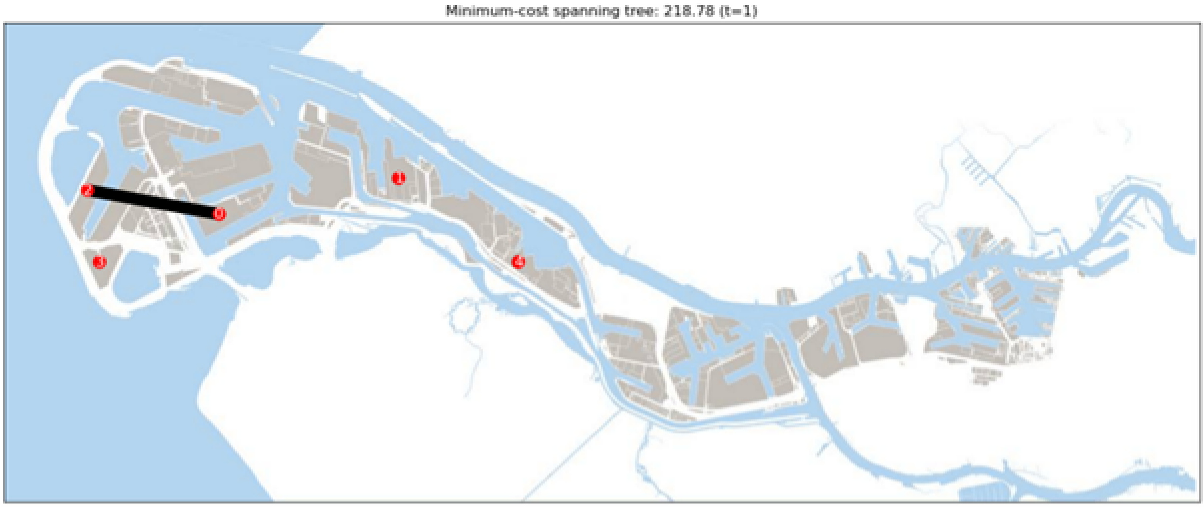


Figure D.22: Simulation Results

D.2.2 Import Terminals First

Figure D.23: Simulation Results



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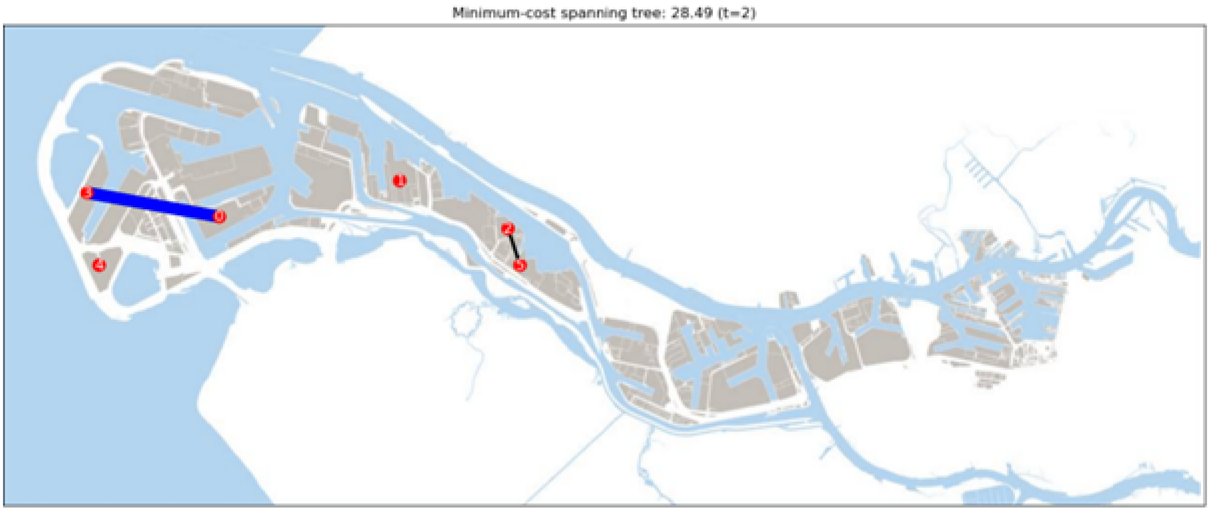

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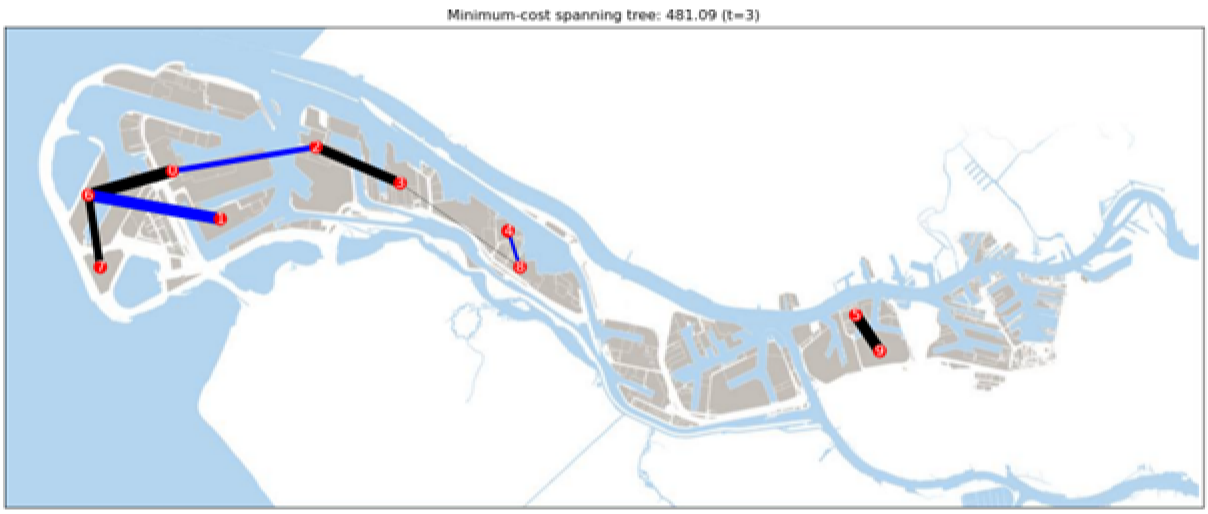


Figure D.26: Simulation Results

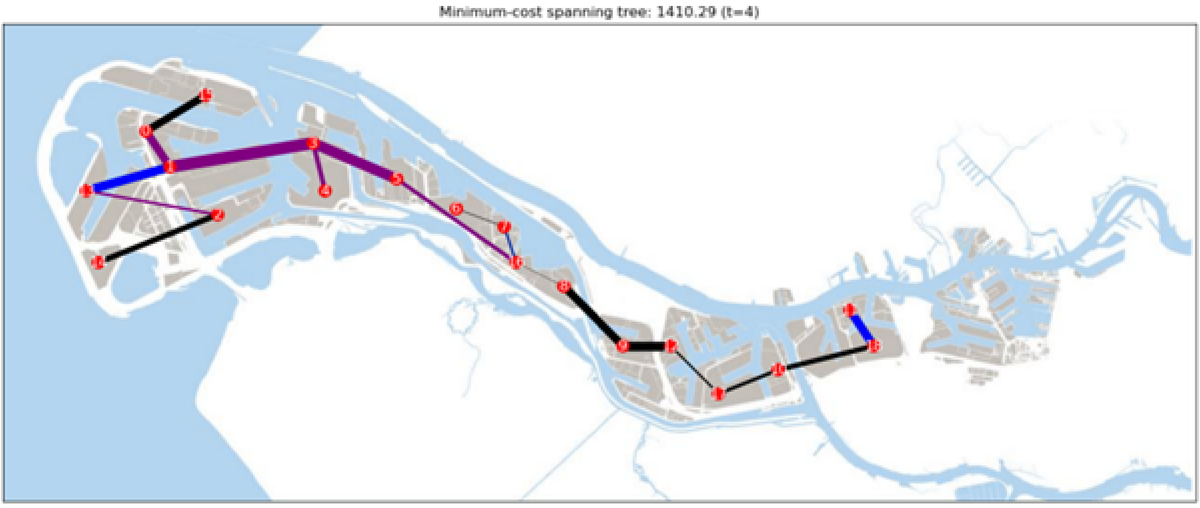
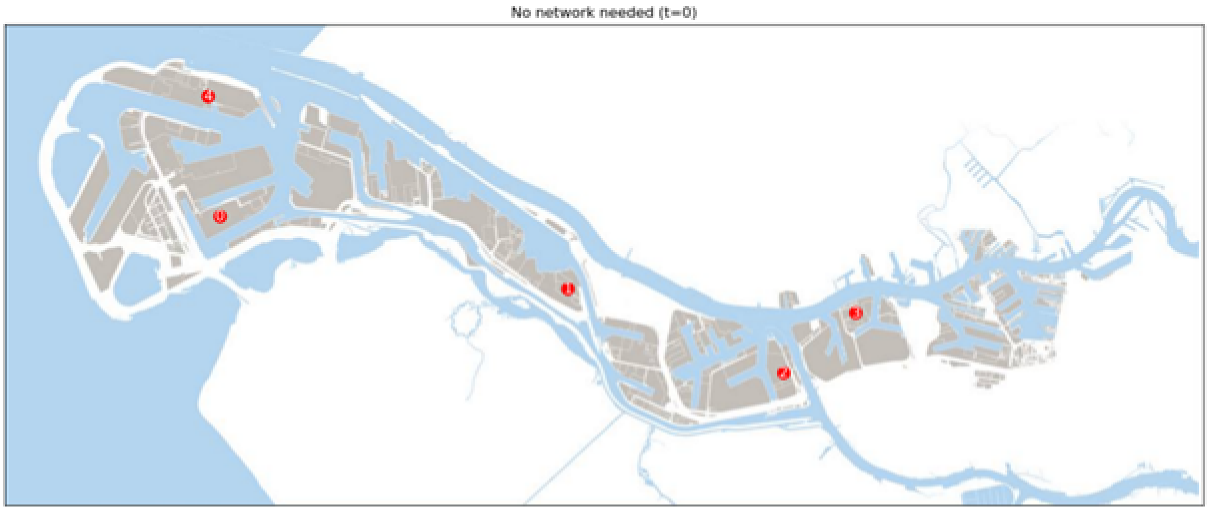


Figure D.27: Simulation Results

D.2.3 Storage Providers First



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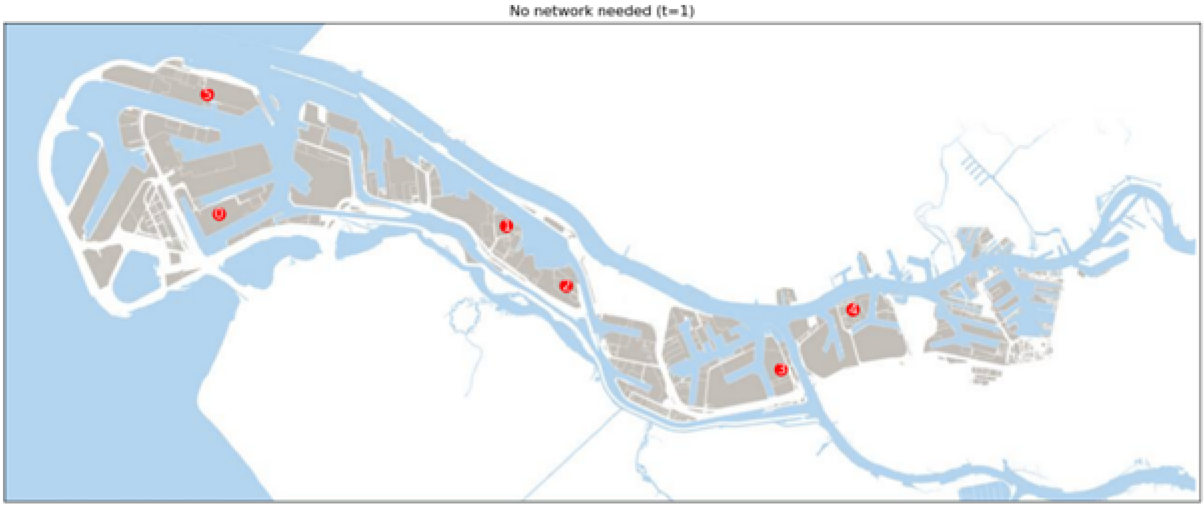

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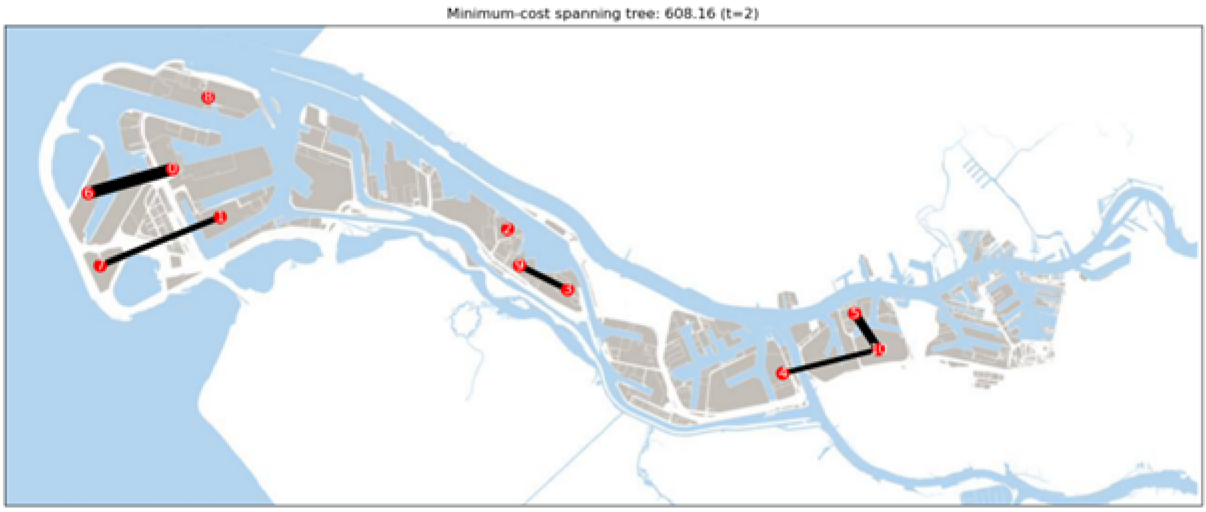

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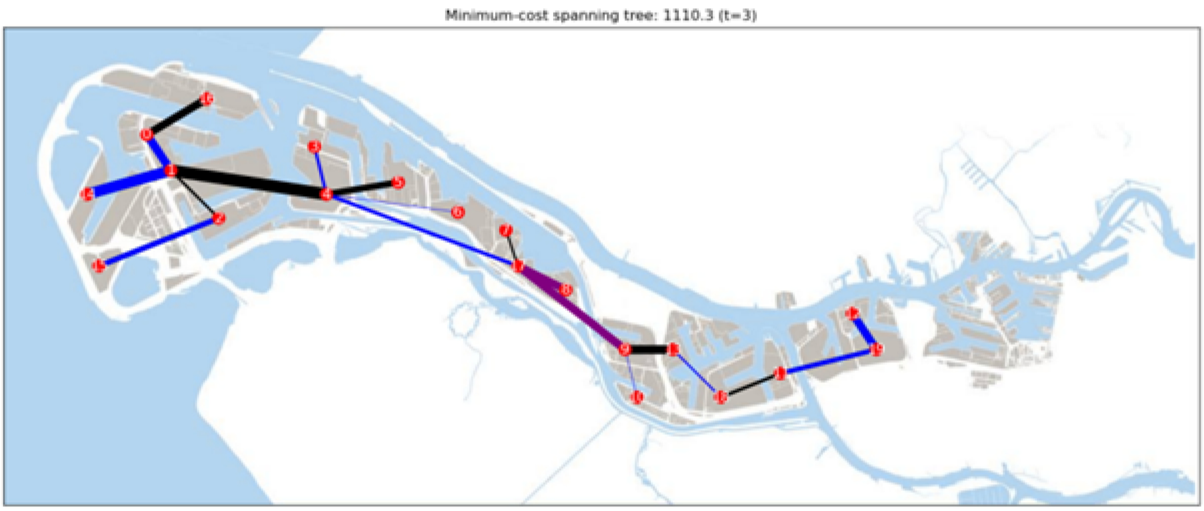


Figure D.31: Simulation Results

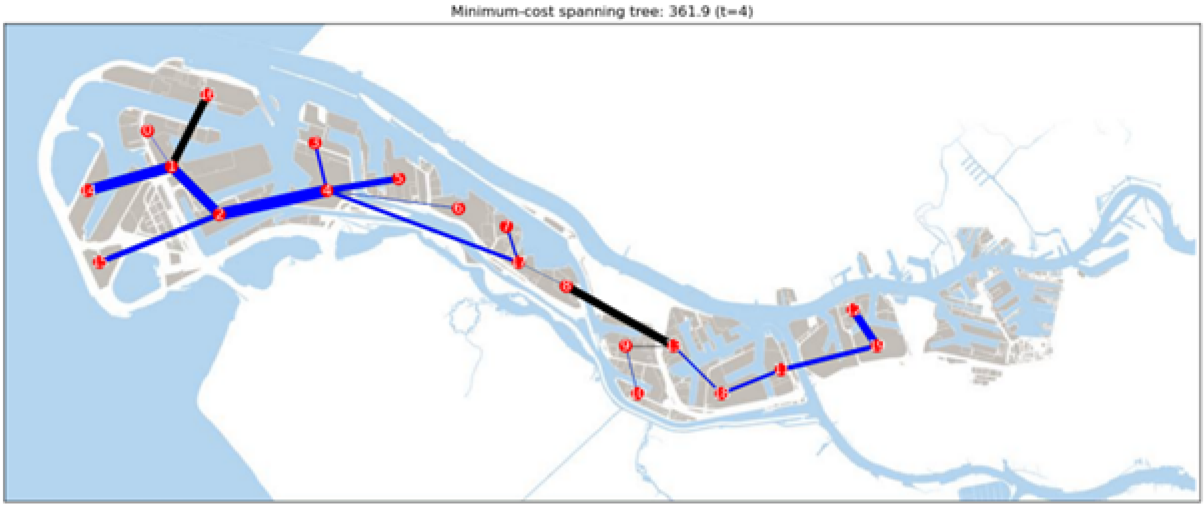


Figure D.32: Simulation Results

D.3 High Hydrogen Demand Scenario

D.3.1 Hydrogen Supplier First

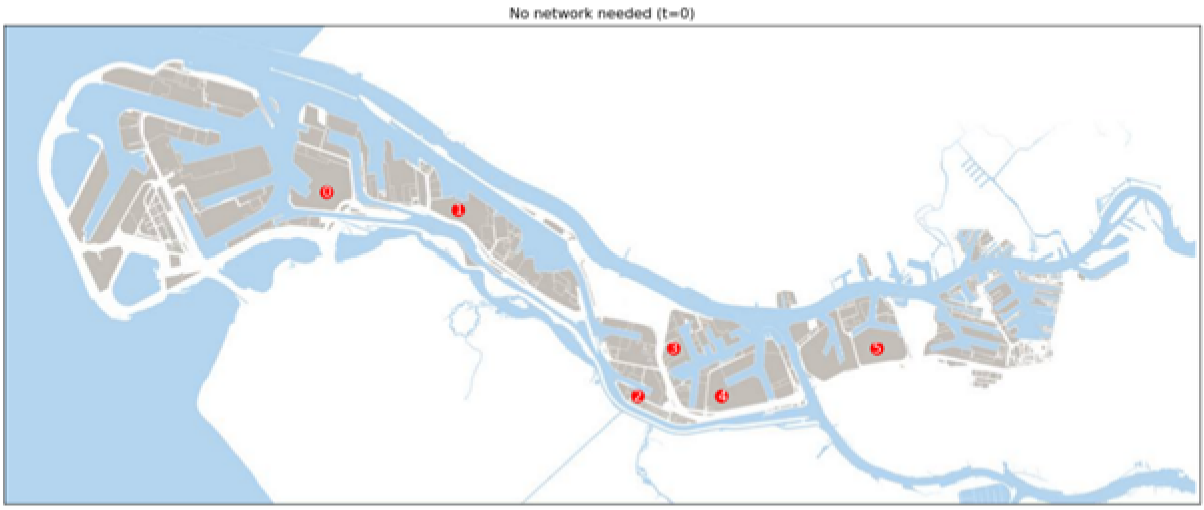
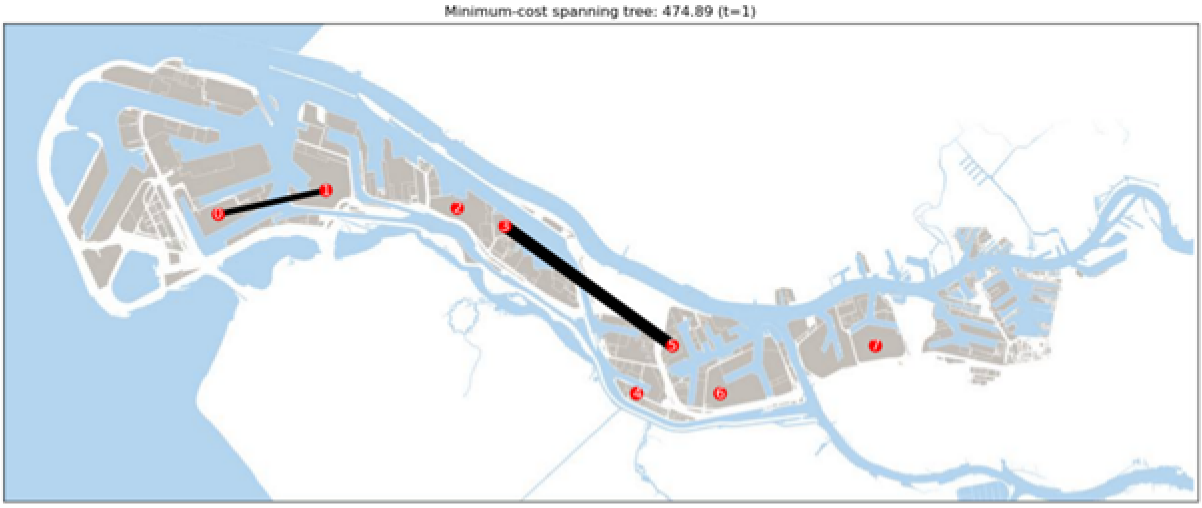


Figure D.33: Simulation Results



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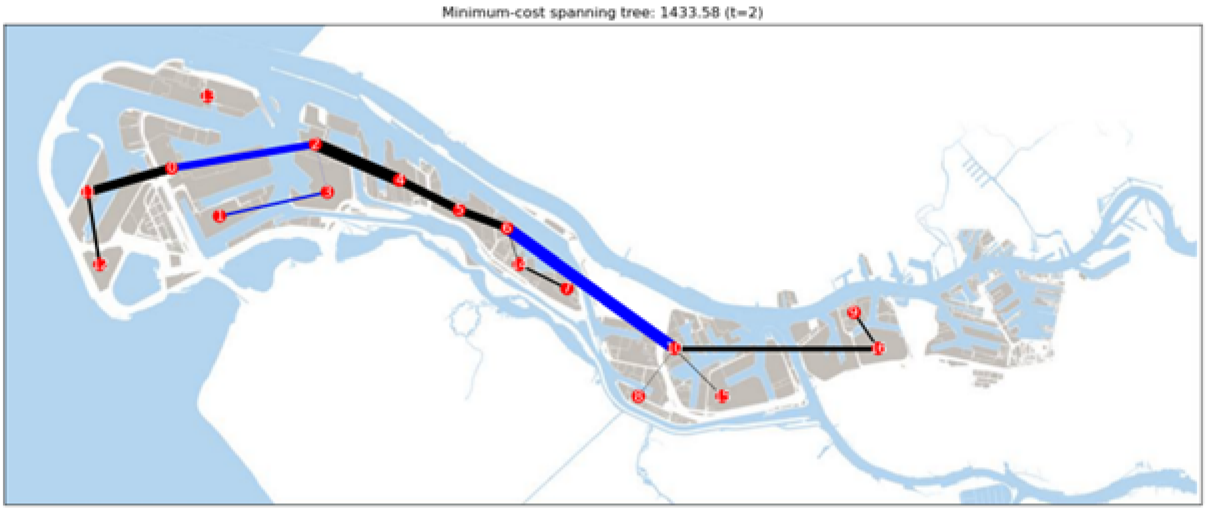


Figure D.35: Simulation Results

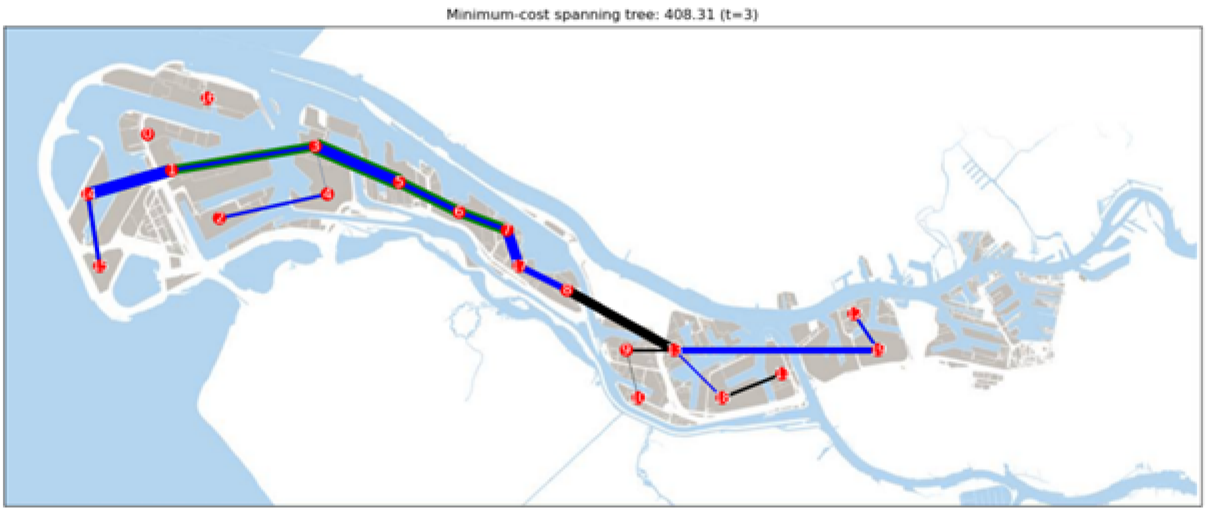


Figure D.36: Simulation Results

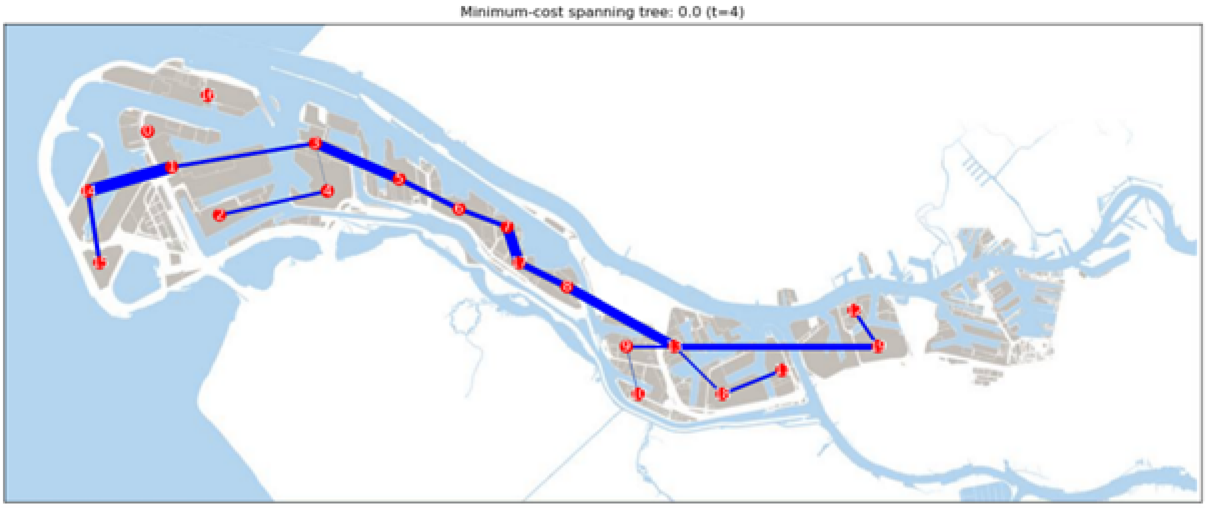


Figure D.37: Simulation Results

D.3.2 Import Terminals First

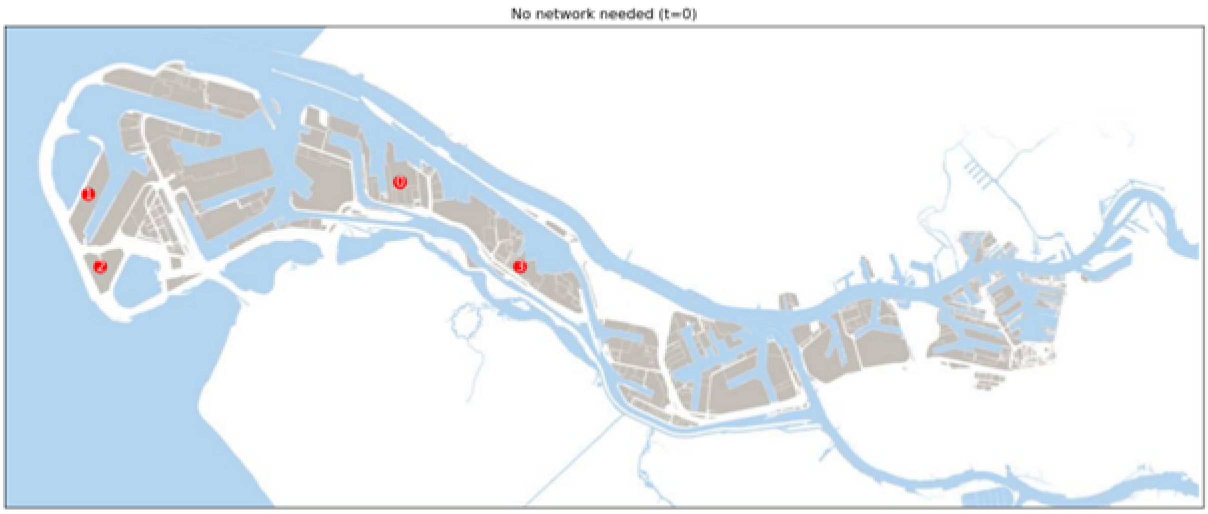


Figure D.38: Simulation Results

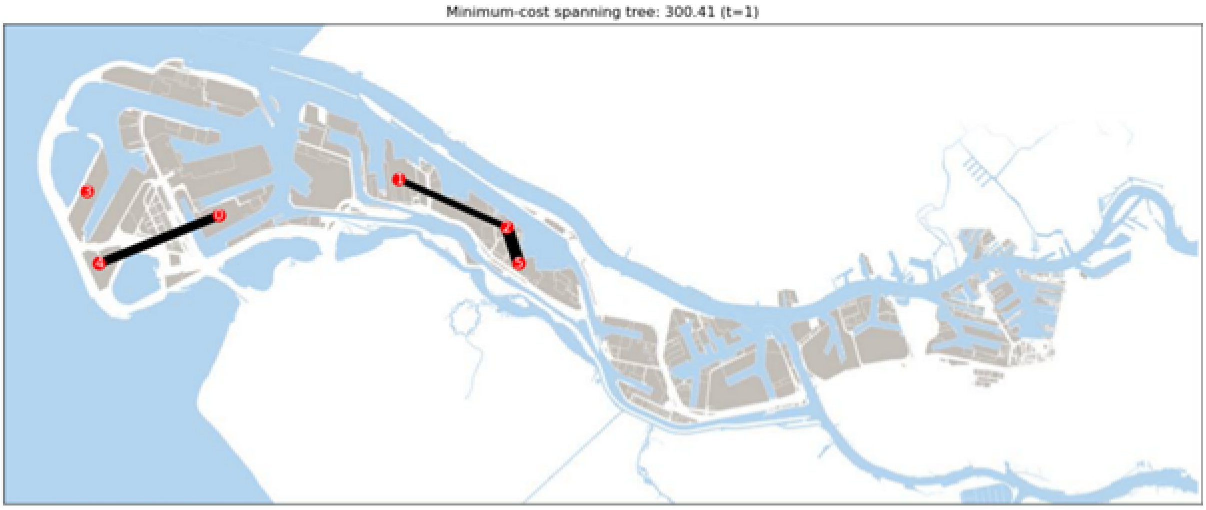


Figure D.39: Simulation Results

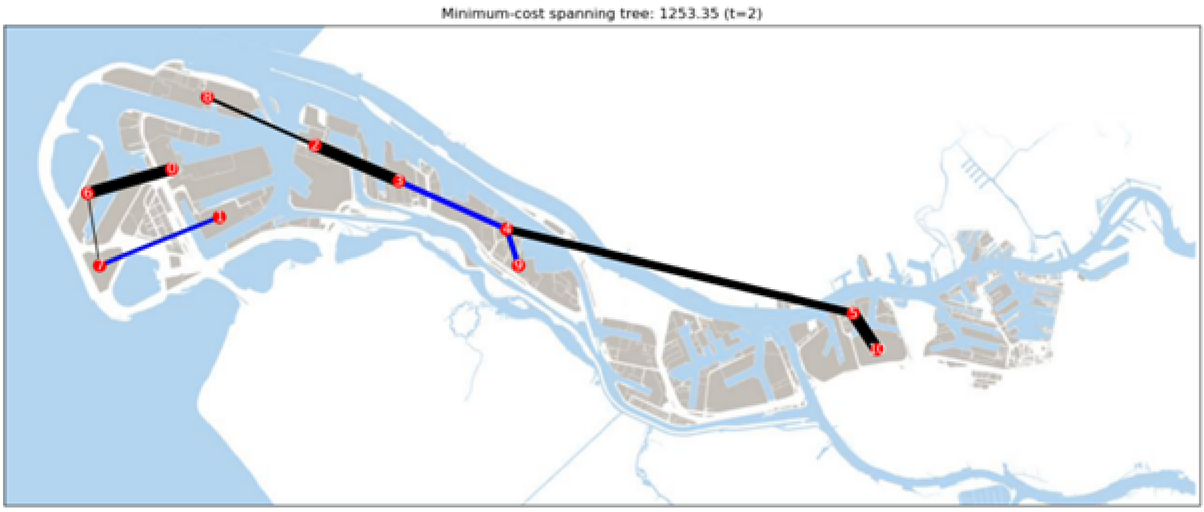


Figure D.40: Simulation Results

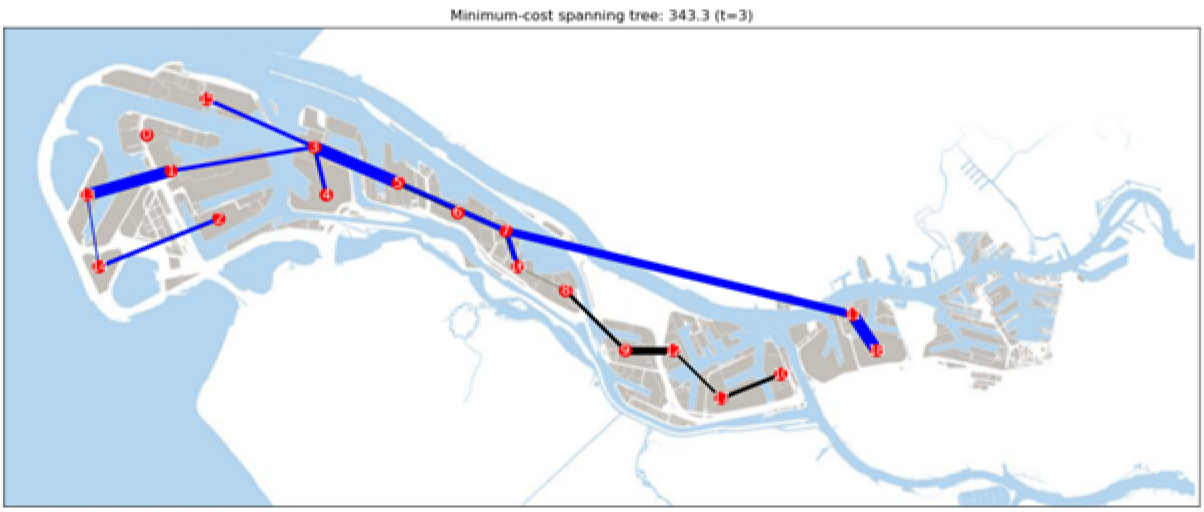


Figure D.41: Simulation Results

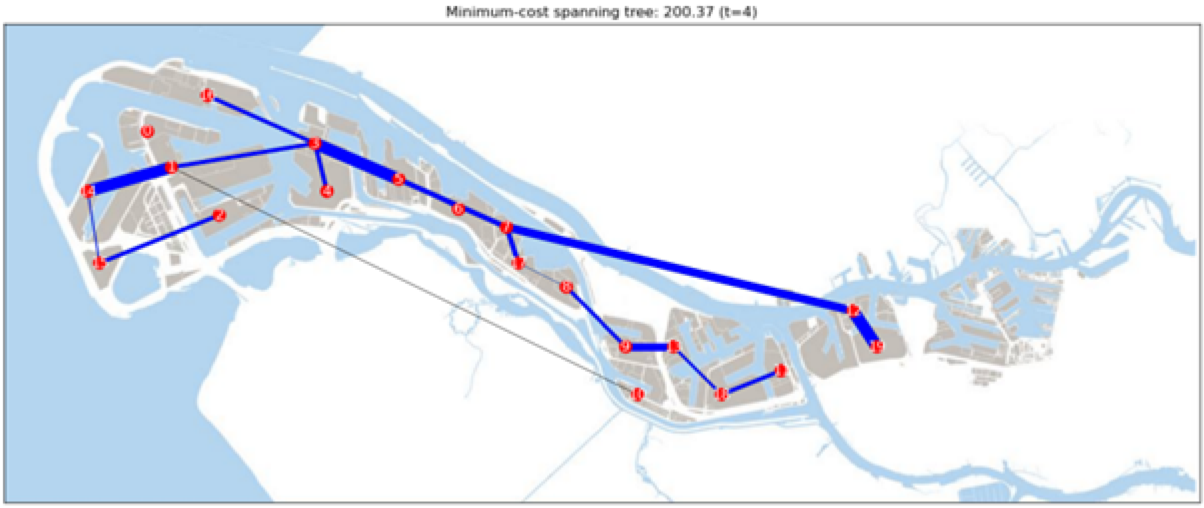


Figure D.42: Simulation Results

D.3.3 Storage Providers First

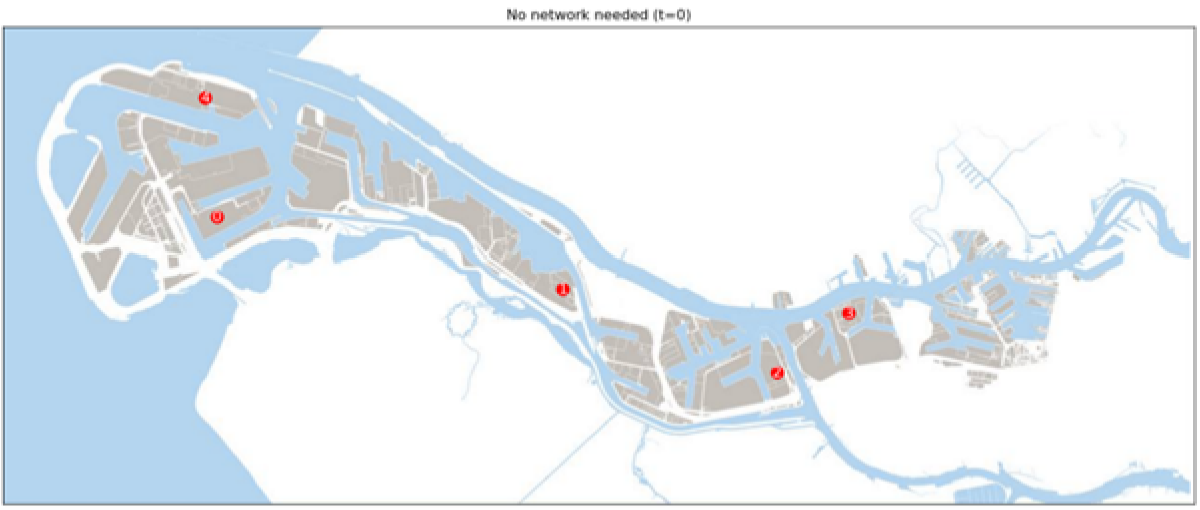


Figure D.43: Simulation Results

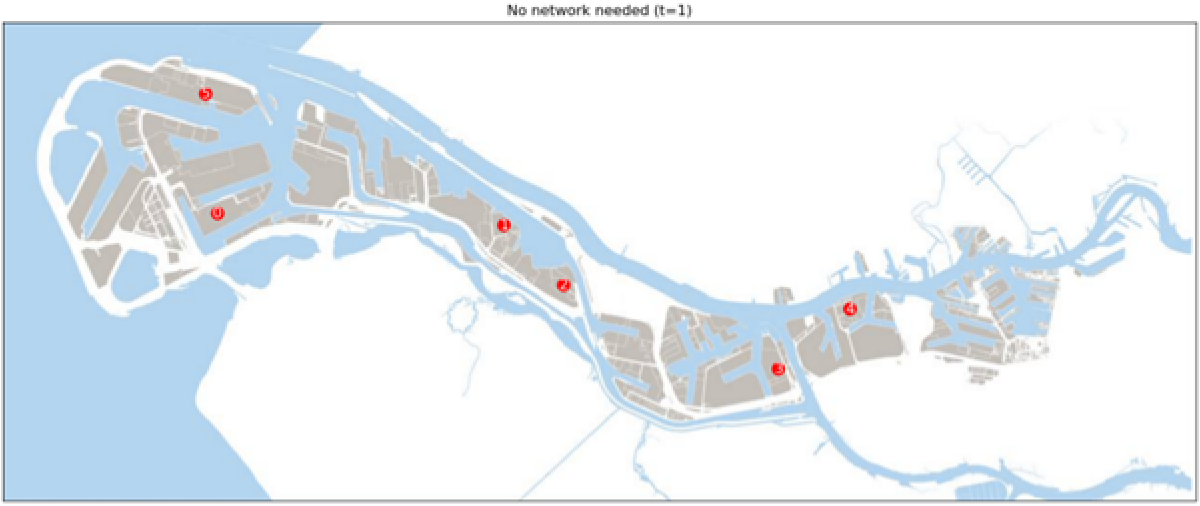


Figure D.44: Simulation Results

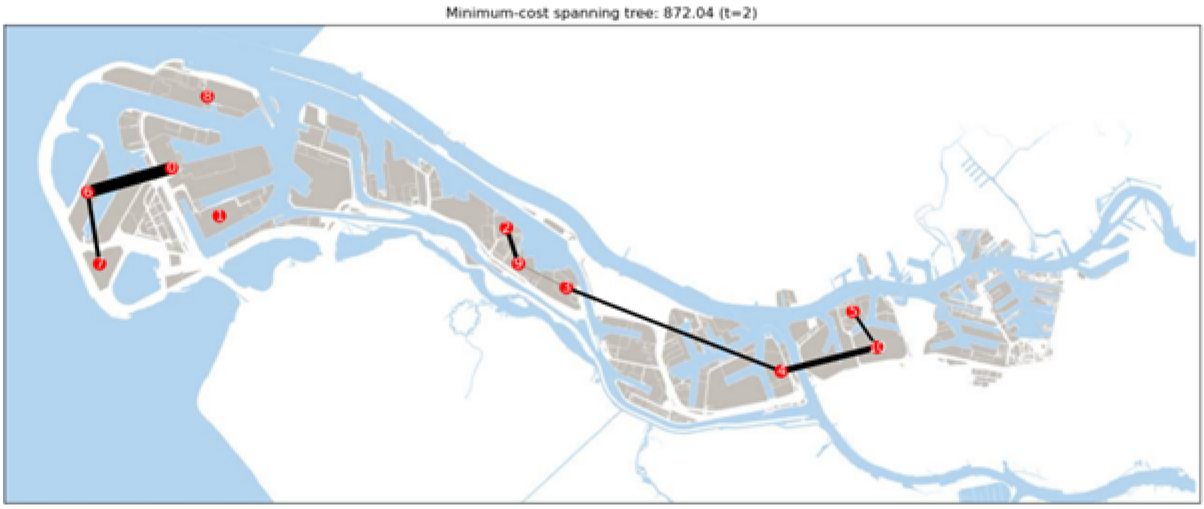


Figure D.45: Simulation Results

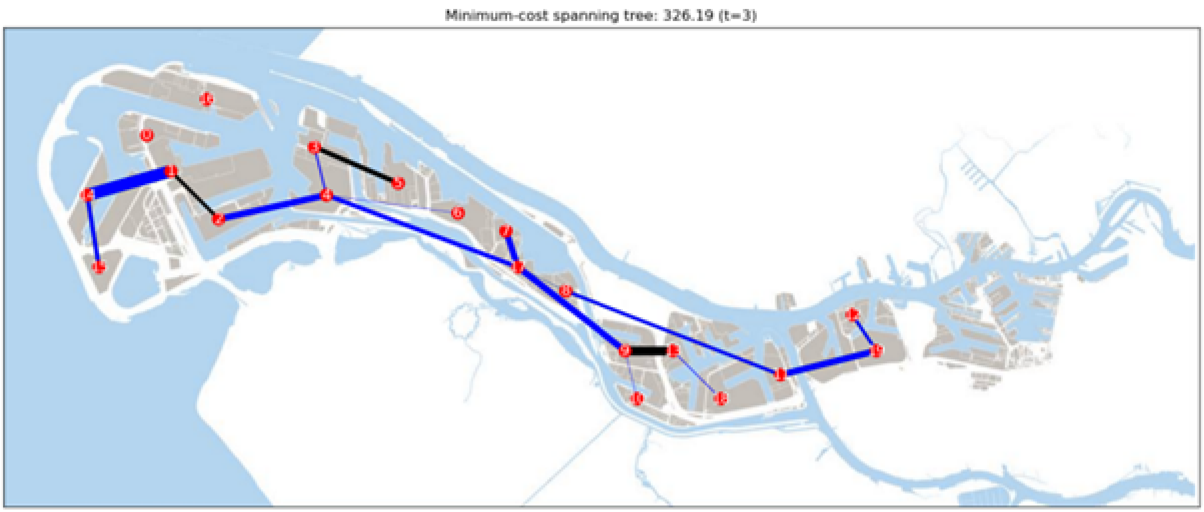


Figure D.46: Simulation Results

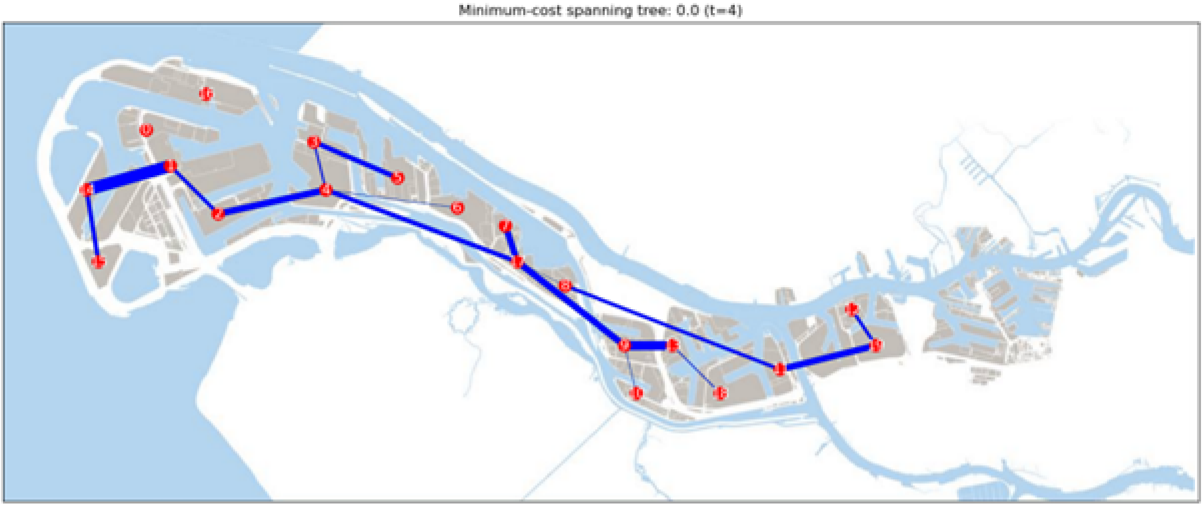


Figure D.47: Simulation Results

D.4 Low Ammonia Import Scenario

D.4.1 Hydrogen Supplier First

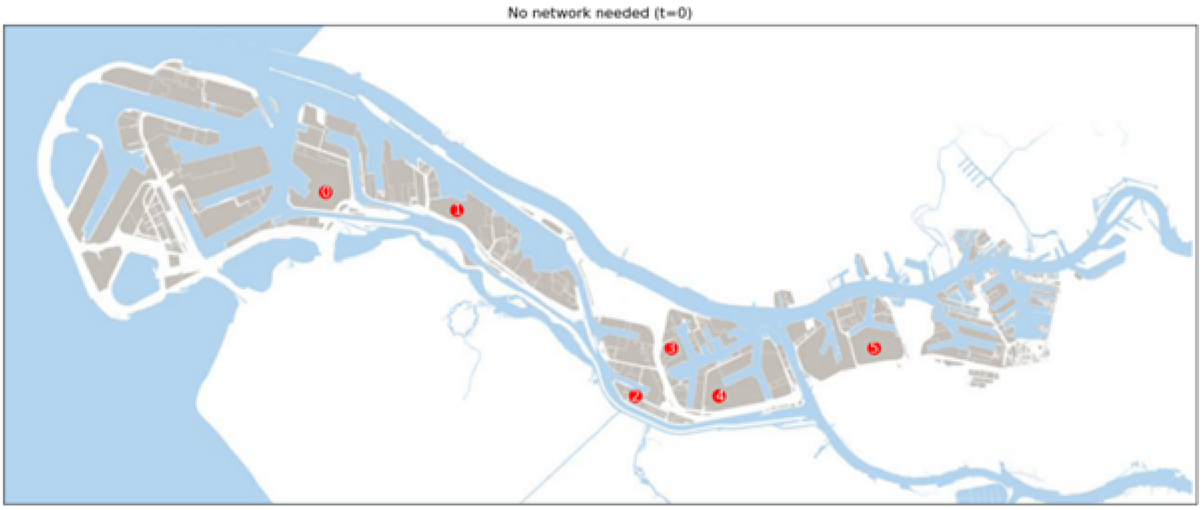


Figure D.48: Simulation Results

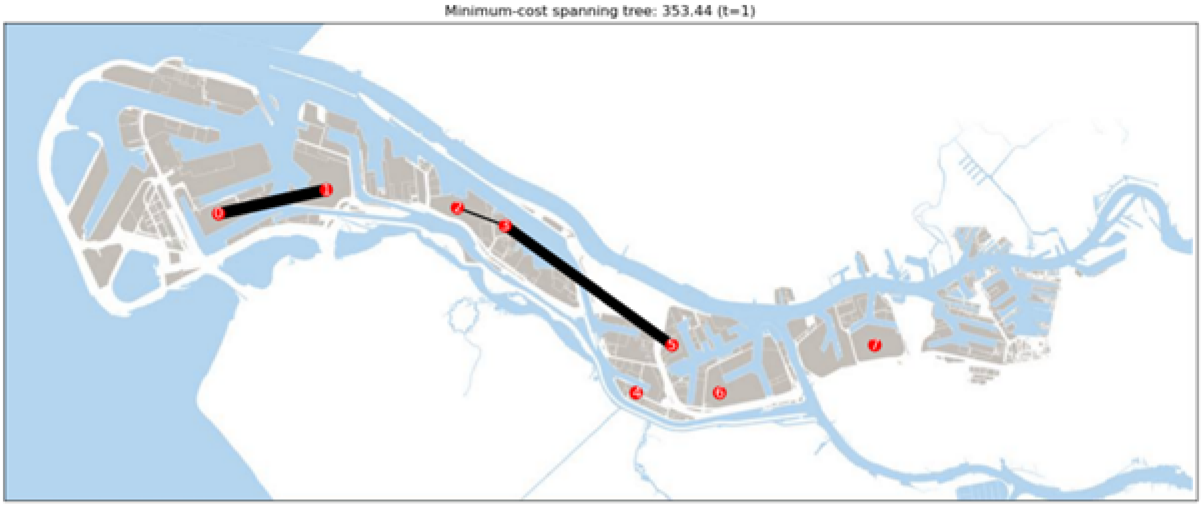
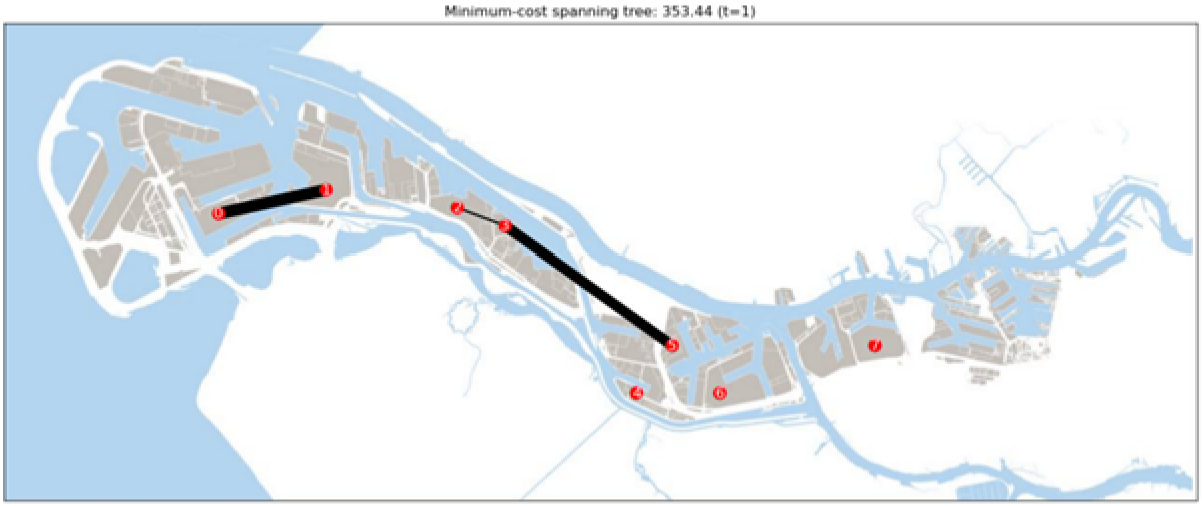


Figure D.49: Simulation Results



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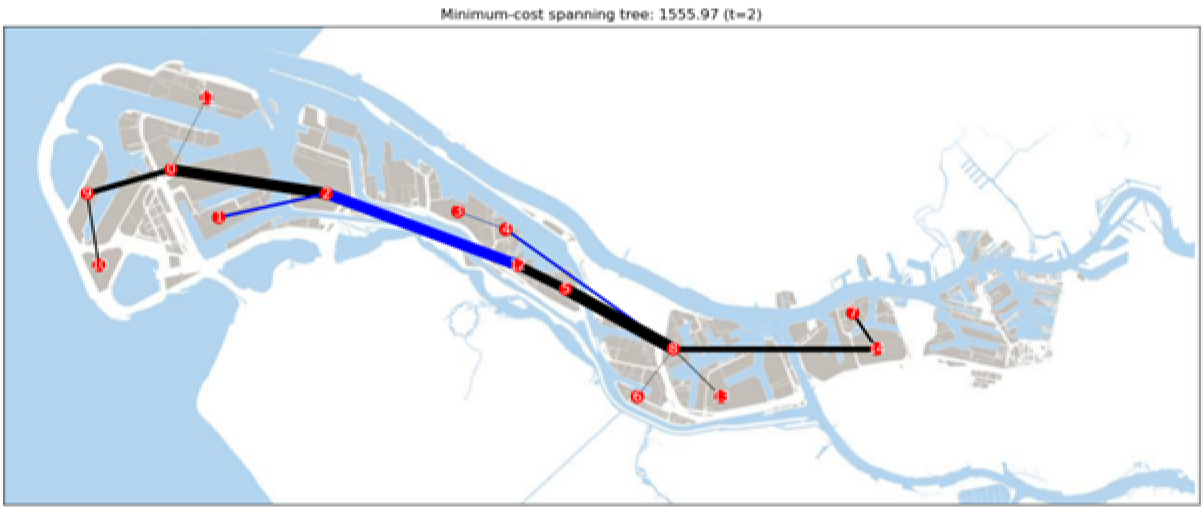

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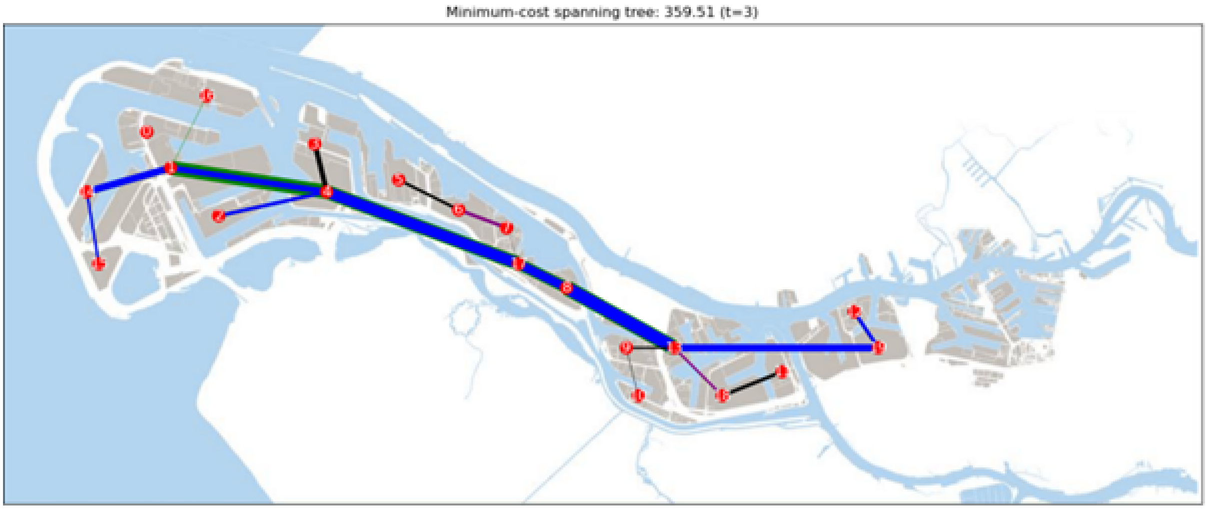


Figure D.52: Simulation Results

D.4.2 Import Terminals First

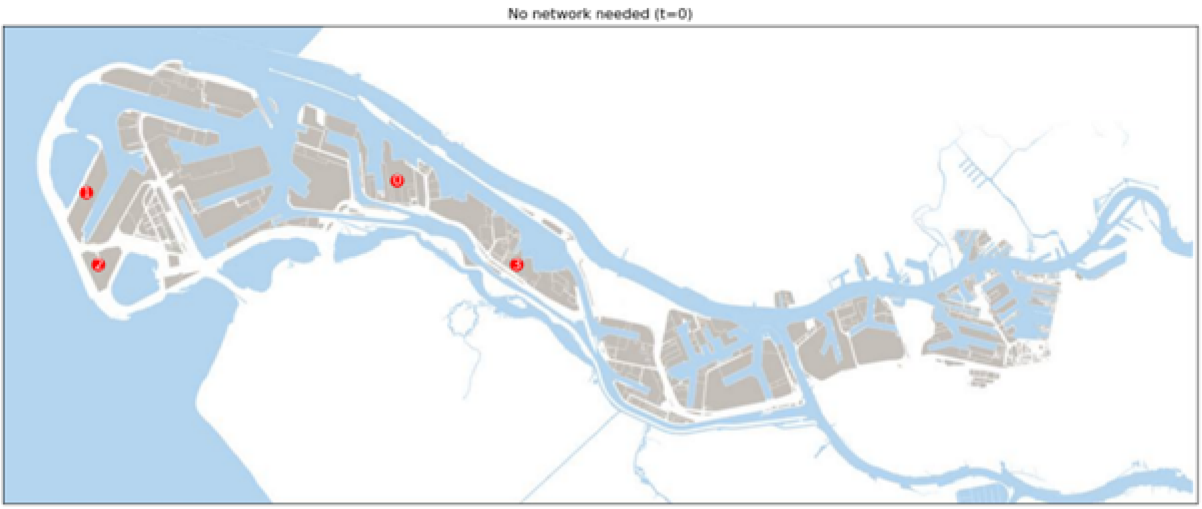


Figure D.53: Simulation Results

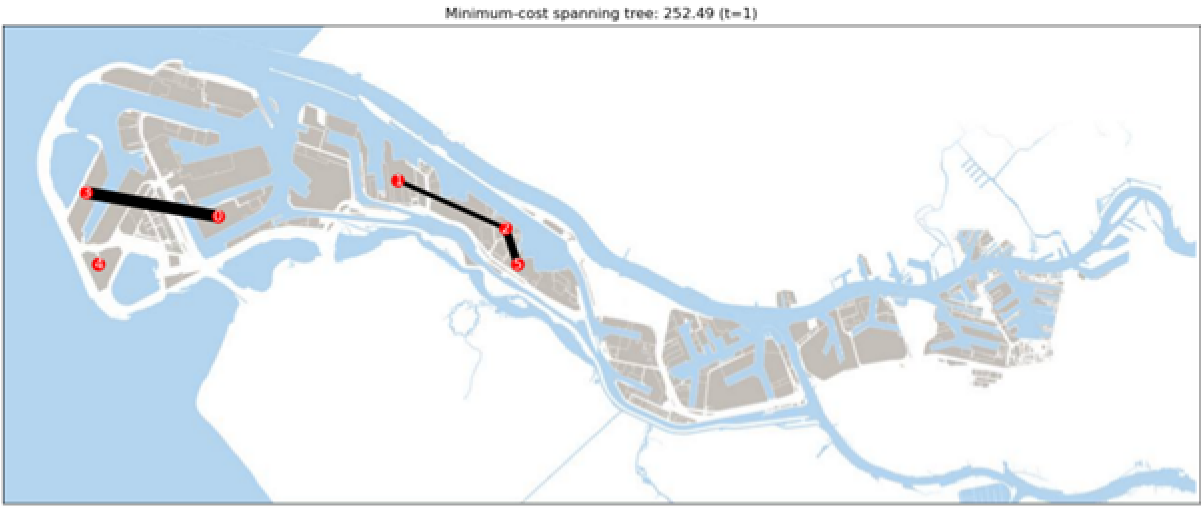


Figure D.54: Simulation Results

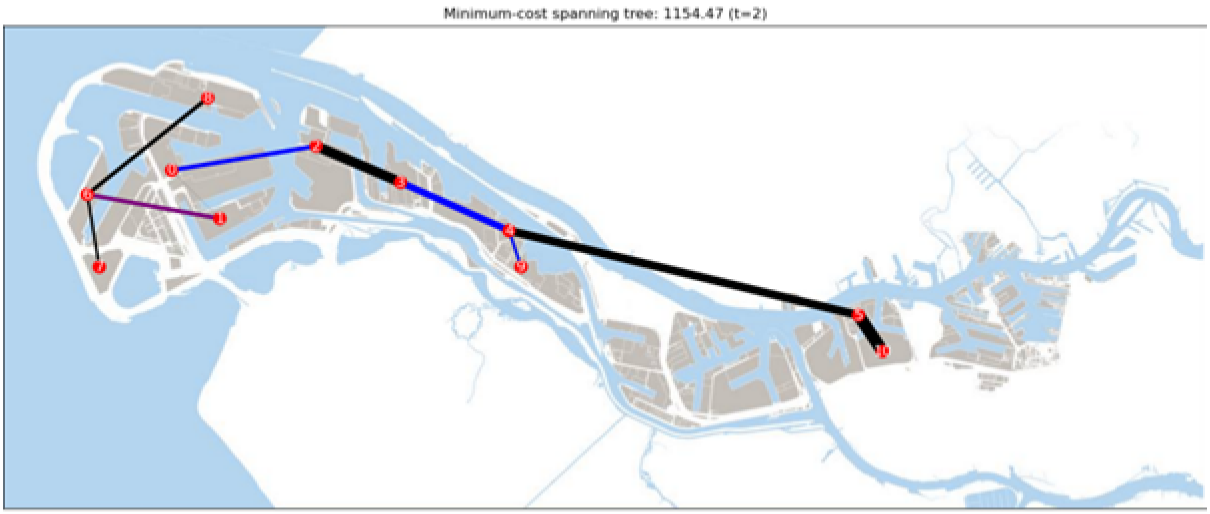
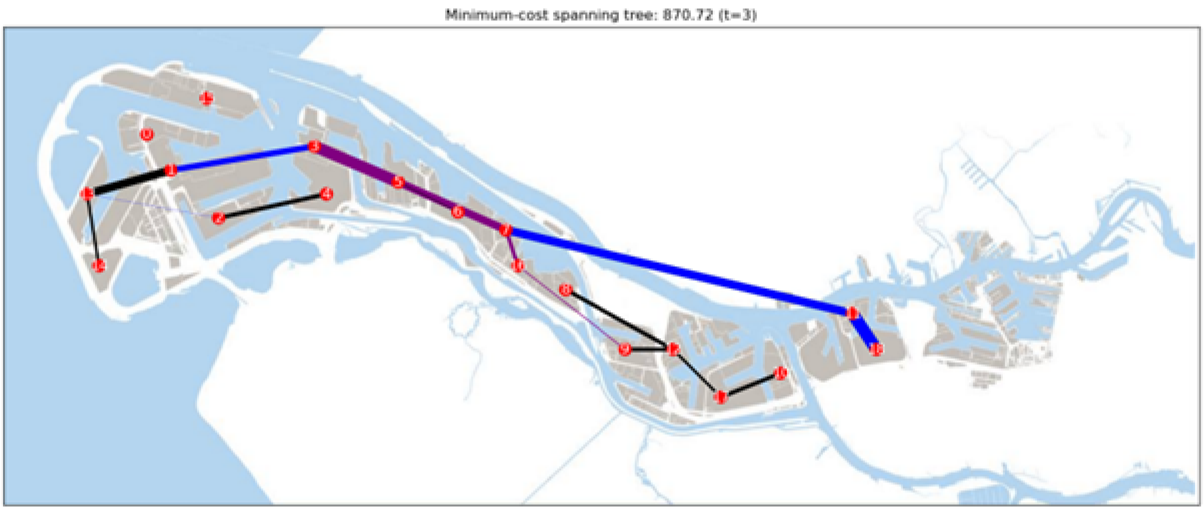


Figure D.55: Simulation Results



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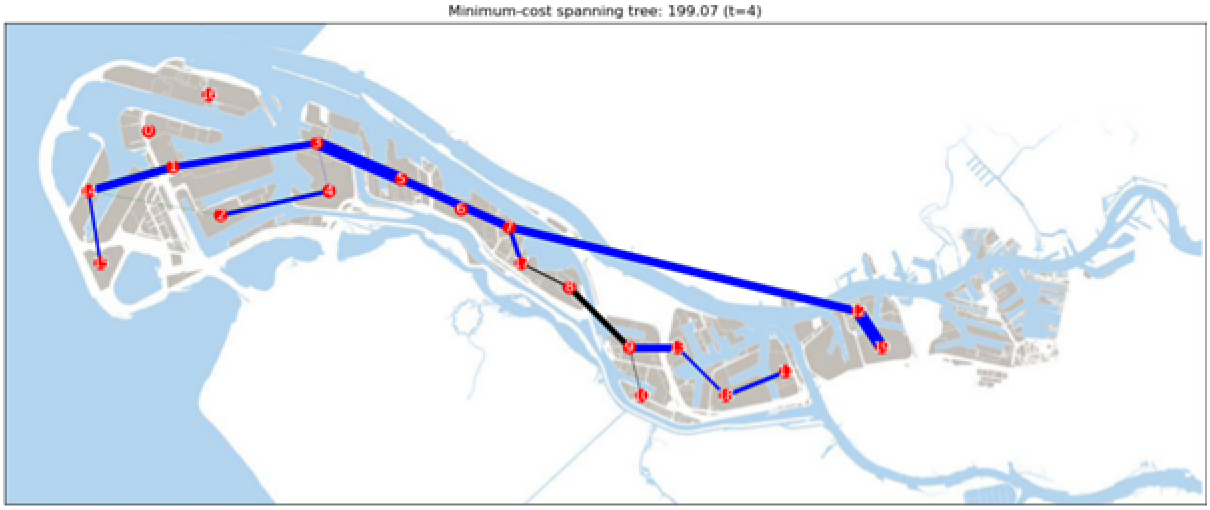
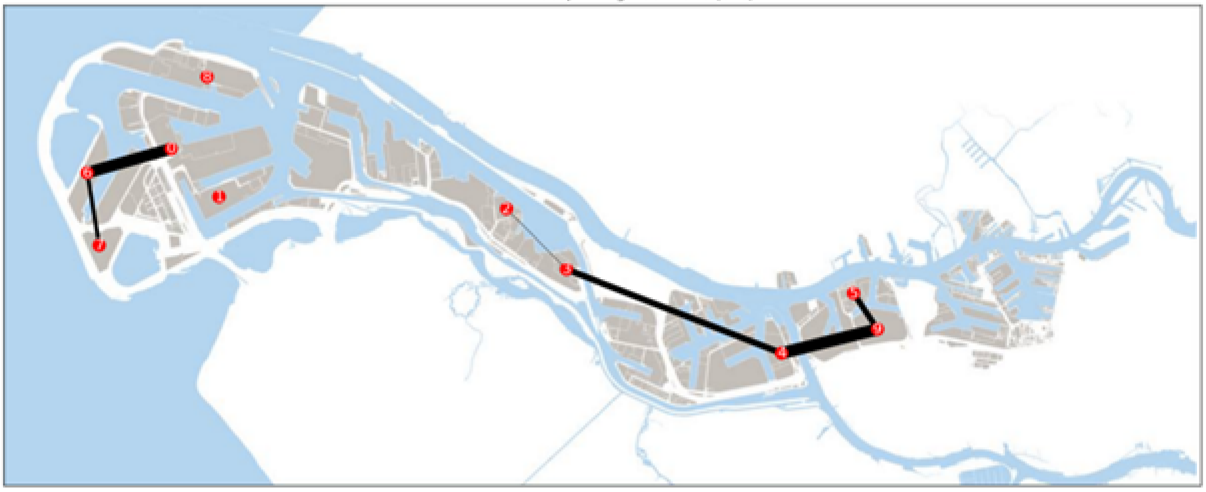


Figure D.57: Simulation Results

D.4.3 Storage Providers First

Figure D.58: Simulation Results

Figure D.59: Simulation Results



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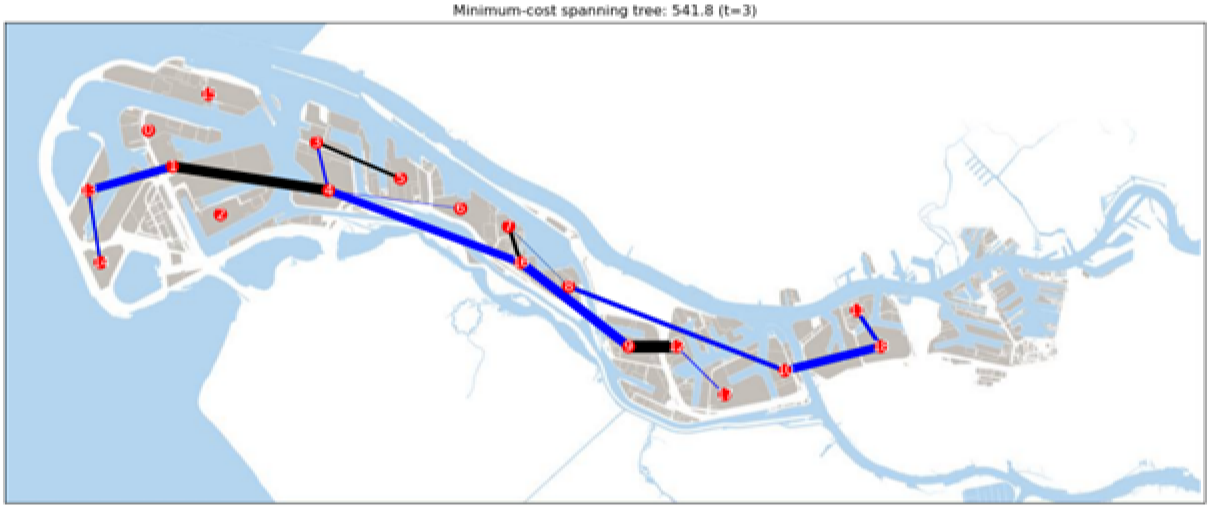


Figure D.61: Simulation Results

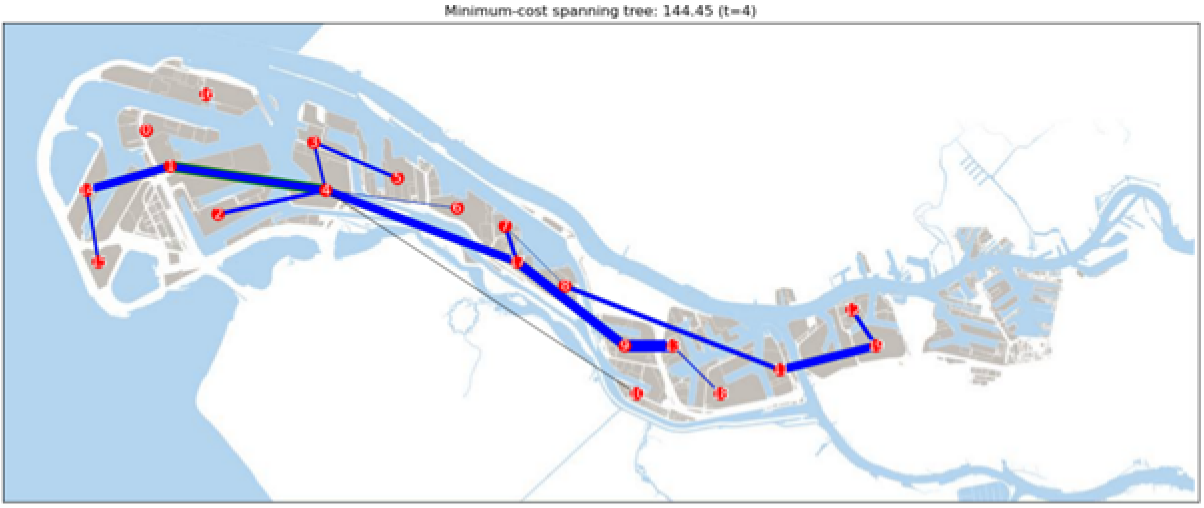


Figure D.62: Simulation Results

D.5 High Ammonia Import Scenario

D.5.1 Hydrogen Supplier First

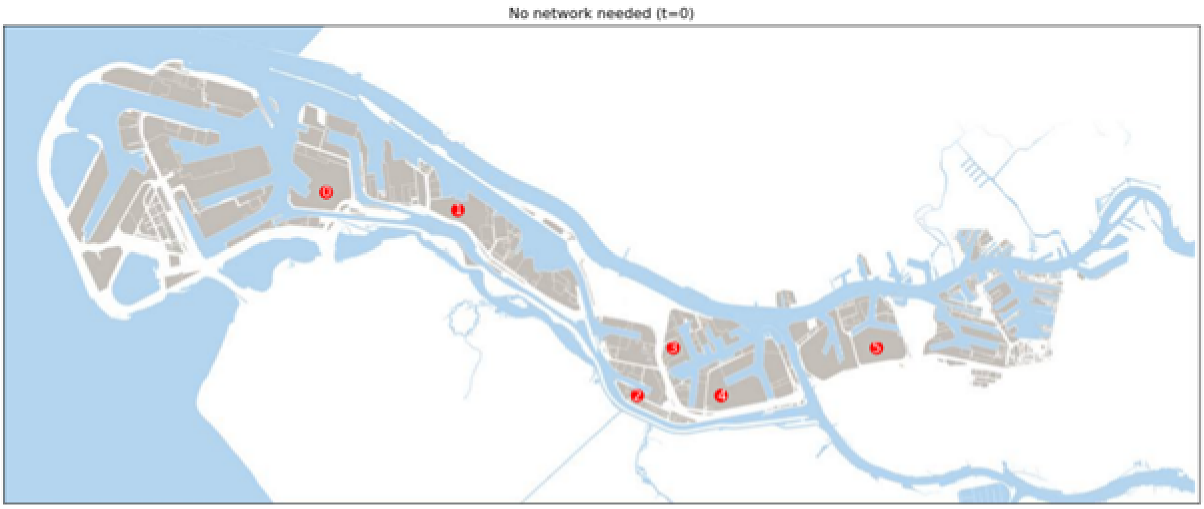
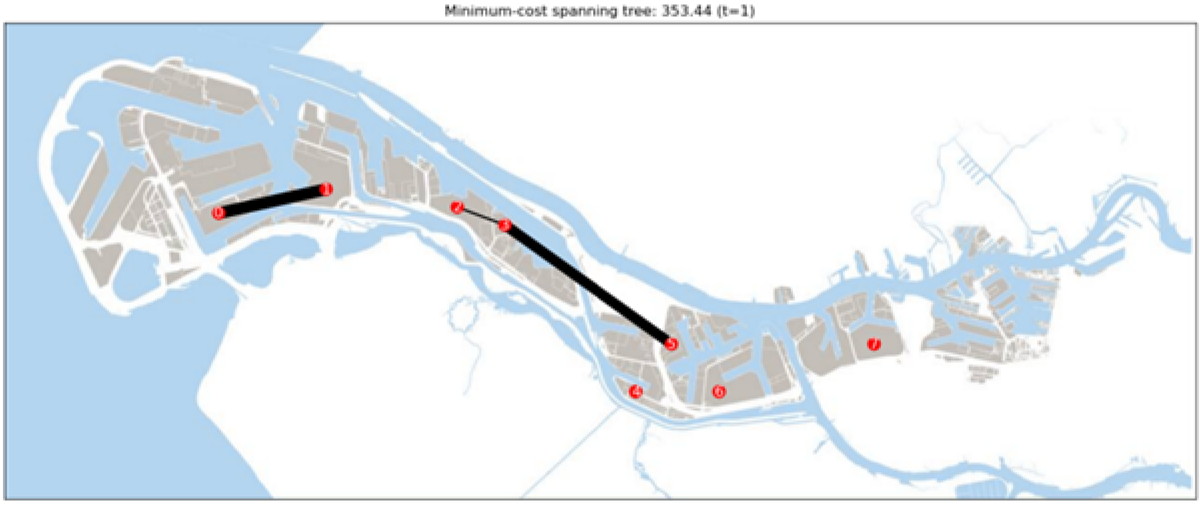


Figure D.63: Simulation Results



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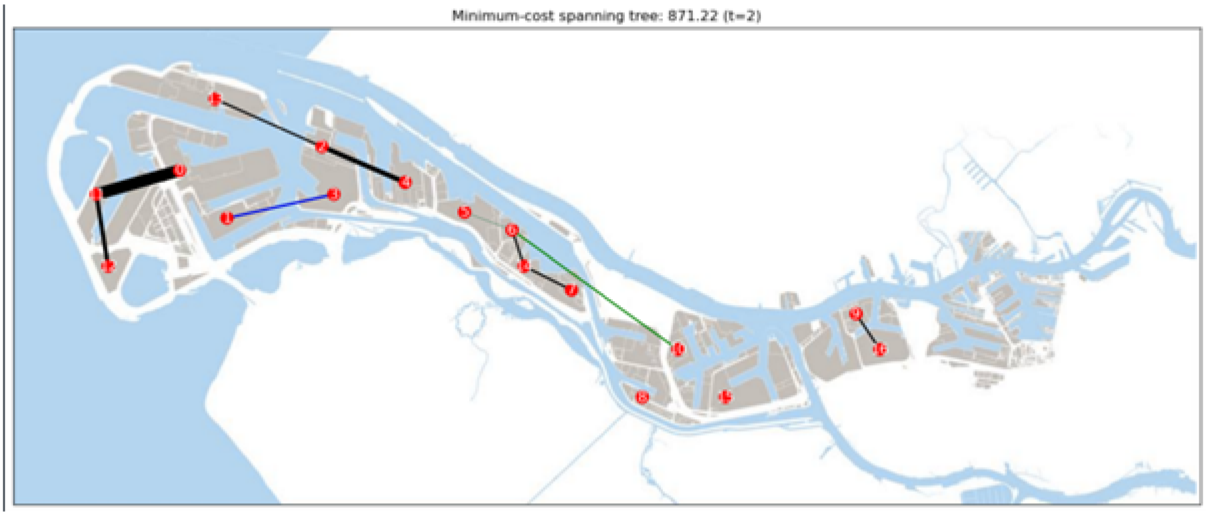

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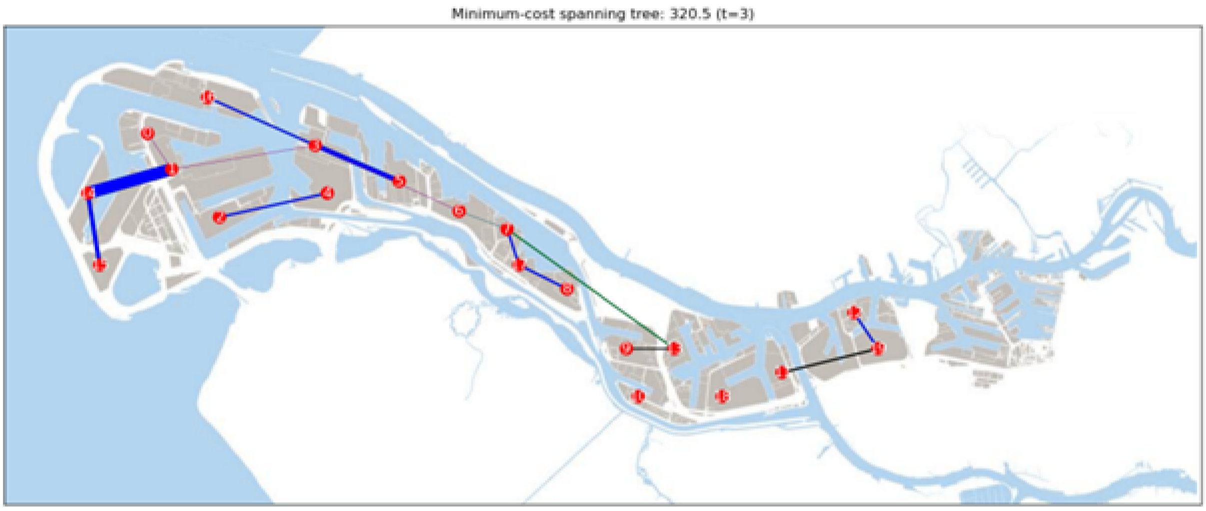


Figure D.66: Simulation Results

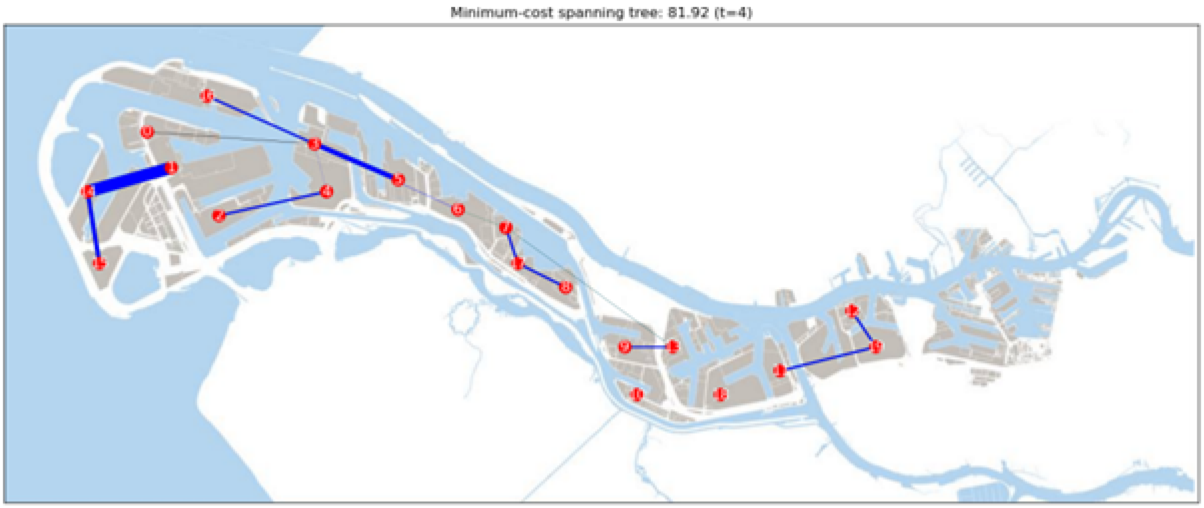


Figure D.67: Simulation Results

D.5.2 Import Terminals First

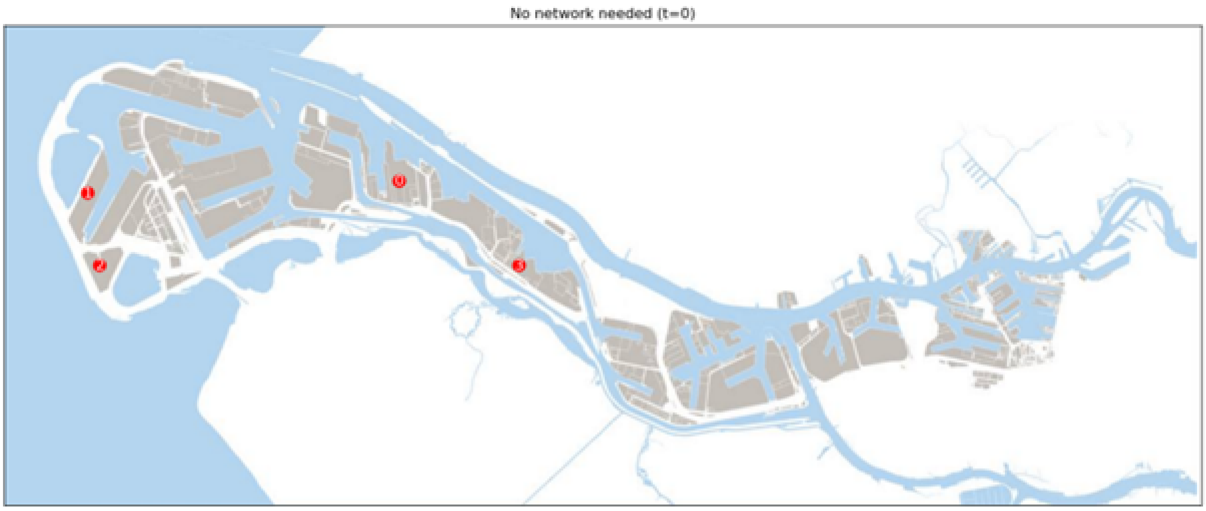
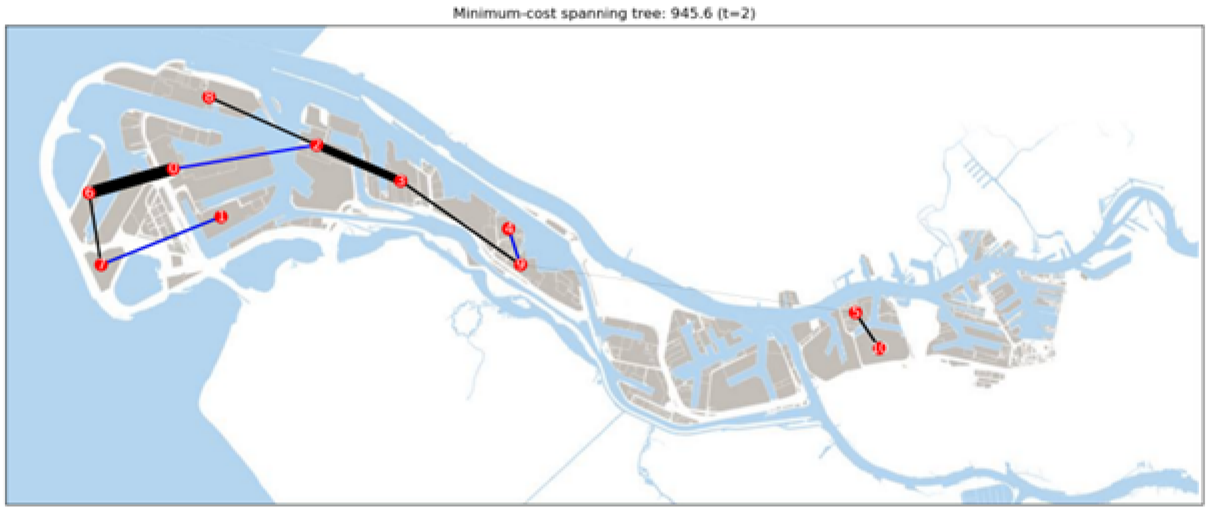


Figure D.68: Simulation Results

Figure D.69: Simulation Results



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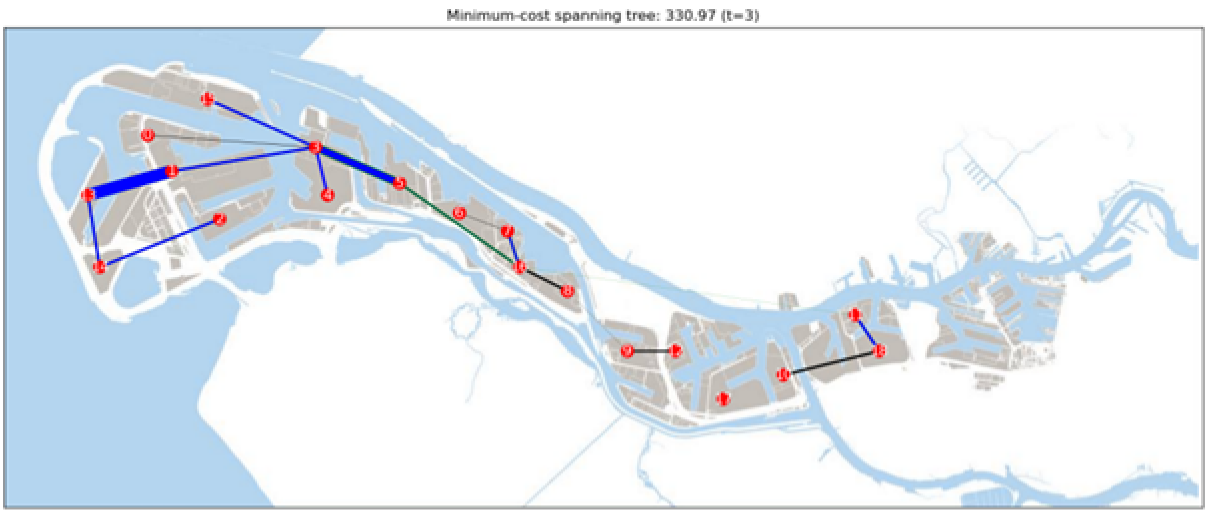

Figure D.71: Simulation Results

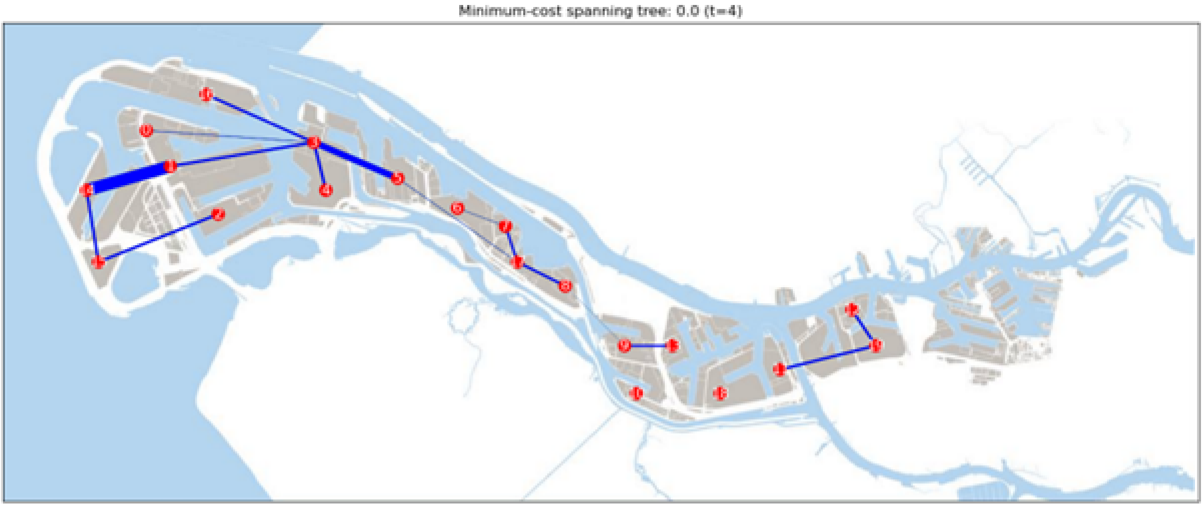

Figure D.72: Simulation Results

D.5.3 Storage Providers First

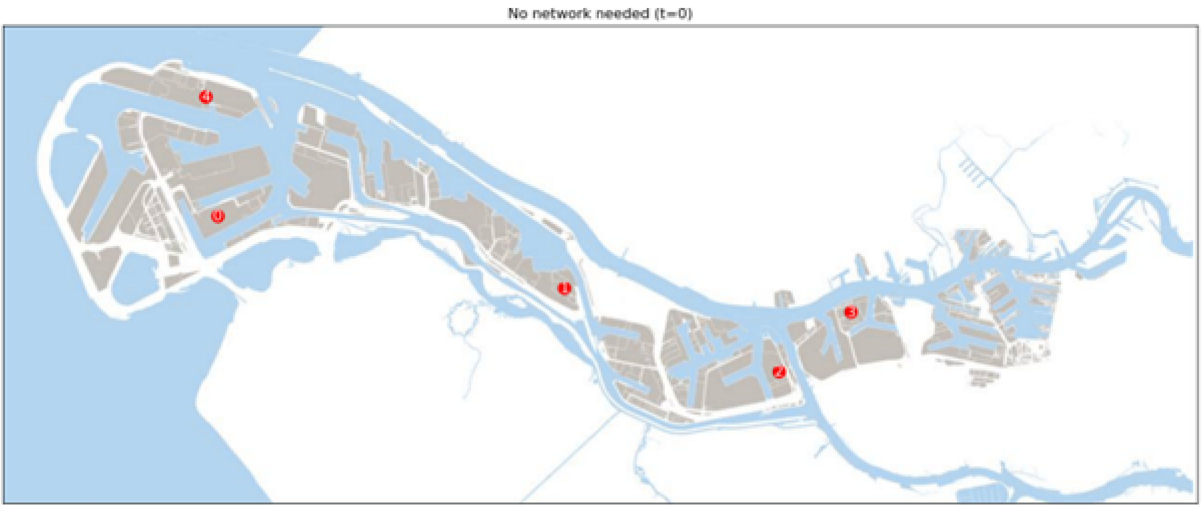

Figure D.73: Simulation Results

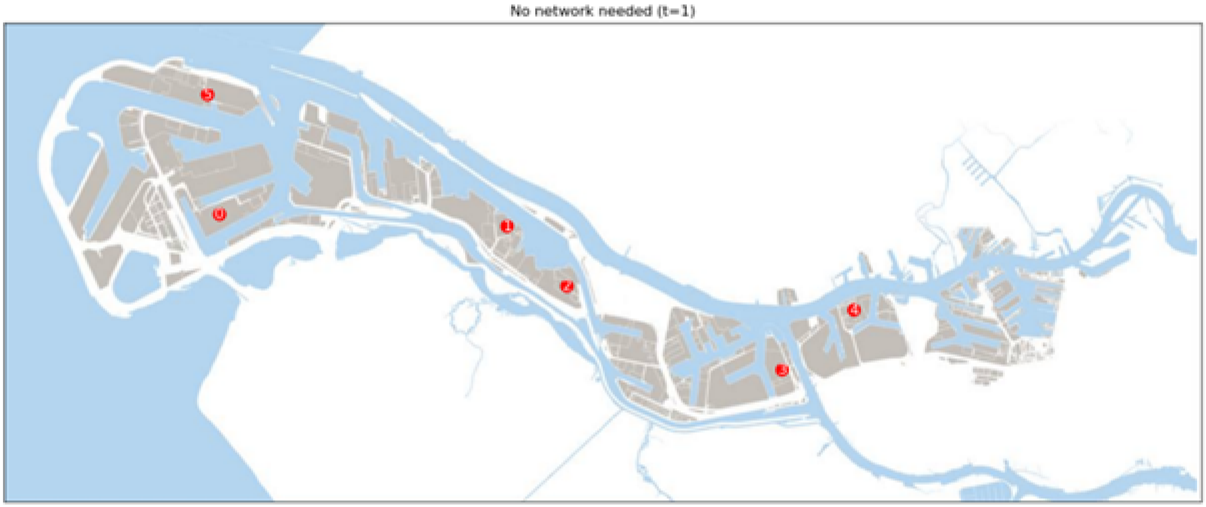

Figure D.74: Simulation Results

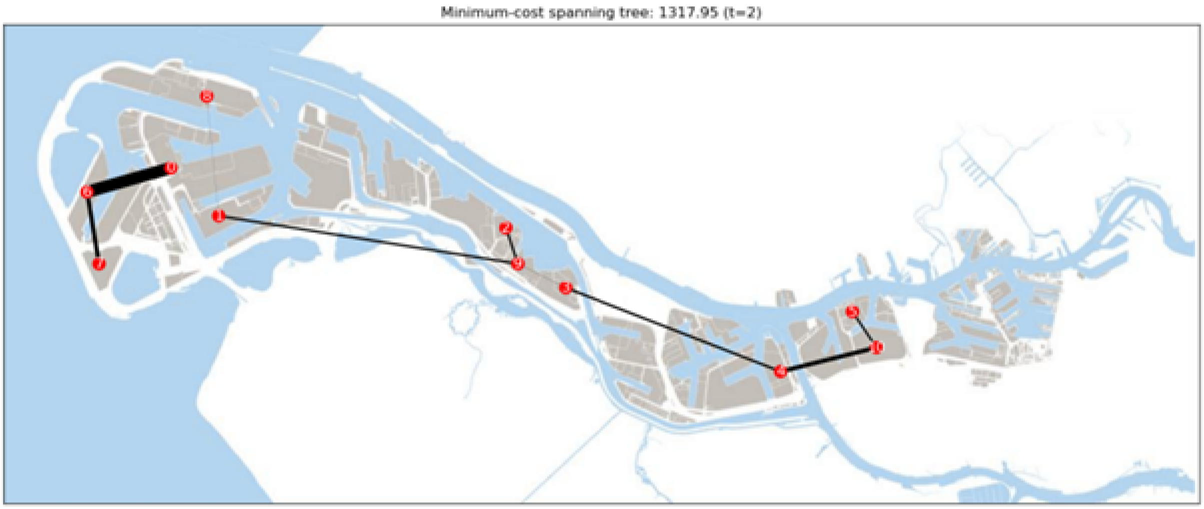

Figure D.75: Simulation Results

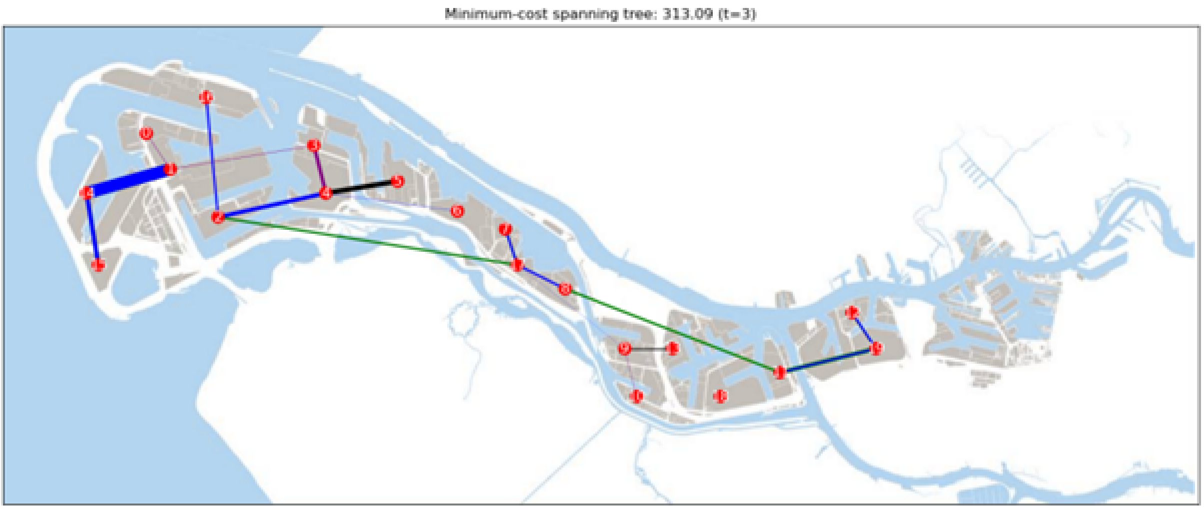

Figure D.76: Simulation Results

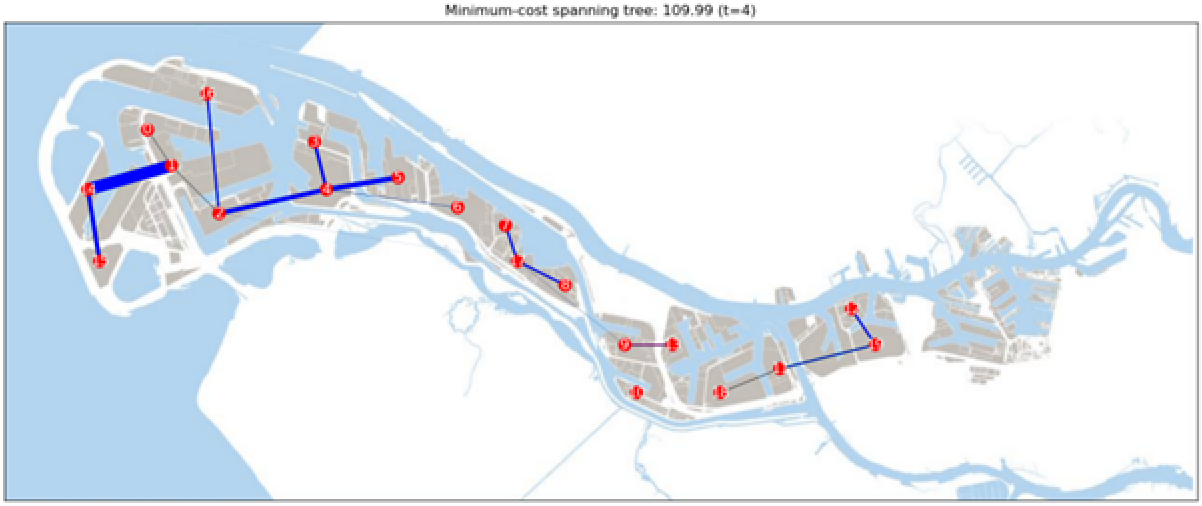

Figure D.77: Simulation Results

Bibliography

[1] E. Ackerman et al. "On grids in topological graphs". In: *Computational Geometry* 47.7 (2014), pp. 710–723. DOI: 10.1016/j.comgeo.2014.02.003.

[2] Anthropic. *Claude (Claude 3.5 Sonnet)*. Large language model. 2024. URL: https://claude.ai (visited on 07/21/2024).

[3] Peace Ayegba et al. "A Comparative Study of Minimal Spanning Tree Algorithms". In: *2020 International Conference in Mathematics, Computer Engineering and Computer Science (ICMCECS)*. Accessed June 3, 2025. IEEE, 2020, pp. 1–6. DOI: 10.1109/ICMCECS47690.2020.240900. URL: https://www.researchgate.net/publication/340975690.

[4] Arie Ben-David. "A pairwise comparison approach to ranking methods for large-scale problems". In: *Journal of the Operational Research Society* 50.10 (1999), pp. 1101–1109. DOI: 10.1057/palgrave.jors.2600805.

[5] S. C. Bhattacharyya and G. R. Timilsina. "A review of energy system models". In: *International Journal Of Energy Sector Management* 4.4 (2010), pp. 494–518. DOI: 10.1108/17506221011092742.

[6] T. Capurso et al. "Perspective of the role of hydrogen in the 21st century energy transition". In: *Energy Conversion And Management* 251 (2021), p. 114898. DOI: 10.1016/j.enconman.2021.114898.

[7] S. Chatterjee, R. K. Parsapur, and K. Huang. "Limitations of Ammonia as a Hydrogen Energy Carrier for the Transportation Sector". In: *ACS Energy Letters* 6.12 (2021), pp. 4390–4394. DOI: 10.1021/acsenergylett.1c02189.

[8] C. Chen, M. Pinar, and T. Stengos. "Renewable energy and CO2 emissions: New evidence with the panel threshold model". In: *Renewable Energy* 194 (2022), pp. 117–128. DOI: 10.1016/j.renene.2022.05.095.

[9] Yingying Chen and Jian Zhu. "A Graph Theory-Based Method for Regional Integrated Energy Network Planning: A Case Study of a China–U.S. Low-Carbon Demonstration City". In: *Energies* 12.23 (2019), p. 4491. DOI: 10.3390/en12234491. URL: https://www.mdpi.com/1996-1073/12/23/4491.

[10] J. Cui and M. Aziz. "Techno-economic analysis of hydrogen transportation infrastructure using ammonia and methanol". In: *International Journal of Hydrogen Energy* 48 (2023), pp. 15737–15747. DOI: 10.1016/j.ijhydene.2023.01.096.

[11] J. De La Cruz et al. *Multiobjective Optimization of the Transport in Oil Pipelines Networks*. https://doi.org/10.1109/etfa.2003.1247757. 2004. DOI: 10.1109/etfa.2003.1247757.

[12] Y. Deng et al. “Fuzzy Dijkstra algorithm for shortest path problem under uncertain environment”. In: *Applied Soft Computing* 12.3 (2011), pp. 1231–1237. DOI: 10.1016/j.asoc.2011.11.011. URL: https://doi.org/10.1016/j.asoc.2011.11.011.

[13] Jinxu Ding and Arun Somani. “A Long-Term Investment Planning Model for Mixed Energy Infrastructure Integrated with Renewable Energy”. In: *Proceedings of the IEEE International Conference*. Accessed via TU Delft Library. IEEE. Ames, Iowa, USA, 2010. URL: https://ieeexplore.ieee.org/document/5485986.

[14] P. A. Dreyer and F. S. Roberts. “Irreversible k-threshold processes: Graph-theoretical threshold models of the spread of disease and of opinion”. In: *Discrete Applied Mathematics* 157.7 (2008), pp. 1615–1627. DOI: 10.1016/j.dam.2008.09.012.

[15] T. Galimova et al. “Feasibility of green ammonia trading via pipelines and shipping: Cases of Europe, North Africa, and South America”. In: *Journal of Cleaner Production* 427 (2023), p. 139212. DOI: 10.1016/j.jclepro.2023.139212.

[16] R. L. Graham and Pavol Hell. “On the History of the Minimum Spanning Tree Problem”. In: *Annals of the History of Computing* 7.1 (1985). Downloaded via TU Delft Library, June 3, 2025, pp. 43–57. DOI: 10.1109/MAHC.1985.10011.

[17] P. Heijnen, É. J. Chappin, and I. Nikolic. “Infrastructure Network Design with a Multi-Model Approach: Comparing Geometric Graph Theory with an Agent-Based Implementation of an Ant Colony Optimization”. In: *Journal of Artificial Societies and Social Simulation* 17.4 (2014). DOI: 10.18564/jasss.2533. URL: https://doi.org/10.18564/jasss.2533.

[18] P. W. Heijnen, E. J. Chappin, and P. M. Herder. “A method for designing minimum-cost multisource multisink network layouts”. In: *Systems Engineering* 23.1 (2020), pp. 14–35.

[19] Petra Heijnen. *Minimum-cost network-layout tool with multi-sinks and multi-sources: Version 4*. Version 4, Tutorial document. 2025. URL: https://gitlab.tudelft.nl/pheijnen/optimal-network-layout.

[20] M. Hermesmann and T. M”uller. “Green, Turquoise, Blue, or Grey? Environmentally friendly Hydrogen Production in Transforming Energy Systems”. In: *Progress in Energy And Combustion Science* 90 (2022), p. 100996. DOI: 10.1016/j.pecs.2022.100996.

[21] H. Ishaq and C. Crawford. “Review of ammonia production and utilization: Enabling clean energy transition and net-zero climate targets”. In: *Energy Conversion And Management* 300 (2024), p. 117869. DOI: 10.1016/j.enconman.2023.117869.

[22] Aled W. Jones. “Perceived Barriers and Policy Solutions in Clean Energy Infrastructure Investment”. In: *Elsevier Manuscript (Open Access)* (2015). Based on CMCI Delphi process, London, 2011-2012. URL: https://www.elsevier.com/open-access/userlicense/1.0/.

[23] Taghi M. Khoshgoftaar, Lofton A. Bullard, and Kehan Gao. “A Rule-Based Software Quality Classification Model”. In: *International Journal of Reliability, Quality and Safety Engineering* 15.3 (2008), pp. 247–259. DOI: 10.1142/S0218539308003064. URL: https://doi.org/10.1142/S0218539308003064.

[24] C. Kim et al. "Review of hydrogen infrastructure: The current status and roll-out strategy". In: *International Journal of Hydrogen Energy* 48 (2023), pp. 1701–1716. DOI: 10.1016/j.ijhydene.2022.10.053.

[25] A. Klerke et al. "Ammonia for hydrogen storage: challenges and opportunities". In: *Journal Of Materials Chemistry* 18.20 (2008), p. 2304. DOI: 10.1039/b720020j.

[26] Y. Kojima and M. Yamaguchi. "Ammonia as a hydrogen energy carrier". In: *International Journal of Hydrogen Energy* 47.54 (2022), pp. 22832–22839. DOI: 10.1016/j.ijhydene.2022.05.096.

[27] Gang Kou et al. "Pairwise Comparison Matrix in Multiple Criteria Decision Making". In: *Technological and Economic Development of Economy* 22.5 (2016), pp. 738–765. DOI: 10.3846/20294913.2016.1210694. URL: https://doi.org/10.3846/20294913.2016.1210694.

[28] M. T. Kyi and L. L. Naing. "Application of Ford-Fulkerson Algorithm to Maximum Flow in Water Distribution Pipeline Network". In: *International Journal of Scientific and Research Publications* 8.12 (2018), pp. 1–5. DOI: 10.29322/ijsrp.8.12.2018.p8441. URL: https://doi.org/10.29322/ijsrp.8.12.2018.p8441.

[29] M Lafeber. "Hydrogen Infrastructure planning under uncertainty in an industrial port cluster". In: *Scientific paper* X.Y (2024). A robust over time approach of pipeline infrastructure, p. 122. DOI: x.

[30] X. Li et al. "Safe transfer of ammonia in pipelines: An analysis of risk". In: *Green and Low-Carbon Economy* 1.1 (2024), pp. 1–9. DOI: 10.47852/bonviewGLCE42022827.

[31] A. N. Madsen and P. D. Andersen. "Innovative regions and industrial clusters in hydrogen and fuel cell technology". In: *Energy Policy* 38.10 (2009), pp. 5372–5381. DOI: 10.1016/j.enpol.2009.03.040. URL: https://doi.org/10.1016/j.enpol.2009.03.040.

[32] C. Makhloufi and N. Kezibri. "Large-scale decomposition of green ammonia for pure hydrogen production". In: *International Journal Of Hydrogen Energy* 46.70 (2021), pp. 34777–34787. DOI: 10.1016/j.ijhydene.2021.07.188.

[33] J. Meckling and N. Goedeking. "Coalition cascades: The politics of tipping points in clean energy transitions". In: *Policy Studies Journal* 51.4 (2023), pp. 715–739. DOI: 10.1111/psj.12507.

[34] V. Negro, M. Noussan, and D. Chiaramonti. "The potential role of ammonia for hydrogen storage and transport: A critical review of challenges and opportunities". In: *Energies* 16.6192 (2023). DOI: 10.3390/en16176192.

[35] M. Niermann et al. "Liquid Organic Hydrogen Carriers and alternatives for international transport of renewable hydrogen". In: *Renewable and Sustainable Energy Reviews* 135 (2021), p. 110171. DOI: 10.1016/j.rser.2020.110171.

[36] S. Oh and M. Al-Juaied. "Decarbonizing industrial hubs and clusters: Towards an integrated framework of green industrial policies". In: *Energy Research & Social Science* 118 (2024), p. 103777. DOI: 10.1016/j.erss.2024.103777. URL: https://doi.org/10.1016/j.erss.2024.103777.

[37] OpenAI. *ChatGPT (GPT-4)*. Large language model. 2024. URL: https://chat.openai.com (visited on 07/21/2024).

[38] Port of Rotterdam Authority. *Planned 800MW Eneco Electrolyser Brings the Target of 25GW Hydrogen*. https://www.portofrotterdam.com/en/news-and-press-releases/planned-800-mw-eneco-electrolyser-brings-the-target-of-25-gw-hydrogen. Accessed: 2025-06-30. June 2025.

[39] E. Ridha, L. Nolting, and A. Praktiknjo. "Complexity profiles: A large-scale review of energy system models in terms of complexity". In: *Energy Strategy Reviews* 30 (2020), p. 100515. DOI: 10.1016/j.esr.2020.100515.

[40] I. Riepin et al. "Adaptive robust optimization for European strategic gas infrastructure planning". In: *Applied Energy* 324 (2022), p. 119686. DOI: 10.1016/j.apenergy.2022.119686.

[41] W. S. Rossi, G. Como, and F. Fagnani. "Threshold Models of Cascades in Large-Scale Networks". In: *IEEE Transactions On Network Science And Engineering* 6.2 (2017), pp. 158–172. DOI: 10.1109/tnse.2017.2777941. URL: https://doi.org/10.1109/tnse.2017.2777941.

[42] Nicholas Salmon and René Bañares-Alcántara. "Green ammonia as a spatial energy vector: a review". In: *Sustainable Energy Fuels* 5.11 (2021), pp. 2814–2839. DOI: 10.1039/d1se00345c.

[43] Sascha Samadi et al. *Decarbonization pathways for the industrial cluster of the Port of Rotterdam: final report*. en. Tech. rep. Wuppertal: Wuppertal Institute for Climate, Environment and Energy, 2016, p. 176. URL: http://nbn-resolving.de/urn:nbn:de:bsz:wup4-opus-66565.

[44] Bridie Schmidt. *Hydrogen Hype Meets Hard Costs: Europe's Pipeline Plan in Trouble*. Accessed: 2025-06-22. CleanTechnica. 2025. URL: https://cleantechnica.com/2025/02/21/hydrogen-hype-meets-hard-costs-europes-pipeline-plan-in-trouble/.

[45] C. Schneider, S. Lechtenb"ohmer, and S. Samadi. "Risks and opportunities associated with decarbonising Rotterdam's industrial cluster". In: *Environmental Innovation And Societal Transitions* 35 (2019), pp. 414–428. DOI: 10.1016/j.eist.2019.05.004.

[46] O. Serpell et al. *Ammonia's role in a net-zero hydrogen economy*. https://kleinmanenergy.upenn.edu. Accessed: [Insert date of access]. 2023.

[47] D. Shin, D. Qian, and J. Zhang. "Cascading effects in interdependent networks". In: *IEEE Network* 28.4 (2014), pp. 82–87. DOI: 10.1109/mnet.2014.6863136.

[48] Johan Simonsson, Khalid Tourkey Atta, and Wolfgang Birk. "A Graph Theoretical Approach to Modeling of District Energy Networks". In: *IEEE Transactions on Control Systems Technology* 32.5 (2024). Open Access, pp. 1616–1626. DOI: 10.1109/TCST.2023.3345213. URL: https://doi.org/10.1109/TCST.2023.3345213.

[49] Ardy Stemerding. *EU komt met klimaatdoel, inclusief geitenpaadjes*. Geraadpleegd op August 20, 2025. July 2025. URL: https://nos.nl/artikel/2573288-eu-komt-met-klimaatdoel-inclusief-geitenpaadjes.

[50] K. N. Suding and R. J. Hobbs. "Threshold models in restoration and conservation: a developing framework". In: *Trends in Ecology & Evolution* 24.5 (2009), pp. 271–279. DOI: 10.1016/j.tree.2008.11.012.

[51] X. Sun et al. "Ammonia as hydrogen carrier: Advances in ammonia decomposition catalysts for promising hydrogen production". In: *Renewable and Sustainable Energy Reviews* 159 (2022), p. 112918. DOI: 10.1016/j.rser.2022.112918.

[52] K. Trangwachirachai et al. "Recent progress on ammonia cracking technologies for scalable hydrogen production". In: *Current Opinion in Green and Sustainable Chemistry* 49 (2024), p. 100945. DOI: 10.1016/j.cogsc.2024.100945.

[53] United Nations Framework Convention on Climate Change. *Paris Agreement*. Presented to Parliament by Command of Her Majesty. Treaty Series No. 4 (2017), Cm 9395. Presented to Parliament by the Secretary of State for Foreign and Commonwealth Affairs. Jan. 2017. URL: https://www.gov.uk/government/publications/the-paris-agreement.

[54] Thomas W. Valente. "Social Network Thresholds in the Diffusion of Innovations". In: *Social Networks* 18.1 (1996), pp. 69–89. DOI: 10.1016/0378-8733(95)00256-1. URL: https://doi.org/10.1016/0378-8733(95)00256-1.

[55] M. Van Den Boomen et al. "Optimized Expansion Strategy for a Hydrogen Pipe Network in the Port of Rotterdam with Compound Real Options Analysis". In: *Sustainability* 13.16 (2021), p. 9153. DOI: 10.3390/su13169153.

[56] Z. Wan et al. "Ammonia as an effective carrier and a clean fuel for solid oxide fuel cells". In: *Energy Conversion and Management* 228 (2020), p. 113729. DOI: 10.1016/j.enconman.2020.113729.

[57] J. Wang et al. "Literature review on modeling and simulation of energy infrastructures from a resilience perspective". In: *Reliability Engineering & System Safety* 183 (2018), pp. 360–373. DOI: 10.1016/j.ress.2018.11.029.

[58] Ruichi Wang et al. "A Graph Theory Based Energy Routing Algorithm in Energy Local Area Network (e-LAN)". In: *IEEE Transactions on Industrial Informatics* 16.4 (2020), pp. 2651–2662. DOI: 10.1109/TII.2019.2947439. URL: https://doi.org/10.1109/TII.2019.2947439.

[59] G. Xu et al. "Evaluating the effect of renewable energy investment on renewable energy development in China with panel threshold model". In: *Energy Policy* 187 (2024), p. 114029. DOI: 10.1016/j.enpol.2024.114029.

[60] Zhaohui Yang et al. "The Effect of Soil and Topography Factors on Larix gmelinii var. Principis-rupprechtii Forest Mortality and Capability of Decision Tree Binning Method and Generalized Linear Models in Predicting Tree Mortality". In: *Forests* 15.12 (2024), p. 2060. DOI: 10.3390/f15122060. URL: https://www.mdpi.com/1999-4907/15/12/2060.

[61] Y. Ye, Y. Chen, and W. Han. "Influence maximization in social networks: Theories, methods and challenges". In: *Array* 16 (2022), p. 100264. DOI: 10.1016/j.array.2022.100264.

[62] L. Zhang et al. "The role of hydrogen in the energy transition of the oil and gas industry". In: *Renewable and Sustainable Energy Reviews* 185 (2024), p. 100090. DOI: 10.1016/j.enrev.2024.100090.

[63] L. Zhou et al. "Data-driven robust optimisation of hydrogen infrastructure planning under demand uncertainty". In: *Renewable and Sustainable Energy Reviews* 159 (2022), p. 112230. DOI: 10.1016/j.rser.2022.112230. URL: https://doi.org/10.1016/j.rser.2022.112230.