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Review

Current and Future Role of Natural Gas Supply Chains in the Transition to a Low-Carbon Hydrogen Economy: A Comprehensive Review on Integrated Natural Gas Supply Chain Optimisation Models

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Abstract: Natural gas is the most growing fossil fuel due to its environmental advantages. For the economical transportation of natural gas to distant markets, physical (i.e., liquefaction and compression) or chemical (i.e., direct and indirect) monetisation options must be considered to reduce volume and meet the demand of different markets. Planning natural gas supply chains is a complex problem in today's turbulent markets, especially considering the uncertainties associated with final market demand and competition with emerging renewable and hydrogen energies. This review study evaluates the latest research on mathematical programming (i.e., MILP and MINLP) as a decision-making tool for designing and planning natural gas supply chains under different planning horizons. The first part of this study assesses the status of existing natural gas infrastructures by addressing readily available natural monetisation options, quantitative tools for selecting monetisation options, and single-state and multistate natural gas supply chain optimisation models. The second part investigates hydrogen as a potential energy carrier for integration with natural gas supply chains, carbon capture utilisation, and storage technologies. This integration is foreseen to decarbonise systems, diversify the product portfolio, and fill the gap between current supply chains and the future market need of cleaner energy commodities. Since natural gas markets are turbulent and hydrogen energy has the potential to replace fossil fuels in the future, addressing stochastic conditions and demand uncertainty is vital to hedge against risks through designing a responsive supply chain in the project's early design stages. Hence, hydrogen supply chain optimisation studies and the latest works on hydrogen–natural gas supply chain optimisation were reviewed under deterministic and stochastic conditions. Only quantitative mathematical models for supply chain optimisation, including linear and nonlinear programming models, were considered in this study to evaluate the effectiveness of each proposed approach.

Keywords: natural gas; hydrogen; optimisation; supply chains; flexibility

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Citation: Yusuf, N.; Al-Ansari, T. Current and Future Role of Natural Gas Supply Chains in the Transition to a Low-Carbon Hydrogen Economy: A Comprehensive Review on Integrated Natural Gas Supply Chain Optimisation Models. *Energies* **2023**, *16*, 7672. https://doi.org/10.3390/en16227672

Academic Editor: Luca Gonsalvi

Received: 12 September 2023
Revised: 11 November 2023
Accepted: 13 November 2023
Published: 20 November 2023

1. Introduction

The world's energy demand is increasing rapidly. The U.S. Energy Information Administration (EIA) projects an energy consumption increase of 50% by 2050 relative to 2018, wherein most of this growth will be driven by the Asian industrial sector [1]. Amongst the different primary energy sources, renewables are the fastest-growing energy source. Nevertheless, natural gas has grown rapidly in the energy mix as a cleaner fossil fuel, with further reliance on natural gas anticipated until 2050 [2,3]. Gas consumption is forecast to increase by more than 40% by 2050 relative to 2018 [1]. Additionally, by 2050, more than 50% of power generation will come from cheaper renewable resources rather than fossil-fuelled plants, followed by natural gas and coal [4]. The shift to natural gas and renewables is mainly driven by the need for cleaner energy sources to reduce the environmental impact,

especially after the Paris Agreement on climate change [5,6]. Extensive efforts have been made to investigate affordable solutions for using renewable resources or cleaner fuels, such as natural gas, in different sectors due to their environmental characteristics. Natural gas emits fewer air pollutants, including NOx, CO, and CO_2, to generate the same energy as other fossil fuels [7]. For generating 1.06 GJ of energy, natural gas emits around 26% less CO_2 than gasoline and 44% less CO_2 than coal [8]. Exceptional efforts to utilise natural gas in the road transport sector have been recognised, supported by emission mitigation legalisation [9]. Replacing diesel with natural gas (i.e., liquefied or compressed) in transport not only reduces emissions [10]; the shift revealed additional advantages, including lower noise, lower costs, and a longer engine life [11]. Consequently, countries such as China promoted the coal-to-gas policy for climate mitigation targets [12]. Exporting countries, such as the U.S. and Qatar, have focused on developing natural gas projects and expanding supplies to meet the surge in demand for liquefied natural gas.

Natural gas is primarily composed of methane, along with heavier hydrocarbons such as ethane, propane, and butane. Moreover, it contains inorganic components such as nitrogen, carbon dioxide, water vapour, hydrogen sulphide, helium, and mercury. The composition of the produced raw natural gas differs from one reservoir to another, and sometimes it varies from one well to another located in the same field [13]. Consequently, natural gas projects utilise different technologies, treatments, and processing routes based on the feedstock conditions. However, one major drawback associated with the oil and gas industry is the release of methane in daily operations. As one of the greenhouse gases, methane's emission to the atmosphere is a significant driver of global warming [14]. Similarly, methane is released from other sectors, such as livestock, agriculture, and organic municipal solid wastes [15,16]. In terms of organic wastes, biogas produced from biomass has acquired attention for integration within natural gas networks [17–20]. In this approach, generated biomethane is pumped into existing natural gas networks, resulting in capital expenditure cost savings.

The emergence of new markets and demands has increased interest in utilising natural gas from standard fields, which requires high capital costs and market security through signing long-term agreements with importing countries [21]. However, the increased competitiveness and uncertainty in the markets due to the emergence of new suppliers have impacted the planning of different parts of the natural gas supply chains (NGSCs), from exploration until transportation to final markets. This, in turn, influences the selection of monetisation options when starting new projects or expanding existing ones has been challenging. Subsequently, extensive research has been carried out to develop different natural gas monetisation options and to study the optimal combination of employed technologies based on economic and technical factors [22]. In addition to the significance of selecting monetisation options, optimising NGSCs is critical to assess the combination of monetisation options in achieving economic profitability, hedging against risk, and supporting environmental sustainability.

Different entities in the natural gas industry manage each function of the supply chain, as demonstrated in Figure 1. The NGSCs comprise a single or multiple monetised products, such as gaseous-state natural gas, liquefied natural gas (LNG), and compressed natural gas (CNG), along with various storage facilities and transportation modes. Hence, optimising the design and operation of the NGSC is complex and can be accomplished under different planning horizons depending on the project's phase: strategic, tactical, and operational [23,24]. Strategic decisions involve selecting technologies, production capacities, storage, transportation, and the allocation of facilities. The tactical level is a medium-term planning interval where seasonal production capacities are determined based on demand forecasts. Lastly, the operational planning level deals with shorter-term planning intervals, such as days, where the process's responsiveness to risks due to unexpected shocks and/or shutdowns is considered.

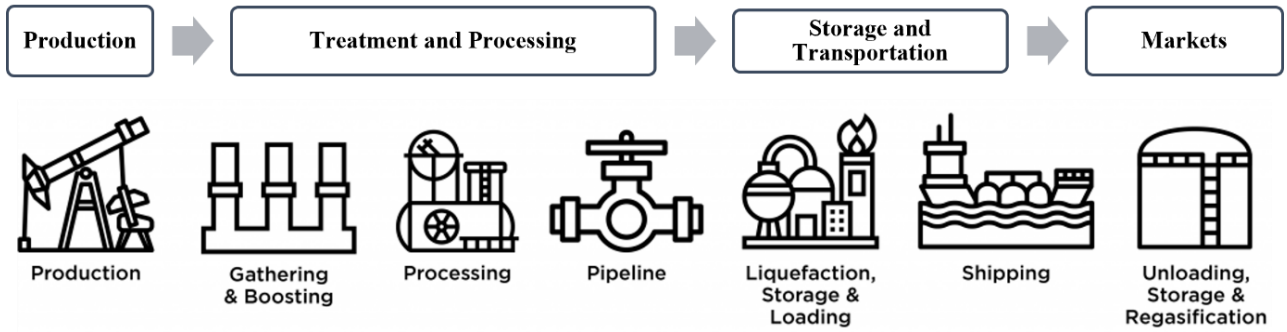

Figure 1. The supply chain's main functions.

On the other hand, decision-makers must address potential uncertainties in the early design stages of projects to hedge against risks. Different approaches exist for dealing with exogenous uncertainties, based on reducing the uncertainty or enabling the system to respond. The approach to managing uncertainties includes controlling uncertainty, protecting passively by increasing the robustness of the system, or protecting the system actively by embedding flexibility to react to uncertainties. Flexibility could be introduced on different decision-making levels (i.e., strategic, tactical, and operational) for single or multiple decisions, such as flexibility in production capacity, storage capacity, construction of facilities, suppliers, transportation modes, and selling strategies. However, the decision-making level and flexibility must be evaluated in the project's early design stages to account for potential capital, operating costs, and spatial or technological constraints. In the literature, the concept of flexibility in energy and manufacturing supply chains has become interestingly important in increasing supply chains' responsiveness to uncertainties arising from dynamic environments [25–29].

Although flexible NGSCs sustain the economic profitability of the business, net-zero energy system policies and the EU's carbon border tax could slash the profits generated by hydrocarbon exporters. For hydrocarbon economies with less resilience to the EU's carbon pricing scheme, immediate decarbonisation actions are required to support the environmental and economic sustainability of the oil and gas business. Hydrogen has the potential to combat global warming and meet the increase in future energy demand by providing solutions at different economic, financial, social, and energy-efficiency levels [30–32]. Liquid hydrogen exhibits a high energy density of 143 MJ/kg, which is three times greater than that of conventional liquid fossil fuels [33]. Hence, it is a promising alternative to fossil fuels in industry, transportation, residential heating, and electricity generation sectors. Integrating hydrogen with existing NGSCs will facilitate the transition to renewables to achieve the net-zero carbon emissions vision by 2050. In integrated hydrogen–natural gas supply chains (H_2-NGSCs), existing infrastructure can be utilised for hydrogen production, monetisation, storage, and transportation. For hydrogen produced from natural gas (i.e., grey hydrogen), introducing carbon capture, utilisation, and storage (CCUS) technologies is crucial to reduce embodied CO_2 (i.e., blue hydrogen). In the literature, carbon capture and storage (CCS) technologies have been questioned in large-scale implementation due to costs and technical constraints [34–38]. CCS is a mitigation strategy to reduce CO_2 emissions without sustaining business profitability. In CCS, CO_2 is stored underground in geological formations such as depleted gas reservoirs. On the other hand, carbon capture and utilisation (CCU) has economic value, since valuable byproducts can be produced from CO_2. Hence, CCU technologies can financially support CCS when built together [39].

This review highlights strategic- and tactical-level optimisation models discussed in the literature for deterministic and stochastic optimisation of NGSCs, hydrogen supply chains, and integrated H_2-NGSCs. In this regard, demand and price uncertainties are key parameters influencing decision-making when studying and optimising supply chains. Hence, accounting for uncertainties in the early design stages is essential to increase the supply chain's robustness and/or flexibility to future shocks. The investigation of de-

carbonisation efforts to reduce the CO_2 footprint by introducing CCUS technologies and H_2 production units is also addressed. The integration of the three aspects (i.e., decarbonisation, existing natural gas supply chains, and hydrogen supply chains) contributes to the resilience of the overall system against uncertainties. This, in turn, enhances the cost-effectiveness, operational flexibility, and environmental sustainability of the business, as demonstrated in Figure 2.

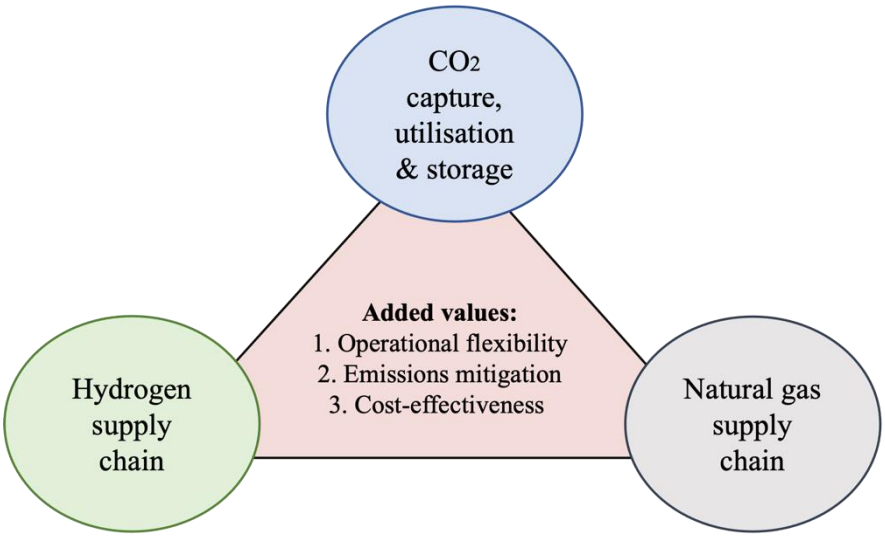

Figure 2. Scope of this review paper.

Integrating the three addressed aspects adds flexibility in production to the comprehensive NGSC. In an integrated NGSC, different products can be produced to be sold for markets or utilised internally. To the best of the authors' knowledge, the literature lacks multidisciplinary reviews linking these three aspects. Most review papers have addressed previous mathematical optimisation models in single-product NGSC optimisation [23,40] and hydrogen supply chain optimisation [41–44]. On the other hand, reviews on hydrogen production, storage, and transportation technologies occupy a large proportion of studies in the literature [45–48]. Reviewing the literature has identified a gap for review studies evaluating advanced deterministic and/or stochastic optimisation techniques for integrated, multiproduct H_2-NGSCs. This is the first review paper to evaluate the current status and future capabilities of integrating H_2-NGSCs. Fundamentally, understanding single-product supply chains is essential prior to analysing integrated multiproduct supply chains. Hence, this review achieves five main objectives: (1) evaluating promising physical and chemical monetisation options for natural gas, (2) investigating the value of flexibility in supply chain management to cope with uncertainties, (3) emphasising the potential of producing low-carbon hydrogen from natural gas when coupled with CCUS technologies, (4) reviewing mathematical optimisation studies on natural gas and hydrogen supply chain optimisation, and (5) reviewing the studies on integrating H_2-NGSCs for decarbonising systems and adding flexibility.

Review Structure

The main contribution of this review is to provide a multidisciplinary overview of the up-to-date research on natural gas monetisation and decision-making and the future of NGSCs in the era of decarbonisation and renewables. This is achieved through reviewing different journal and review papers on natural gas monetisation decision-making, NGSC optimisation, hydrogen supply chain optimisation, and the latest published works on integrating hydrogen facilities with NGSCs. This comprehensive analysis is essential to assess natural gas systems' status and future prospects in the low-carbon hydrogen economy era. A sustainable NGSC combines social responsibility with environmental and economic values. Hence, this study emphasises the active role of natural gas in smoothening

the transition towards renewables by filling the gap between current systems and future requirements.

This review highlights the decision-making process for natural gas monetisation technologies based on future market demands in Sections 3 and 4. Section 5 reviews NGSC optimisation models, which are addressed with an emphasis on uncertainties in stochastic modelling. The role of hydrogen in today's economy and the potential of hydrogen supply chain optimisation are discussed in Section 6. Section 7 highlights the flexibility opportunities arising from integrating H_2-NGSCs for moving forward. Optimisation-based supply chains in this study are classified based on mathematical models, objective functions, planning levels, and time windows, as illustrated in Figure 3.

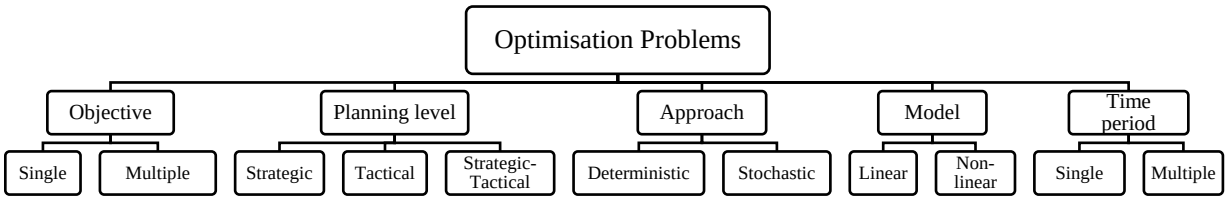

Figure 3. Classification of supply chain optimisation problems.

2. Scope and Review Methodology

With the objective of supporting decision-makers in understanding the opportunities and challenges of a net-zero economy, evaluations of strategies to decarbonise the oil and gas industry have become crucial [49,50]. In the recent literature, Khorasani et al. [51] identified 14 strategies from the literature to decarbonise different functions of oil and natural gas supply chains. Cherepovitsyn [50] expanded the theoretical discussion on green diversification processes in the oil and gas industry and elaborated on the feasibility of implementing renewables. Most recently, a systematic review by de Queiroz et al. [49] identified the energy transition constraints prioritised by industry. The review revealed that renewable energy implementation and carbon capture and mitigation were the most cited aspects in the literature. However, the studies broadly highlighted different aspects of decarbonising and diversifying oil and gas natural gas supply chains, with a lack of focus on quantitative tools for providing insights when deciding on the combinations of technologies in the integrated supply chains. This work provides a comprehensive review of the evolution of the natural gas industry, from a quantitative selection of natural gas monetisation tools to quantitative decision-making in integrated hydrogen and natural gas supply chains. The final list of papers considered in this study was obtained through three fundamental steps: First, the search engine Google Scholar was used to search for English-language publications from 2015 onwards. Search terms such as "natural gas supply chain", "natural gas monetisation", "hydrogen supply chain", "hydrogen value chain", "integrated supply chain", "uncertainty", and "quantitative models" were used to create a primary list of papers. This was followed by a second list of papers, created using the snowball method [52]. In the second list, publications from before the year 2000 were excluded.

Finally, a final list was determined upon filtration of the secondary list based on three criteria: First, the research questions had to align with the review paper's objectives. Second, the reviewed articles had to include quantitative decision-making approaches, such as mixed-integer linear programming (MILP), mixed-integer nonlinear programming (MINLP), linear programming (LP), stochastic modelling, and optimisation algorithms. These tools are essential to quantitatively measure the effectiveness of each proposed framework in analysing complex natural gas and hydrogen systems. Finally, a few qualitative studies were reviewed to consider the subjective perspective of policymakers in shaping future energy decisions. When analysing optimisation models throughout the different sections of the review paper, 56 studies classified based on the strategic, tactical, or strategic–tactical planning levels were analysed, as summarised in Figure 4. Moreover, 11 other

operational planning studies were addressed to identify the different mathematical models utilised in the literature. Fundamentally, the evaluations of the studies presented herein assess decision-makers with an understanding of the value of mathematical programming as a decision-making tool when investigating the optimal configuration of infrastructure and technologies in integrated supply chains. Hence, we suggest combining technical knowledge with applied mathematics for optimal planning under uncertainties.

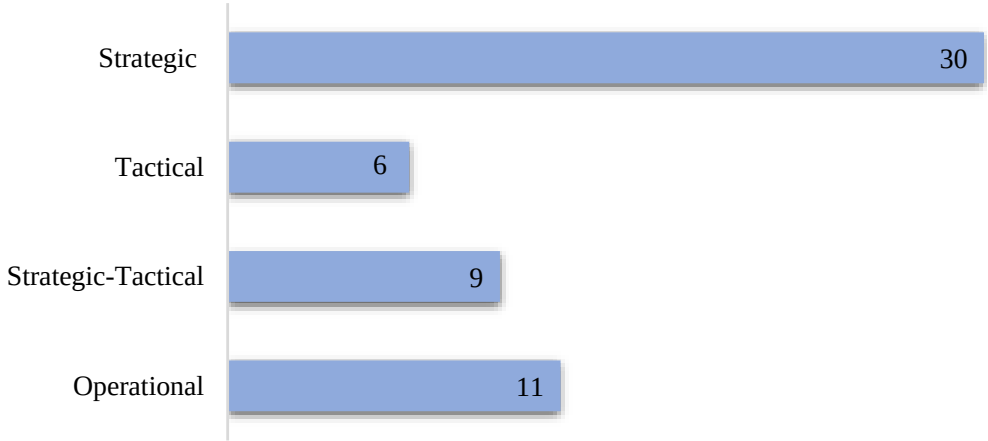

Figure 4. Numbers of published articles focusing on the three supply chain planning modes.

3. Methane Monetisation

The gaseous state of natural gas makes transportation to distant local and international markets significantly challenging [22,53]. For nearby markets, treated natural gas can be economically transported via pipelines [54]. On the other hand, different monetisation techniques have been developed to economically transport natural gas to distant markets, as well as for efficient long-term natural gas storage. Natural gas monetisation techniques include either physical or chemical conversions. In physical monetisation, cryogenic techniques are used to reduce the volume of gas (i.e., liquefaction and compression), with the objective of economical storage and transportation. Chemical monetisation options aim to convert the hydrocarbons in natural gas into higher-value products for an increased economic value of natural gas and a diversified product portfolio.

Standard natural gas can be converted through physical processes into liquefied natural gas (LNG), compressed natural gas (CNG), or natural gas hydrates (NGHs) for transportation to international markets. On the other hand, direct and indirect gas-to-liquid (GTL) processes are chemical routes that are used to convert standard natural gas into products such as methanol, ethylene, diesel, and dimethyl ether. Different GTL processes yield different products based on the operating conditions and the technology utilised. Furthermore, other natural gas monetisation options include gas-to-commodity (GTC), where the gas is converted into thermal or electric power that is then used in the production of aluminium and iron, and gas-to-wire (GTW) [55]. Overall, selecting monetisation technologies is a critical decision-making process in natural gas projects that depends on various external and internal factors, such as the size and type of reservoir, market demands, distance to markets, and political changes [53,55–57].

3.1. Description of Chemical and Physical Monetisation of Natural Gas into Products

Standard natural gas can be monetised through chemical conversion into multiple value-added products. The treated and dehydrated natural gas is fractioned into streams with different hydrocarbon compositions: a methane-rich stream, natural gas liquids (NGLs), and liquefied petroleum gases (LPGs). NGLs and LPGs possess high economic value and can be sold directly in markets or cracked within the same facility for the production of high-value products [13,56,58,59]. These include ethane (converted to the intermediate ethylene, a primary feedstock for polyethylene production), propane, and

butane. Each hydrocarbon extracted from natural gas can be used as a feedstock for multiple industries. Consequently, each hydrocarbon extracted from the standard natural gas mixture has a separate value chain with multiple products and monetisation routes, all under the overall natural gas value chain.

Since methane comprises 70–90% of the composition of natural gas, special attention has been given to the monetisation techniques for the methane-rich stream [38,60]. The methane-rich steam is commonly known as natural gas, with various uses in heating, electricity generation, and various industries. For economical storage and transportation, pipelines, LNG, and CNG have been identified as the most viable options [61,62], while other direct and indirect chemical monetisation approaches have been deployed for producing high-value products shipped to international markets. The indirect approach is the most industrially mature route, wherein natural gas is converted into the intermediate syngas (a mixture of CO_2, CO, and H_2), which acts as a feedstock for the Fischer–Tropsch GTL process, methanol process, Haber–Bosch ammonia process, etc.

3.1.1. Liquefied Natural Gas (LNG)

In natural gas liquefaction, LNG is obtained by cooling down treated natural gas below −162 °C, reducing its original volume by 600 times [56]. LNG is then transported to the final markets via LNG tankers. At the receiving terminal, the chilled product is regasified and distributed to local markets for power generation in households and industries, or as a feedstock in industries. For satellite regasification stations, LNG trucks or trains can be used to transport LNG from receiving terminals to regasification stations [63].

The selection of a liquefaction technology depends on several factors, such as the reservoir's size, the plant's location (i.e., onshore or offshore), weather conditions, and market demand. The most industrially mature LNG technologies are propane precooled mixed refrigerant, mixed-fluid cascade, dual mixed refrigerant, and optimised cascade [64]. These technologies vary based on the number of refrigeration cycles, the refrigerants used, the production capacity, and the operational conditions.

3.1.2. Compressed Natural Gas (CNG)

In natural gas compression, natural gas is compressed to less than 1% of its volume and stored at a pressure of up to 24.8 MPa for easier transportation to markets via tankers or vessels [65]. At receiving stations, CNG undergoes decompression for distribution to domestic markets via pipelines. The natural gas compression process is less complicated than liquefaction, with more than a 50% reduction in capital costs [55]. Moreover, the transportation of the compressed product is less costly and easier to manage, making it a convenient mode of transportation to markets with small gas capacity requirements [66]. However, CNG occupies more space than LNG due to its greater volume and requires a larger cargo size for long-distance transportation [53].

3.1.3. Gas-to-Liquid (GTL)

Gas-to-liquid (GTL) processes are chemical processes in which methane is converted into high-value hydrocarbon liquid products and fuels, offering market expansion and diversification for gas-producing countries [67,68]. In the GTL route, different direct and indirect technologies and operating conditions can be used for converting methane into higher-value products, subject to market demand and reservoir conditions. Amongst the developed GTL technologies, the Fischer–Tropsch (F-T) technologies dominate both large-scale and small-scale projects [67]. This process yields high-quality liquid products, including naphtha, jet fuels, diesel, lubes, and waxes. In fact, the diesel produced by the F-T process is of high quality compared to the diesel produced through crude oil refineries, due to its high cetane number, low sulphur and aromatics contents, and low density [69,70]. By contrast, the yield of the high-value middle distillate produced through the F-T GTL process is relatively one-third more of the same products produced from a conventional oil refinery [71].

The F-T process consists of three steps: (1) production of syngas through steam reforming and/or partial oxidation; (2) catalytic F-T synthesis to process and polymerise the hydrogen and carbon monoxide in syngas into long-chain hydrocarbon molecules using F-T reactors; (3) product upgrading, where conventional cracking processes take place to break down the syncrude into products such as naphtha, diesel, lube oils, and waxes for commercial markets [13,67,72]. The cracking process is flexible in terms of the operating conditions. The operating conditions can be adjusted to produce more products in demand based on the market performance [13,70]

GTL products can be shipped directly via trucks or tankers. In contrast, GTL products received at the receiving terminals can be transported directly to the final consumers without deploying decompression and regasification facilities, as needed by CNG and LNG, respectively [53].

3.1.4. Gas-to-Chemical (GTC)

Natural gas can be chemically converted into valuable products such as methanol and hydrogen at lower costs than the F-T GTL process. On the other hand, the GTL process provides more flexibility in changing the operating conditions to produce certain products based on market performance. Economic factors fundamentally impact the decision as to which production routes to deploy.

Methanol

Methanol produced from methane is a profitable product that can be used as fuel in the transportation sector or as a feedstock for the manufacturing of chemicals, paints, solvents, and adhesives [38,73,74]. Similar to the first step of GTL, the methane is chemically converted to syngas via steam reforming and/or partial oxidation reactions. The syngas is then converted to methanol at high temperatures and in the presence of a catalyst such as copper [73,75].

Methanol has gained attention in maritime logistics for utilisation as a ship fuel, representing a great potential for methanol utilisation in the future [74,76,77]. Like natural gas markets, methanol markets are regionally segmented based on production and consumption hubs. The Asia–Pacific region is anticipated to dominate the global market share due to the projected increase in industrial demand. By 2050, methanol produced from biomass and green hydrogen with captured CO_2 will compete with methanol produced from fossil fuels [78]. Consequently, strategic critical decisions must be made on natural gas's monetisation to methanol in terms of production capacity and produced grade to sustain sales in profitable markets. Moreover, methanol produced from methane could add flexibility to the same methane value chain by constructing production facilities for dimethyl ether (DME), acetic acid, olefins, formaldehyde, MTBE, and gasoline.

Hydrogen

Syngas produced from methane via steam reforming and/or partial oxidation can also be separated into hydrogen and carbon monoxide/carbon dioxide. At ambient temperature, the hydrogen can be liquefied at a temperature of −253 °C for shipping, reducing its volume by 1/848 [79]. Additionally, gaseous hydrogen can be utilised domestically in the fertiliser production, metal treatment, and food processing industries. Within the midstream natural gas value chain, hydrogen is a fundamental feedstock for producing ammonia via the Haber–Bosch process, which acts as a hydrogen carrier for economical transportation to international markets. When integrated with CCUS technologies, blue hydrogen plays a significant role in decarbonising sectors and accelerating the energy transition. The hydrogen supply chain design has been given special attention in the literature, especially after the Paris Agreement.

3.2. Other Products Produced from Natural Gas

In addition to the abovementioned monetisation routes, different high-pressure steam cracking approaches can be utilised to produce ethylene and propylene from ethane and propane, respectively. Ethylene is a feedstock for producing various chemicals, such as high-density and low-density polyethylene, ethylene dichloride, acetaldehyde, and ethylene oxide [13]. Propylene is a feedstock for producing polypropylene and propylene oxide [80,81]. However, with the introduction of strict governmental regulations on the use of plastics, the market growth of ethylene and propylene is expected to tumble [82]. Figure 5 summmarises the most common methane-based products.

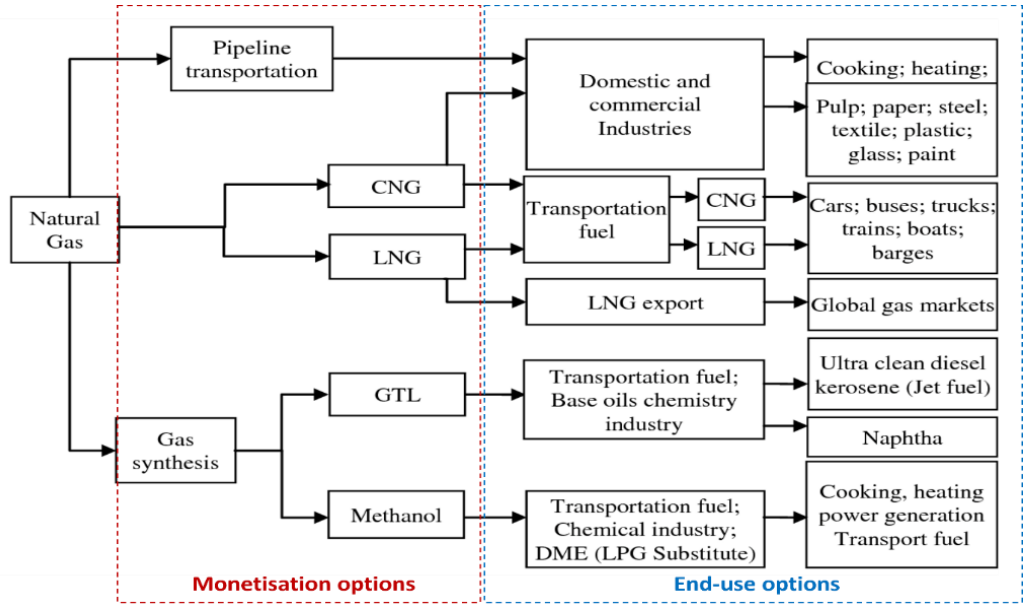

Figure 5. Natural gas (methane) products' value chain.

4. Selection of Natural Gas Monetisation Options under Deterministic and Stochastic Conditions

Natural gas megaprojects are capital-intensive and require billions of USD in investment. Hence, the selection of monetisation options, technologies, shipping routes, and markets is pivotal in the pre-final investment decision process, affecting the project's performance and profitability. Producers control unique natural gas value chains that differ based on infrastructure, monetisation options, transportation modes, and targeted final markets.

The illiquidity and market segmentation of the natural gas market has raised complexities in the natural gas trade. The increase in energy market uncertainties driven by policy changes and unexpected events have complicated the management and planning of NGSCs [65,83]. A disruption in one part of the supply chain of one natural gas project impacts the operation of other components within the same supply chain and, potentially, the overall global natural gas industry [83]. Accordingly, each part of the NGSC must be planned, managed, and operated efficiently to ensure the reliability of the flow of natural gas from wells to the final markets [84,85]. Previous studies in the literature have qualitatively evaluated and compared the techno-economic aspects of different natural gas monetisation options (LNG, CNG, GTL, and NGH) based on reservoir type, distance to final markets, capital and operating expenditures, and safety [55,86]. However, decision-making and implementing findings based on qualitative approaches are risky due to the limited understanding of consumer behaviour. Later studies focused on the quantitative selection of natural gas monetisation options in different regions, such as the U.S. Gulf of Mexico [87], Canada [88], Iran [89], Nigeria [2,60,90], and Russia [91]. With the increased interest in monetising unconventional hydrocarbon resources, there has been a focus on conducting techno-economic feasibility assessments of the production, transportation, and storage of

natural gas hydrates (NGH)s [92–96]. However, NGHs are still under research and are less commercially mature than other monetisation options utilised in the market [97]. CNG, LNG, and GTL were the most discussed technologies in the literature due to the maturity of these technologies. Although studies on optimising the operation of different processes are still in progress for optimal productivity, environmental effectiveness, and energy usage, a few studies have highlighted the dynamic operation of the abovementioned monetisation options under operational or market uncertainties. Qualitative and scenario-based risk management approaches cannot capture the full picture when analysing future megaproject uncertainties. Hence, quantitative evaluation of the performance of different monetisation options under demand uncertainties is vital when addressing uncertainty in natural gas monetisation.

Natural Gas Monetisation under Uncertainty

In today's turbulent energy markets, uncertainties in energy products due to seasonality, competitiveness with other energy resources, and geopolitical issues significantly impact the natural gas trade [3,28,98–100]. Hence, quantitative assessments of natural gas monetisation options are crucial prior to starting new projects or expanding existing facilities [27,101]. Fundamentally, uncertainties influencing natural gas projects are classified as endogenous and exogenous uncertainties. Endogenous uncertainties include internal disruptions in production and transportation facilities, such as natural gas composition variations, flow rate changes, and technical disturbances [102,103]. On the other hand, exogenous uncertainties arise from external market variabilities, including changes in fuel prices, utility prices, and product prices [104–106]. Project owners can better manage endogenous uncertainties by diversifying suppliers or embedding operational flexibility to contain variabilities. However, some projects may fail in spite of great technical performance, due to poor forecasts and/or failure to consider exogenous uncertainties in the early design stages of projects [107–109]. Evaluating uncertainties is critical to understanding the project's future performance and addressing potential tools and techniques for managing possible drawbacks. Consequently, some studies in the literature have widely investigated the impacts of uncertainties on different parts of the NGSCs [110,111], whilst others have studied the impacts of uncertainties on the selection of monetisation technologies when developing or expanding natural gas projects [28,112,113]. Figure 6 illustrates the layers of uncertainties model, as described by De Weck et al. [107] and Lessard [114]. Moving from inner layers (endogenous uncertainties) to outer layers (exogenous uncertainties), the degree of influence in mitigating risks or exploiting opportunities arising from uncertainties decreases sharply. Despite being able to choose its technical architecture, suppliers, and operational strategy, a firm may have little impact on future regulations and be unable to control natural disasters. However, a firm may prepare for the consequences of exogenous uncertainties by investing in different risk mitigation strategies in the project's early design stages, including vigorous investments in advanced quantitative decision-making tools.

In the literature, authors have studied the impact of uncertainties on selecting monetisation options when developing natural gas projects by using techno-economic and/or mathematical optimisation approaches [22,53]. Liu et al. [115] developed and modelled a systematic monetisation approach for strategic large-scale shale gas monetisation to polymers by considering different endogenous and exogenous uncertainties. This techno-economic study considered the impacts of endogenous uncertainties related to variabilities in the feedstock composition and exogenous uncertainties of the entire project related to market variability by focusing on process modelling and synthesis. The study did not address the impacts of the uncertainties on other parts of the supply chain, such as transportation and distribution.

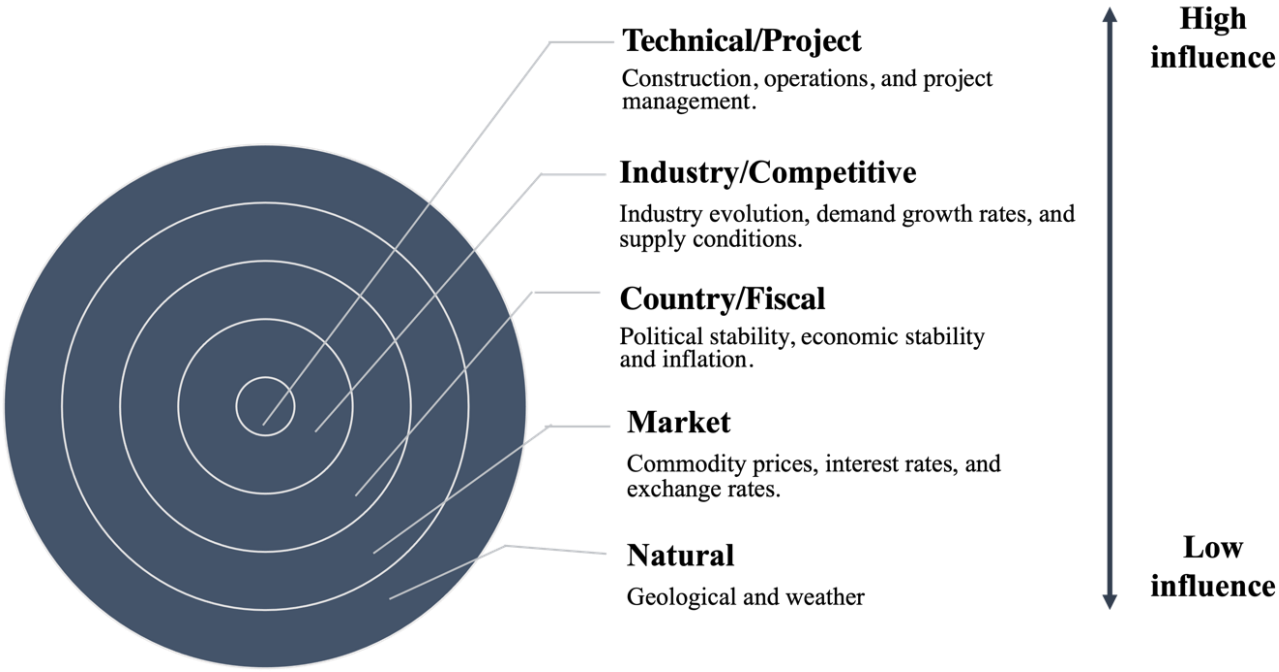

Figure 6. Layers of uncertainty and their influence on project performance.

Moreover, Khalilpour and Karimi [22] presented a two-stage optimisation approach for making investment decisions for a company that wishes to develop a natural gas reserve for transportation to nearby markets. Three monetisation options were considered: GTL, LNG, and CNG, under uncertain product demands, crude oil prices, and feed gas prices. The authors used a mixed-integer linear program (MILP) that yields the maximum expected net present value (ENPV) and optimal production capacities for each technology. Moreover, the MILP model was integrated with costs and decisions related to shipping. A scenario-based approach was finally used to allocate product amounts to markets throughout the production period. Similarly, a later study by Khalilpour and Karimi [53] identified the best gas monetisation options under natural gas and oil price uncertainty through considering the overall supply chain, from production to transportation to markets. The techno-economic analysis suggested that GTL is the best option compared to LNG and CNG for a large reservoir and distant markets. However, other factors, such as technology reliability, political stability, and market structures, were not considered.

A study by Tan and Barton [116] presented a framework for decision-makers for the optimal allocation of small-scale mobile LNG and GTL technologies to monetise standard or associated gas under stochastic supply, price, and demand of the various products in international markets. A multi-period MILP model was proposed to maximise the net present value (NPV) of the project, and the model was then implemented in a real-world case study on the Bakken Play to determine the optimal NPV. The authors reported that the profitability of implementing mobile plants depends on the project and its circumstances. The authors extended the framework in a later study and proved the robustness and effectiveness of mobile plants under uncertain supply, price, and demand [117].

Overall, the reported studies considered systematic approaches for evaluating upstream natural gas monetisation investment decisions under uncertainty. The literature screening revealed sufficiency in the technical evaluations of monetisation approaches in response to exogenous uncertainties. As production processes are the core of the natural gas supply chains, the technical fundamentals are inputs for the evaluation of comprehensive supply chains. In fact, most of the recent research evaluated the reliability of shale gas monetisation processing under endogenous uncertainties (i.e., varied natural gas flow rate and composition) under environmental, economic, and/or technical key

performance indicators [118,119]. Endogenous uncertainties in the upstream operation of shale gas facilities are extremely vital due to the high capital and operating expenditures associated with the production and processing of shale gas. Hence, shale gas projects encounter greater planning and operational challenges, associated with endogenous uncertainties in processing shale gas and exogenous uncertainties in monetising processed gas to value-added products.

5. Natural Gas Supply Chain Optimisation

While supply chains have existed ever since businesses began to transfer services and/or products to customers, supply chain management and optimisation have been recent areas of research to analyse and study the impact of different parts of the supply chain on the overall business performance. In the last couple of decades, supply chain optimisation has been an area of interest for firms to study the inter-organisational and inter-functional integration of the different parts of the supply chain in order to make better supply decisions. Different authors have presented extensive literature reviews on the approaches used in supply chain modelling and optimisation in the literature, such as big data and the internet of things [120,121], metaheuristics [122], and artificial intelligence [123,124]. Most studies highlight the approaches to solving mathematical optimisation problems in supply chain management. This section highlights the mathematical optimisation problems described in the literature in the planning and operation of NGSCs under deterministic and stochastic conditions.

In the area of NGSC optimisation, different authors have studied the modelling and optimisation of different parts of the NGSC, including production, processing, storage and transportation, contract management, and market sales. Hasle et al. [58] studied a company's NGSC with a portfolio of production fields from an upstream point of view. The authors studied the impacts of spot and forward markets and the technological innovations of transportation and processing on the operations and planning of the NGSC. A static one-period MILP model was reported to optimise the natural gas transportation network to ensure that the planned production meets demand, i.e., the nominated volumes are delivered to the receiving terminals within a pre-specified time period. The model was extended to consider multiple periods, storage capacities, contracts, and markets to discuss the portfolio perspective of NGSC management by considering the stochastic behaviour of prices and demand in the European markets. Additionally, technical aspects such as pressure drop, contracts' predetermined pressure and quality standards, and minimal energy consumption were considered in the model. The proposed model is a useful tool for operators to meet the customers' demand based on a certain network state, either to optimise the routing of natural gas in pipelines or to adjust the production in the fields, in the event that a flexible production strategy has been implemented.

In NGSCs, the natural gas pipeline network plays a significant role in natural gas resource allocation. The network acts as an intermediary link connecting upstream gas supply and downstream customer demand [125,126]. With the increased growth in natural gas demand and the expansion of natural gas networks, the optimal allocation and operation of natural gas networks have become crucial for sufficient, reliable, economical, and safe transmission [40]. In the literature, studies have reported mixed-integer nonlinear programming (MINLP) and MILP optimisation models for the distribution planning (operational planning level) and/or design of natural gas pipelines' transmission and distribution networks (strategic planning level), considering single or multiple objectives [84,127–132]. Considering the nonlinear characteristics in the MINLP models developed in previous studies, different algorithms have been used to solve the models, such as the partial swarm optimisation algorithm (PSO), ant colony optimisation algorithm (ACO), and genetic algorithm (GA). In most studies, the multi-objective optimisation problems were simplified into a single-objective optimisation problem by converting some of the objectives to constraints. However, most of the reported studies focused mainly on the design and/or operation, transmission, and distribution in the natural gas network under deterministic conditions,

regardless of sustainability aspects and stochastic demand. Fundamentally, the instability in natural gas demand jeopardises the operational efficiency of the natural gas pipeline network. A recent work by Wen et al. [133] reported a multi-period MINLP approach to respond to the instability in user demand. Through three cases with diverse characteristics, the model was used to derive the optimal decision-making scheme for different topological structures and engineering situations that may occur in real-life natural gas pipeline network systems, with the objective of minimising costs and carbon dioxide emissions. The recent consideration of CO_2 minimisation is crucial for natural gas companies to stay aligned with national CO_2 regulations and policies. Table 1 summarises the natural gas optimisation problems based on the research purpose, addressing the part of the supply chain, modelling approach, and planning level. Economic and environmental objectives in natural gas transmission problems, with the objectives of maximising gas allocations, minimising fuel consumption, and minimising CO_2 emissions, have been heavily researched in the literature. On the other hand, pipeline safety has received attention recently in the literature, since pipeline failure would lead to disasters and economic losses [134]. Consequently, considering the objective of pipeline reliability in existing models is auspicious for multi-objective problems to study economic, environmental, and safety aspects [135].

Table 1. Summary table of the reviewed articles related to natural gas supply chain optimisation models.

Reference	Decision Problem	Supply Chain Type	Deterministic/ Stochastic	Modelling Approach	Planning Level	Region
Hasle et al. [58]	Portfolio optimisation model for the natural gas value chain	Natural gas pipeline network (transportation, storage, and markets)	Stochastic	Two-stage MILP	Strategic/ tactical	Norway and import terminals in the UK, France, Belgium, and Germany
Alves et al. [84]	Design optimisation of natural gas transmission network	Natural gas pipeline network (single source and sink)	Deterministic	Multi-objective NLP	Tactical	Not applicable
Chebouba [127]	Optimisation of power consumed in a natural gas supply chain	Natural gas pipeline network	Stochastic	Dynamic optimisation	Operational	Hassi R' mell-Arzew gas pipeline, Algeria
Martin et al. [128]	Optimising the flow of natural gas	Natural gas pipeline network	Deterministic	MINLP	Operational	Ruhrgas network, Germany
Mikolajková et al. [129]	Design optimisation of natural gas pipeline network	Natural gas pipeline network	Deterministic	MILP	Strategic	Pori in Southwest Finland
Turan and Falmand [130]	Design and planning optimisation of natural gas supply chain with producers and mid-streamers with respect to new infrastructure investment decisions	Natural gas pipeline network (regasification, storage, and distribution)	Deterministic	MILP	Strategic	EU
Wang et al. [131]	Design optimisation of natural gas pipeline network	Natural gas pipeline network	Deterministic	Multi-period MILP	Strategic	Shanxi Province in China
Zarei and Amin-Naseri [132]	Design and planning optimisation of the overall natural gas supply chain	Natural gas supply chain	Deterministic	MILP	Strategic	Iran
Wen et al. [133]	Allocation and optimisation of the natural gas transmission network subject to changes in downstream users' demand	Natural gas pipeline network	Stochastic	Multi-period MINLP	Tactical	China
Hamedi et al. [136]	Distribution planning of the natural gas network	Natural gas pipeline network	Deterministic	Multi-period MILP	Operational	Not applicable
Demissie et al. [137]	Distribution planning of natural gas pipeline network	Natural gas pipeline network	Deterministic	Multi-objective NLP	Operational	Not applicable

With the growth of demand for LNG in the last two decades, optimisation of LNG supply chains has become a trending research topic, where different deterministic and

stochastic MILP and LP models have been reported in the literature [138–142]. Two scenario-based two-stage stochastic MINLP models were proposed by Li et al. [143] for tactical natural gas infrastructure planning under supply and demand uncertainties. The first stage of the decision aims to determine whether to deploy the infrastructure. The second-stage decisions determine multiple long-term operating conditions under uncertain parameters. To solve the large-scale nonconvex MINLP, the authors proved the efficiency of using the nonconvex generalised Benders decomposition (NGBD) algorithm over the state-of-the-art global optimisation solver. On the other hand, the complexity of LNG inventory and transportation management is anticipated to increase due to introduced constraints caused by demand expansion, capacity restrictions, and LNG fleet availability. With GTL optimisation studies being less common in the literature, only a few scholars have reported the optimisation of GTL supply chains, such as Elia et al. [144,145], who reported an MILP model for strategic planning of a GTL supply chain in the U.S. A summary of LNG/GTL supply chain optimisation studies is presented in Table 2. The addressed studies are concerned with supply chain design and planning, wherein transportation problems were excluded.

Table 2. Summary of LNG/GTL supply chain optimisation studies.

Reference	Decision Problem	Supply Chain Type	Deterministic/ Stochastic	Modelling Approach	Planning Level	Region
Bittante et al. [138]	Optimisation of the supply chain from the point of view of shipping	LNG supply chain	Stochastic	MILP	Strategic	Gulf of Bothnia
Bittante et al. [139]	Design and multi-period planning optimisation of an LNG supply chain with sea and land transportation	LNG supply chain	Deterministic	Multi-period MILP	Strategic/ tactical	Gulf of Bothnia
Bittante and Saxén [140]	Design and multi-period planning optimisation of a small-scale supply chain with sea and land transportation	LNG supply chain	Deterministic	Multi-period MILP	Strategic/ tactical	Gulf of Bothnia
Utku and Soyöz [141]	Design and planning of the supply chain subject to demand uncertainty	NG/LNG supply chain	Stochastic	LP	Strategic/ tactical	Not applicable
Zhang et al. [142]	Planning for developing infrastructure and inventory routing	LNG supply chain	Stochastic	Three-stage MINLP	Operational	China
Elia et al. [144,145]	Design and planning optimisation of the supply chain	GTL supply chain	Deterministic	MILP	Strategic/ tactical	The U.S.
Bittante et al. [146]	Design and planning optimisation of a small-scale supply chain with sea and land transportation	LNG supply chain	Deterministic	MILP	Strategic/ tactical	Gulf of Bothnia
Li et al. [143]	Planning of natural gas infrastructure development under uncertainty	LNG supply chain	Stochastic	Two-stage MINLP	Tactical	Malaysia

Multistate Natural Gas Supply Chain Optimisation

Natural-gas-producing countries embrace various monetisation approaches to diversify their product portfolio, tackle CO_2 emissions, and optimise profitability. This contributes to complexities in planning and managing NGSCs, with multiple production processes, storage technologies, transportation modes, and targeted markets (see Figure 7).

Mathematical optimisation has been a widely used decision-making approach to investigate the optimal design, planning, and operation of multistate NGSCs. Different technical, economic, legal, and policy constraints can be introduced to the problem, depending on the decision level. In the literature, integrated simulation–optimisation models have been reported to economically optimise multistate upstream and midstream natural gas processing facilities [147–150]. The simulation–optimisation framework presented by Al-Sobhi et al. [149,150] and Al-Sobhi and Elkamel [148] strictly focuses on upstream or midstream processing units. The authors considered the modelling, simulation, and optimisation of the processing units, where the output data were used to improve the optimisation model's results. The study's results justified the significance of incorporating rigorous simulation models in decision-making when designing gas networks. However, the studies did not address the storage and transportation of the produced products to international markets. The upstream natural gas studies in the literature mainly reported MIP models for natural gas purification and processing units considering different objectives, such as minimising emissions, minimising costs, and maximising profits [147,150,151]. Upstream optimisation studies are mainly subject to endogenous uncertainties, including variabilities supplied by natural gas production, composition, and flow rates.

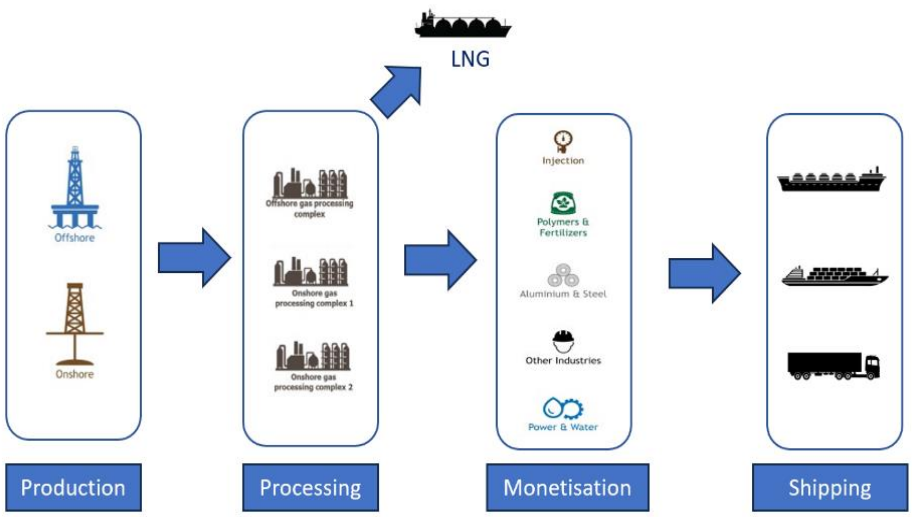

Figure 7. Overview of a multistate natural gas supply chain comprising different monetisation and shipping options.

Additionally, Zhang et al. [152] presented an optimisation approach to design and operate a multistate local NGSC with three options—PNG, LNG, and CNG—and four transportation modes: pipelines, LNG ships, LNG road tankers, and CNG road tankers, subject to uncertainty to minimise construction and operation costs. The multi-simulation MILP model was developed based on the Monte Carlo simulation, featuring uncertainties in demands and prices. The results of the study reported that the construction of such a network increases the flexibility of the integrated transportation system. Moreover, the results of the analysed cases revealed that the price uncertainties impacted the total costs more than the construction scheme of the supply chain. Similarly, Zhang et al. [153] reported three scenario-based MIP models for designing a multistate NGSC consisting of PNG, LNG, and CNG with different transportation schemes. The models aimed to optimise economic performance by maximising the annual profits of the NGSC under uncertain future gas demand. The designed supply chain scheme was then evaluated environmentally by considering CO_2 emissions from the production, transmission, storage, and transportation stages.

With the growing demand for renewable energy, the integration of renewable systems with fossil-based systems is expanding. In integrated renewables–natural gas systems, renewables can be used as a source of energy or as a primary feedstock for various processes.

This represents the utilisation of upgraded biogas in NGSCs, as discussed by Mikolajková-Alifov et al. [154], who proposed an MILP model for optimising a domestic multiproduct NGSC composed of LNG, CNG, and upgraded biogas. Other studies in the literature have discussed optimising the design and/or operation of integrated systems subject to uncertainties, such as integrated crude oil systems [155,156] and multiproduct supply chain projects [157–159]. In fact, incorporating uncertainties into planning models using stochastic optimisation has been challenging due to the complexity involved in the computational requirements. According to Oliveira et al. [160], two-stage stochastic programming has been the most common framework to deal with uncertainties in optimisation models. The authors presented a framework for the network design and capacity expansion of a multiproduct, multi-period supply chain investment planning problem under demand uncertainty, in which a Lagrangian decomposition scheme was proposed to solve the mixed-stage MILP model. The model was applied to a petroleum product supply chain and can be generalised for stochastic integer programming problems. With NGSCs being more vulnerable to market disruptions, stochastic programming is a valuable approach to deal with market uncertainties. Table 3 below summarises multistate natural gas supply chain optimisation studies.

Table 3. Summary of multistate natural gas supply chain optimisation studies.

Reference	Decision Problem	Supply Chain Type	Deterministic/ Stochastic	Model	Planning Level	Region
Al-Sobhi and Elkamel [148]	Simulation and optimisation of a natural gas production network consisting of LNG, GTL, and methanol facilities	Natural gas processing units: LNG, GTL, and methanol, with byproducts	Deterministic	LP	Strategic	Not applicable
Al-Sobhi et al. [149]	Simulation and optimisation of a natural gas production network consisting of LNG, GTL, and methanol facilities	Natural gas processing units: LNG, GTL, and methanol, with byproducts	Deterministic	MILP	Strategic	Not applicable
Zarei and Amin-Naseri [151]	Enviro-economic design and planning optimisation of the overall natural gas supply chain	Multi-product natural gas supply chain	Deterministic	Multi-objective MILP	Strategic/ tactical	Iran
Zhang et al. [152]	Design and operational optimisation of the natural gas supply chain subject to demand and purchase price uncertainties	Natural gas supply chain: gaseous, LNG, and CNG	Stochastic	MILP	Strategic/ tactical	China
Zhang et al. [153]	Enviro-economic design and operation optimisation under three risk attitude scenarios caused by uncertain gas demand	Natural gas supply chain: gaseous, LNG, and CNG	Stochastic-Scenario based	Risk neutral: MILP Risk aversion: MIQP Risk-taking: MINLP	Strategic/ tactical	China
Mikolajková-Alifov et al. [154]	Design optimisation of gas supply to customers	Natural gas supply chain: LNG, GTL, and upgraded biogas	Deterministic	MILP	Strategic	Western Finland

6. Emergence of Hydrogen and the Future of Natural Gas Supply Chains

For countries that are highly dependent on coal, natural gas can be a transition fuel on the road to net-zero objectives with less emitted CO_2. Modern gas-fired electricity plants emit 50–60% less CO_2 than traditional coal-fired plants [161]. Hence, the first climate change mitigation step adopted by several countries has been to increase the share of natural gas in their energy portfolios. However, switching from coal to gas is a short-term solution, and further actions are needed in the long term to support the goal of achieving net-zero by 2050. This includes adopting cleaner energy resources (i.e., renewables and nuclear) in different sectors and investing in carbon capture, utilisation, and storage (CCUS) technologies in existing fossil-based supply chains. Carbon adjustment policies have been

adopted on imported products based on the embodied CO_2 in consumer markets. For example, the Carbon Border Adjustment Mechanism (CBAM) regulation announced by the European Commission considers imposing emissions pricing on the direct emissions of imported products, including fertilisers and steel [162]. Some of the burden of emissions pricing (i.e., carbon taxes) may be shifted to sellers, such as Qatar. The new policies imposed on natural gas monetised products and energy commodities, along with the long-term shifts to renewables as energy resources, intensify the risk to existing natural gas supply chains. Consequently, various strategies can be qualitatively and quantitatively investigated for sustaining natural gas businesses. These include decarbonising existing natural gas production systems, integrating natural gas production systems with hydrogen production along with CCUS, and deploying renewable technologies in NGSCs. The latter will support the role of natural gas in securing a smooth transition towards renewables by filling the gap between existing systems and the future demand for cleaner energy resources. Moreover, the integration of NGSCs, hydrogen supply chains (HSCs), and CCUS results in various economic and environmental added values, including decarbonisation and enhanced product portfolios.

6.1. Hydrogen Supply Chain and Production Technologies

The concept of employing hydrogen as a potential clean energy carrier has been of great interest in the last few years for supporting energy sustainability and system flexibility [42,163,164]. In addition to hydrogen's role in decarbonising the transportation and residential sectors, hydrogen has unlocked the efficient production of e-fuels, such as ammonia, methanol, and synthetic gas, when coupled with CCUS and renewables [38,73,165]. However, the costs of green technologies for producing green hydrogen (i.e., carbon-free hydrogen produced from renewables) have been a limiting factor in large-scale hydrogen deployment. Hence, other low-carbon alternatives have been introduced by researchers and industry leaders to accelerate the economic deployment of hydrogen on an industrial scale, including decarbonising fossil-based hydrogen production.

In the literature, several review studies have highlighted up-to-date available technologies and advancements for hydrogen's production, storage, and transportation from environmental, economic, social, and technical perspectives [165–169]. As illustrated in Figure 8, the hydrogen production route strongly depends on the feedstock [166]. The transportation mode and storage technologies rely on the physical form of the produced hydrogen [42,170]. On the other hand, the maturity of hydrogen storage technologies has been an area of debate in the literature. Technical comparative assessments of the most feasible storage solutions revealed that compressed gas, cryogenic liquids, chemical hydrides, metal hydrides, and nanomaterials are the most viable options [163,171,172].

Despite the intensified efforts to investigate economical methods of producing hydrogen from renewables, green hydrogen production costs substantially more than fossil-fuel-based technologies [173,174]. Natural gas is the primary source for hydrogen production, with a global natural gas use of 6% [175]. In practice, the term "grey hydrogen" is used to refer to hydrogen sourced from natural gas or any other fossil fuel. Pairing grey hydrogen production facilities with CCUS supports the production of low-carbon hydrogen, or "blue hydrogen", with a maximum cost increase of 0.5 USD/kg [170]. Consequently, cost-effective blue hydrogen will significantly contribute to tackling CO_2 emissions for countries with limited renewables potential. This translates to assessing strategies and investment decisions for integrating blue hydrogen within NGSCs.

Various assessments on hydrogen production routes from natural gas have been reported in the literature, such as steam methane reforming (SMR), autothermal reforming (ATR), and partial oxidation of methane (POM). Amongst the different production methods, SMR was revealed to be the most used and well-established technology for hydrogen production. The present challenges of SMR are related to optimising the process in terms of hydrogen production capacity, natural gas conversion, and reaction temperature reduction [176]. Hence, developing efficient catalysts for the SMR process has attracted

attention in the last few years [177,178]. On the other hand, commercial POM technology has commercially emerged to overcome the catalyst and external heat input required by the SMR process [179,180]. Due to the limited hydrogen yield produced via POM, the ATR process was developed to integrate the beneficial characteristics of both SMR and POM processes in series configuration. In the ATR process, the generated heat from the POM is utilised for the steam reforming part of the process [181]. The commercialisation of ATR is still not comparable to that of SMR [182]. In recent years, research on ATR and POM technologies has become a common area of research to satisfy the need for cost-effective and less pollutant-high conversions in mild reaction environments [183–185]. The main characteristics of three hydrogen production processes from natural gas are summarised in Table 4, adapted from [176].

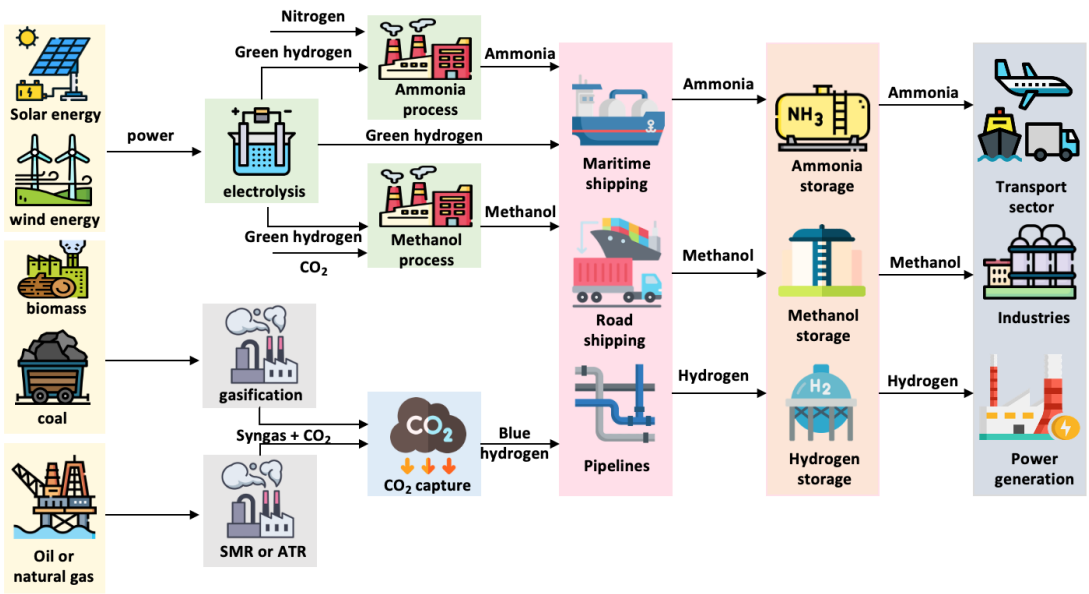

Figure 8. Overview of the hydrogen value chain from production to end-user utilisation, modified from [166].

Table 4. Comparison of hydrogen production processes from natural gas.

	External Heating	Catalyst	Oxidation	Temperature (°C)	Efficiency (%)	CO_2 Capture
Steam methane reforming (SMR)	Required	Required	N/A	800–1100	70–85	Pre- and post-combustion
Partial oxidation of methane (POM)	N/A	N/A	Required	950–1500	55–75	Post-combustion
Autothermal reforming (ATR)	N/A	Required	Required	700–1000	60–75	Post-combustion

To transition from grey hydrogen to blue hydrogen, the selection of a hydrogen production technology is a critical decision. In existing brownfield natural gas–hydrogen production facilities, CO_2 capture is subject to technical limitations, wherein only post-combustion units are applicable. On the other hand, the decision maker has more flexibility in considering different combinations of hydrogen production technologies and CO_2 capture processes in new projects. This indicates that a new ATR unit with CO_2 capture may be more attractive for large-scale deployment when considering CO_2 capture efficiency. Consequently, optimal process configuration and infrastructure planning in either deploying new facilities or retrofitting existing facilities are critical for optimising the hydrogen supply chains based on different environmental, economic, product quality, safety, and social aspects.

6.2. Hydrogen Supply Chain Optimisation

One of the most critical strategic decisions that an organisation can make involves the design of the hydrogen supply chain (HSC), which can be extremely costly and affect the long-term operation of the company. The increased cost complexities are associated with exogenous uncertainties in feedstock costs that impact the HSC. With limited knowledge of exogenous feedstock costs, HSC models are unable to recognise and respond appropriately to the dynamics of other supply chains [44]. In this sense, an optimal HSC must consider the number and capacity of production units, storage facilities, and transportation modes. Additionally, demand, temporal, and spatial factors must be considered in the early design stages of an HSC. In the literature, mathematical programming has been a common approach to optimise the design and operation of low-carbon HSCs. A web search on "Science Direct" for the term "hydrogen supply chain" between 2005 and 2023 resulted in 134 results. By modifying the search term to "hydrogen supply chain optimisation" for the same period, a total of 107 results were obtained, accounting for 80% of the total HSC studies. A final list of 53 HSC optimisation studies was reviewed based on a mathematical programming approach for optimisation. The studies were then filtered based on the feedstock source and type of problem, and only infrastructure planning and operation studies of hydrogen produced from natural gas are discussed herein.

A series of studies reported single-objective and multi-objective optimisation models for the design and operation of regional HSCs under deterministic and stochastic conditions using an MILP model [186–193]. With the increased interest in designing environmentally sustainable HSCs, later studies extensively investigated environmental and/or social factors by introducing CCUS technologies. Almansoori and Betancourt-Torcat [194] extended the approach proposed by Nunes et al. [195] and presented a deterministic MILP model for the infrastructure design and product delivery mode of a domestic HSC with CCUS technologies under constrained GHG emissions. Similarly, Moreno-Benito et al. [196] presented a multi-period spatially explicit MILP model to optimally design a sustainable HSC infrastructure over different timeframes. The reported mathematical model is an extension of a model proposed by Agnolucci et al. [197]. It considers the selection of the facility location, technologies, capacities, storage facilities, transportation modes, international imports, and CCS system, with the objective of minimising the investment cost. The results of a UK-based case study revealed that coupling SMR plants with CCS is the most cost-effective way to maintain low CO_2 emissions. CCS systems are essential when utilising SMR technologies to mitigate the 9 kg of CO_2 emitted per kg of H_2 produced in the process [198]. These findings are consistent with similar HSC optimisation studies that concluded the cost-effectiveness of SMR and CCS technologies in light of economic and/or environmental aspects, especially in the first years of establishing a hydrogen economy [195,199–204]. At the same time, a multi-objective cost-, risk-, and zero-emissions-oriented study by Erdoğan and Güler [205] concluded that a mixed production strategy of SMR and water electrolysis is the most efficient for a 25-year domestic HSC planning horizon. Moreover, a later work by Li et al. [206] presented a multi-period MILP model for the design of a regional HSC network in Dalian, China. The authors investigated the optimal combination and number of technological options, storage types, and transportation modes, subject to primary source availability (i.e., natural gas, coal, biomass, and renewable energy). Applying a Markov chain for a sustainable design indicated that water electrolysis is the most environmentally and economically effective production technology for hydrogen planning subject to the carbon tax.

Although economic and environmental factors represented the most common objectives in HSC infrastructure design and planning, safety risks have been commonly addressed in recent studies, such as [200,205,207]. In the recent literature, safety risks were brought to attention again by Robles et al. [207], who extended a previous framework developed by Almaraz et al. [191] for optimising the hydrogen mobility market in the Midi-Pyrénées region in France. The authors reported a stochastic, spatial-based, multi-objective, multi-period MILP to minimise daily costs, global warming potential, and safety

risks. Decision variables included determining the number, type, capacity, and location of production and storage facilities and transport units, in addition to the flow rate of hydrogen between locations. The study concluded that the safety risk is more difficult to formulate and calibrate compared to the economic and environmental factors. It is worth mentioning that almost all previous regional studies focused on designing and planning domestic HSC networks for the transport sector. As a matter of fact, social responsibility is a crucial measure for assessing the willingness of end consumers to shift to hydrogen fuel cell vehicles. Social aspects of introducing hydrogen as an energy carrier were identified as a research gap [208,209]. The reliability, social responsibility, and economic and environmental aspects of an HSC were studied by Fazli-Khalaf et al. [210]. The study focused on human beings and the quality of their lives when considering social responsibility, such as job creation and meeting customers' demands on time. The authors developed a fuzzy probabilistic flexible programming model to increase the flexibility of the hydrogen network under mixed uncertainties and to maximise the reliability and sustainability of an HSC in Iran. A decentralised network structure was reported with two production technologies (electrolysis and SMR) to produce liquefied and compressed hydrogen. The decentralised structure was reported to catalyse more job opportunities and contribute to minimising the total CO_2 emissions.

Table 5 summarises the main features of the reviewed HSC strategic/tactical design and planning studies. From the reviews of the discussed studies, most of the problems are formulated into MILP. Most of the reported HSC design and planning studies in the literature have not considered feedstock problems and seasonal storage. Addressing seasonal storage is essential for introducing flexibility in the supply chain under demand uncertainty. Nevertheless, introducing hydrogen infrastructure to existing energy supply chains is one of the main challenges in today's industry. The following section highlights the recent studies assessing the integration of hydrogen infrastructure with mature natural gas and energy infrastructures.

Table 5. Summary of the reviewed hydrogen supply chain optimisation models.

Reference	Planning Level	Model	Objective Functions	Demand Uncertainty	Region
Seo et al. [186]	Strategic	Spatially explicit MILP	• Minimise total daily costs	No	South Korea
Almansoori and Shah [187]	Strategic	Multi-period MILP	• Minimise costs	No	Great Britain
Almansoori and Shah [188]	Strategic	MILP	• Minimise costs	No	Great Britain
Almansoori and Shah [189]	Strategic	Multi-period multistage MILP	• Minimise costs	Yes	Great Britain
Dayhim et al. [190]	Strategic	Multi-period two-stage MILP	• Minimise total social costs	Yes	New Jersey, USA
Almaraz et al. [191]	Strategic	Multi-period MILP	• Minimise costs • Minimise environmental impacts • Minimise safety risks	Yes	Midi-Pyrénées region, France
Kim and Moon [192]	Strategic	Two-stage MILP	• Minimise costs • Minimise safety risks	Yes	South Korea
Kim et al. [193]	Strategic	Steady-state two-stage MILP	• Minimise costs	Yes	South Korea
Almansoori and Betancourt-Torcat [194]	Strategic	MILP	• Minimise costs under emissions constraints	No	Germany
Nunes et al. [195]	Strategic	Two-stage MILP	• Minimise costs	Yes	Great Britain
Moreno-Benito et al. [196]	Strategic	Multi-period spatially explicit MILP	• Minimise capital costs	No	The UK
Wickham et al. [199]	Strategic	LP	• Minimise total net present value of costs	No	Great Britain
Erdoğan et al. [200]	Strategic	Multi-period MILP	• Minimise investment and operating costs. • Minimise CO_2 emissions • Minimise safety risks	No	Turkey
Ibrahim and Al-Mohannadi [201]	Strategic	Spatial MILP	• Minimise total costs	No	Qatar

Table 5. *Cont.*

Reference	Planning Level	Model	Objective Functions	Demand Uncertainty	Region
Güler et al. [202]	Strategic	Multi-period MIP	• Minimise total costs	No	Turkey
Forghani et al. [203]	Strategic	Two-stage Multi-period MIP	• Minimise total costs	No	Oman
Cantú et al. [204]	Strategic	Multi-period spatial MINLP	• Minimise total daily costs • Minimise GHG emissions	No	Midi-Pyrénées region, France
Erdoğan and Güler [205]	Strategic	Multi-period MILP	• Minimise investment and operating costs. • Minimise CO_2 emissions • Minimise safety risks	Yes	Turkey
Li et al. [206]	Strategic	Spatiotemporal MILP	• Minimise daily costs	No	Dalian, China
Robles et al. [207]	Strategic	Multi-period MILP	• Minimise total daily costs. • Minimise global warming potential • Minimise safety risks	Yes	Midi-Pyrénées region, France
Fazli-Khalaf et al. [210]	Strategic/Tactical	MILP	• Maximise reliability • Minimise total costs • Maximise demand coverage • Maximise sustainability (environmental and social responsibility)	Yes	Iran

6.3. Integrating Hydrogen Production with Natural Gas Supply Chains

Cost-effective and gradual expansion of hydrogen's market share could be achieved by deploying hydrogen in existing natural gas infrastructure [30]. In fact, introducing hydrogen with existing systems could enhance the sustainability, reliability, and operational flexibility of future low-carbon energy systems [42,211]. As hydrogen produced via SMR is recognised for its efficiency in initiating a hydrogen economy, this section highlights studies that have reported integrating SMR-CCUS with existing NGSCs by focusing on technical, economic, and environmental aspects. In the literature, Hwangbo et al. [212] reported that integrating the HSC with the utilities supply chain is appealing because the steam produced by the utilities network can be utilised for hydrogen production. The authors developed an integrated network model combining a multi-site-scale utilities supply chain with an HSC using a two-stage stochastic MILP model in South Korea. This model optimises the total costs and considers the demand uncertainties of both networks. However, the results revealed that in order to meet the forecasted hydrogen demand, additional independent SMR plants would have to be constructed. On the other hand, the study did not address other production routes or CCUS technologies for decarbonisation.

Samsatli and Samsatli [213] reported a multi-objective MILP model for the design and operation of a multivector energy network comprising different sources converted to final energy services, such as electricity, heat, and mobility. The developed model optimises investment decisions considering both time and space to capture demand variability and resource availability subject to techno-socio-environmental constraints. An investigated multi-scenario case study was conducted in Great Britain to meet local demand for electricity, heat, and mobility. Resources, including natural gas, biomass, and wind power, converted to products such as syngas, electricity, hydrogen, and natural gas, were evaluated. However, the authors only investigated deterministic scenarios and did not highlight the deployment of CCUS technologies. Fundamentally, CCU technologies have been reported to provide more economic incentives compared to CCS for covering the capture costs [38,73]. The decarbonisation and flexibility aspects were addressed in a later work by Quarton and Samsatli [35], who reported a multi-objective spatiotemporal MILP model for a comprehensive, integrated CO_2-HSC with energy. The model was applied to the installed fossil-fuel-based energy system in Great Britain, with the objective of maximising the net present value (NPV). The primary energy resources were natural gas, wind, and biomass, wherein the seasonal availability of biomass was considered. Moreover, the model prioritised satisfying the mandatory demand for heat and electricity, followed by

optional demand for byproducts produced from CCUS to maximise profits. In this study, only methanol produced from CCU was considered, providing great insights for investors and policymakers into the added value of studying CCUS and hydrogen technologies for decarbonising and adding flexibility in the supply chain. Additionally, an integrated system promotes reliance on multiple feedstocks and the production of multiple end products. The potential of introducing other demandable products, such as ammonia and formic acid, could be investigated to diversify the portfolio.

More recent work has been introduced by researchers who investigated the economic benefits of utilising existing natural gas pipelines and hydrogen byproduct infrastructure for the deployment of hydrogen production facilities. A spatially explicit multi-period MILP model was developed to minimise the total costs of the integrated H_2-NGSC. Compared to the non-utilisation scenario, the synergistic effect of utilising existing infrastructure reduced the average levelised cost of hydrogen by 17.53% for the case study in Korea. Moreover, the multi-period analysis suggested that SMR technology for hydrogen production is most appropriate in the early periods until the hydrogen demand matures in the market. Although most studies have reported hydrogen production for local markets, an analysis by Al-Kuwari and Schönfisch [214] addressed a combined natural gas and low-carbon hydrogen market model, covering different stages of hydrogen and natural gas value chains, from production to consumption. Interestingly, the problem was formulated as a mixed complementarity model and run on annual resolutions to maximise the profits of different agents (i.e., exporters, producers, transmission system operators, liquefiers, gasifiers, and shippers). The study concluded that synergies between the LNG and low-carbon hydrogen industries are commercial rather than technical. Given its large-scale engineering and project management capacities, the LNG industry is believed to be well equipped with regard to expertise and assets to develop low-carbon hydrogen. The above reviewed studies are summarised in Table 6. Other studies in the literature have reported MILP and MINLP operational planning optimisation models for local integrated energy systems for economical and reliable operation [59,131,143,215–217]. The energy management studies considered the energy supply and demand, and they did not investigate the production side of energy resources. Such models assist in promoting flexibility in the supply side through planning for storage technologies and storage capacities. However, the decisions would be vigorously influenced when introducing CCUS and hydrogen production technologies into such studies. Overall, the proven synergies between the natural gas industry and low-carbon hydrogen indicate the technical and economic potential of introducing hydrogen production facilities coupled with CCUS in existing systems. Natural-gas-rich economies with constraints in deploying green hydrogen, such as Qatar, can seize market opportunities by retrofitting existing facilities and deploying blue hydrogen infrastructure.

Table 6. Summary of natural gas–hydrogen–renewables/utilities integrated systems.

Reference	Planning Level	Model	Objective Functions	Supply Chain Products/Services	Demand Uncertainty	Region
Quarton and Samsatli [35]	Strategic/ tactical	Spatiotemporal MILP (value web model)	• Maximise net present value	Heat, electricity, liquid fuels, hydrogen, CO_2, and/or methanol	Yes	Great Britain
Hwangbo et al. [212]	Strategic	Multi-period spatially explicit two-stage MILP	• Minimise total costs	Natural gas and utilities, including water and steam	Yes	South Korea
Samsatli and Samsatli [213]	Strategic/ tactical	Spatiotemporal MILP (value web model)	• Minimise costs • Maximise profits • Maximise renewable energy production	Heat, electricity, and hydrogen for mobility	No	Great Britain
Yoon et al. [218]	Strategic	Multi-period spatially explicit MILP	• Minimise total costs	Hydrogen	Yes	South Korea

7. Moving Forward and the Need for Flexibility in Integrated H_2-NGSCs

This literature review shows that NGSC optimisation has been a widely researched field due to the maturity of the existing infrastructure. The covered model-based analyses ranged between strategic and operational planning horizons for different parts of the supply chain, from infrastructure design and planning to delivery. Nevertheless, the increased interest in hydrogen fuel cell vehicles has intensified the number of strategic studies on domestic HSC infrastructure design and planning. In the design of HSCs, it is common for studies to follow a demand-driven approach, whereby predetermined demand estimates are used as input data. The literature showed that new HSC infrastructure is associated with high construction and operation costs in the early periods due to the low demand. In addition to the initial investment burden on hydrogen infrastructure, uncertainties in forecasted hydrogen demand increase the complexity of the decision-making process. The recent literature suggests the economic advantage of utilising existing natural gas infrastructure for the production and transportation of hydrogen in the early stages of establishing a hydrogen economy [214,218]. Additional hydrogen production and monetisation facilities can be introduced as the market grows. Moreover, natural gas facilities could be retired when the market fully transitions to green hydrogen energy and renewables. In the literature, assessments of integrating green hydrogen with existing fossil-based infrastructure are clustered depending on the produced hydrogen's end use (i.e., domestic use and hydrogen for export) [166,219]. For the state of Qatar, a small country with limited renewables potential and significant natural gas reserves, the decarbonisation of hydrogen utilised in the industrial sector has been proposed in the literature [167,219–221]. Babonneau et al. [219] suggested a technology-driven roadmap for reaching a net-zero emissions regime by 2070 in Qatar through several key steps, including fostering electric cars, developing hydrogen production by electrolysis by 2040, and introducing CCS in all industrial sectors. Analysing the results of the implemented linear programming model further suggested that carbon-free hydrogen sales could offset the collapse of natural gas revenues. In a net-zero scenario, where forecasted annual natural gas revenues are expected to decline from USD 76.8 billion to USD 15.8 billion per year, blue hydrogen revenues could reach as high as USD 42 billion per year.

Kazi et al. [167] assessed the industrial decarbonisation of Qatar's existing natural gas sector by replacing a portion of the fossil fuels used in feedstocks with green hydrogen produced via electrolysis. The proposed approach suggested the direct transition from grey hydrogen to green hydrogen. Meanwhile, Okonkwo et al. [220] concluded that shifting from grey to blue hydrogen and monetising the intermediate product to blue ammonia would represent a feasible transition state in the medium term in Qatar. Green hydrogen is foreseen to be as economically attractive as blue ammonia by 2040. This indicates that integrating H_2-NGSCs in the early stages adds product flexibility. A decision-maker would be able to directly sell the produced hydrogen as a product or monetise it to value-added products, such as methanol and ammonia. Moreover, in addition to the environmental attractiveness of CCUS technologies, carbon utilisation technologies allow the producer to offset carbon capture costs by producing value-added products via CO_2 hydrogenation processes. However, an investor must account for the demand uncertainties of the different products produced within an integrated H_2-NGSC with CCUS technologies for informed strategic planning.

Although several studies have accounted for stochastic demand when optimising NGSCs and HSCs, no study has accounted for stochastic demand in integrated H_2-NGSCs. Additionally, multi-period optimisation models were reported for the gradual deployment of infrastructure based on demand growth. In practice, the annual demand fluctuates depending on market dynamics, the emergence of other producers, and competition with other energy resources. Hence, proactively responding to annual market changes represents a new era of energy supply chain planning and operation. The ability to shift the operation and design of one or multiple parts of the supply chain is known as operational flexibility. In the literature, supply chain flexibility has been a trending topic in dealing with exogenous

uncertainties [151,222,223]. Embedding operational flexibility must be considered in the early design stages of a project. Producers first identify operational flexibility in terms of upper and lower operational bounds for a production system. Controllers and valves are then installed to allow the production capacity to be changed throughout the project's lifetime. Finally, flexibility in storage and transportation to markets is addressed. A few studies have considered the flexibility of specific supply chain functions in the literature. Cardin et al. [224] studied the economic value of flexibility of an LNG production system subject to demand uncertainties. The approach justified the role of flexible designs in responding to uncertainties compared with a fixed production system. Reuß et al. [225] studied the opportunities for seasonal storage and alternative carriers for a supply chain model based on hydrogen produced by electrolysis. The authors concluded that seasonal storage enhanced the economic impact and the GHG emissions. He et al. [226] developed a model for HSC planning to identify the minimum costs of production, storage, transmission, and compression facilities. Additionally, flexible scheduling for hydrogen trucks and pipelines was incorporated to serve as both transportation and storage resources based on the changes in demand and production throughout the project's lifetime. Such practices are crucial to enhance the responsiveness of integrated H_2-NGSCs to external shocks.

A flexible supply chain will allow the decision-maker to proactively react to market changes by adjusting the production, storage, and delivery to markets based on market needs. This, in turn, requires maximised technical and commercial coordination between different supply chain entities to evaluate the overall value of embedding flexibility. For example, production process simulation–optimisation studies are crucial to evaluate the impacts of feedstocks and demand uncertainties on the process operations. To date, no research has evaluated the influence of embedding flexibility within integrated systems by considering flexible supply chain functions to cope with market uncertainties. Notably, the technical aspects of flexible production units and the associated requirements of inventory planning and product storage are the most crucial characteristic to be addressed and investigated. Hence, future works should include simulation-based optimisation studies of integrated H_2-NGSCs subject to flexibility constraints. Moreover, technical assessments of the impacts of systems' integration are needed to evaluate potential energy and system efficiency losses. Figure 9 illustrates a comprehensive framework for introducing flexibility in strategic supply chain optimisation.

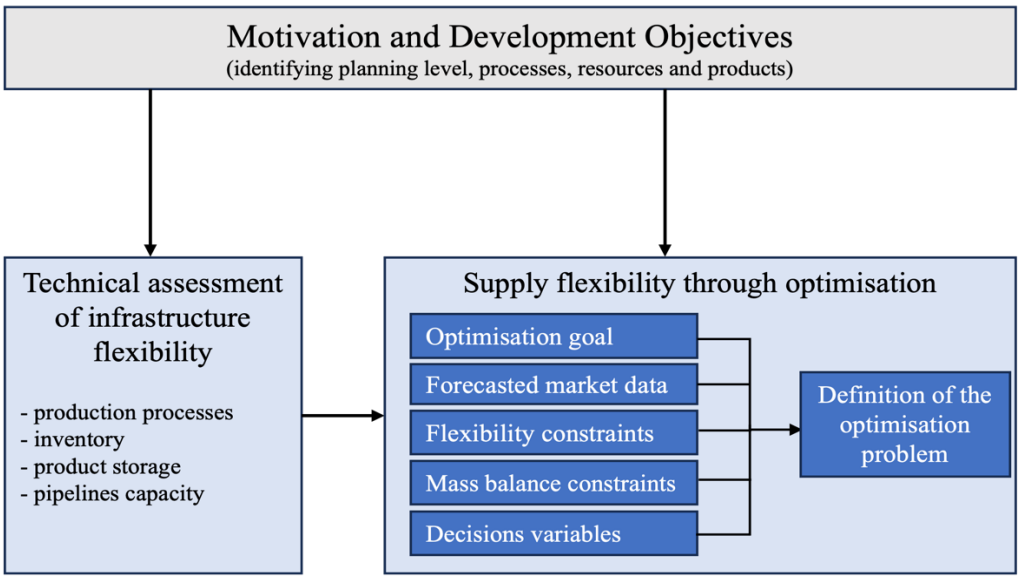

Figure 9. Proposed framework for considering flexibility in integrated supply chain optimisation.

8. Conclusions

With increased interest in mitigating CO_2 emissions, natural gas will be the fastest-growing fossil fuel until 2050. However, in light of demand fluctuations and market restructures, decision-makers must cautiously design and plan monetisation approaches and supply chains. This review investigated mathematical programming models used as quantitative decision-making tools for (1) the selection of monetisation approaches, (2) the design and planning of natural gas supply chains, (3) the design and planning of hydrogen supply chains, and (4) the design and planning of integrated hydrogen–natural gas supply chains. The reviewed aspects represent the systematic evolution of mathematical programming as an optimisation approach in the literature. The increased complexities in today's market are associated with energy supply chains driven by the overlap of different components, such as hydrogen, natural gas, and renewable resources. Hence, this review provides decision-makers and policymakers with a fundamental background on mathematical programming as a tool for the future strategic design of integrated supply chains. While earlier studies in the field evaluated deterministic cases, the deterministic scenario does not capture market volatilities. Hence, more recent studies have focused on stochastic modelling under exogenous uncertainties, especially in studies published after the latest energy market shocks induced by the COVID-19 lockdown in 2020.

Of the natural gas monetisation routes, PNG, CNG, GTL, and LNG were the most investigated in decision-making problems. The economic factor was the main driver in the selection and planning of natural gas supply chains. However, a few more recent studies introduced environmental constraints and/or objectives in multi-objective mathematical programming studies. The incorporation of the environmental factor in the assessments was driven by climate change policies and national roadmaps. On the other hand, several mathematical programming models were reported for the strategic design of hydrogen supply chains. For natural-gas-producing companies with great experience in managing natural gas supply chains, green or blue hydrogen is anticipated to be deployed in the existing infrastructure. Hence, this will require intensified efforts to deploy CCUS technologies to mitigate emissions and reduce the embodied CO_2 contents in the produced products. A large body of the literature qualitatively and quantitatively addresses the added value of exploiting CCUS technologies in existing infrastructure. Amplified efforts are still needed to assess the practicality of integrating CCUS infrastructure with existing natural gas supply chains. Pilot studies should examine the potential decline in process and energy efficiencies induced by integrating technologies (i.e., ATR and CCUS vs. SMR and CCUS). This technical knowledge will reinforce the decision-making process of whether to retrofit existing infrastructure or deploy new infrastructure.

From another perspective, integrating hydrogen and natural gas supply chains can yield operational flexibility, wherein different products can be produced depending on market needs. In turn, flexibility in operation and product portfolio diversification supports the producer to react proactively to market uncertainties. The deployment of CCUS technologies to the integrated supply chains results in further added values, including decarbonisation and enhanced product portfolios. For example, CCU can support the production of products such as methanol and syngas from captured CO_2, while CCS reduces the embodied CO_2 in the produced ammonia. However, there has been a gap in the literature investigating the environmental and economic value of integrating hydrogen and natural gas supply chains along with CCUS. Moreover, further knowledge of the operational flexibility of different processes (i.e., upper and lower bands) is essential for making informed decisions when optimising integrated supply chains.

Funding: This research is supported by Hamad Bin Khalifa University, a member of the Qatar Foundation.

Data Availability Statement: Data will be made available on request.

Acknowledgments: The authors acknowledge the College of Science and Engineering at Hamad Bin Khalifa University, a member of the Qatar Foundation, for supporting this research.

Conflicts of Interest: The authors declare no conflict of interest.

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