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A systematic review of modelling methods for studying the integration of hydrogen into energy systems

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ABSTRACT

Hydrogen could be generated, stored, transported, and consumed in various ways, making it a promising solution to carbon emission reduction. However, key questions still remain in how hydrogen could be appropriately integrated into energy systems over time while coupling with different sectors. This has led to model-based studies of the whole system value of hydrogen in future energy systems, and the near-term actions and long-term strategies required to facilitate the transition to low-carbon energy systems with hydrogen. In this paper, a systematic review of the existing model-based studies in this area was conducted. A summary of hydrogen applications in energy systems was made, with statistics of publications and projects revealing the fast-growing interest in hydrogen in the past several years. The modelling methods used to investigate the system integration of hydrogen was summarised from over 130 publications. This paper also identified the gaps in modelling capability and potential future research topics: 1) balance between the resolution and modelling complexity, 2) inclusion of all uncertain factors of hydrogen pathways, 3) advancement of modelling approaches to address the chicken-and-egg dilemma of hydrogen economy development, and 4) a more detailed and comprehensive coverage of various interactions between hydrogen and other sectors.

Abbreviations and acronyms

Abbreviation or acronym	Definition
AEM	Anion exchange membrane
AEMFC	Anion exchange membrane fuel cell
CCGT	Combined-cycle gas turbine
CCS	Carbon capture and storage
CCUS	Carbon capture, utilisation, and storage
CHP	Combined heat and power
EPS	Electric power system
ESM	Energy system model
FC	Fuel cell
FCEV	Fuel cell electric vehicle
H2-NG	Hydrogen-natural gas
HRS	Hydrogen refuelling station
LCOH	Levelised cost of hydrogen
MILP	Mixed integer linear programming
NGS	Natural gas system
OCGT	Open cycle gas turbine
PDE	Partial differential equation
PEM	Proton exchange membrane electrolyser
PEMFC	Proton exchange membrane fuel cell
RES	Renewable energy source
SMR	Steam methane reforming
SOEC	Solid oxide electrolyser cell
SOFC	Solid oxide fuel cell

(*continued on next column*)

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1. Introduction

1.1. Background

In the context of achieving carbon neutrality, the call for clean fuel alternatives to support the decarbonisation of energy systems has been growing stronger. Among many potential alternatives, hydrogen is expected to play a crucial role in the energy transition because of its potential to reduce emissions in the "hard-to-abate" sectors, such as transport, heat, and industry [1]. Furthermore, it's also expected to offer energy storage capacity to accommodate the intermittent renewable energy in the electric power system. Many countries and international organisations have issued policy papers [2–4] that have set goals and timelines for hydrogen infrastructure scale-up and market development.

Hydrogen first gained attention in the 1970s, as the 1970s energy crisis raised the interest in alternatives to petroleum fuels [5,6]. International collaborations were then launched to investigate and facilitate the production and use of hydrogen [7]. The rising concerns about climate change in the 1990s and the energy crisis in the 2000s expedited the development of hydrogen and fuel cells, particularly their applications in the transport sector [6,8]. However, until the mid-2010s, hydrogen's economic competitiveness against other options had been compromised due to its high production and investment costs. Lithium-ion battery cost reductions through the development of battery electric vehicles have decreased interest in hydrogen fuel cell cars [6]. In addition, the "chicken and egg" problem[1] hindered the development of the hydrogen economy [2,9]. However, since the signing of the Paris Agreement, with recent concerns of energy security, low-carbon hydrogen development is currently gaining unprecedented momentum [4,10].

Hydrogen can be produced from a variety of feedstocks by various methods, transported and stored in different forms, and consumed by numerous technologies to provide a range of energy services. It can support renewable electricity generation deployment by accommodating surplus renewable energy generation and providing certain grid services. Some hydrogen end-users, such as fuel cell electric vehicles (FCEVs) and hydrogen boilers also compete with electrification. Hydrogen is expected to help decarbonise some hard-to-abate applications where direct electrification is not feasible or other decarbonisation options are limited or costly, such as high-temperature heat, heavy goods transport, aviation, and steel production [1]. This means that both the production and use of hydrogen are closely linked with the other energy vectors.

In the many countries targeting net zero by 2050, timely actions are needed if hydrogen is to have a substantial role. This requires all stakeholders to possess a comprehensive understanding of the possible outcomes of potential hydrogen pathways and investment strategies, within the context of integrating hydrogen into the whole energy system. These considerations can be categorised into several research questions to be addressed: when, where, and which type of hydrogen infrastructure is to be integrated into the energy systems, and at what scale; how hydrogen-relevant stakeholders will interact with each other in terms of investment decision making and market trading; will hydrogen be economically, technologically and environmentally viable in future energy scenarios, and how will it contribute to the carbon emission mitigation across multiple sectors. These questions have received significant attention from both the academia and the industry, prompting a great number of model-based studies, such as optimisation models, simulation models, agent-based models, system dynamics models and more, to address them.

1.2. Previous reviews

1.2.1. Review papers examining the use of hydrogen across the economy

The status and outlook of the hydrogen sector have been the subject of extensive reviews, such as papers [11–14]. Some reviews have extended the review scope to hydrogen applications in other sectors including electricity, gas, heat, and transport. These reviews compared the technologies and applications linking hydrogen with other sectors, with discussions from different perspectives (as shown in Table 1). Though these reviews identified the key challenges to upscale the hydrogen use across the economy with some of them discussing the research progress in the field, none of them specifically focused on model-based studies.

1.2.2. Review papers focusing on the model-based analysis of the system integration of hydrogen

There have been many review papers examining energy systems models (ESMs) with multiple energy vectors, but review papers targeting the modelling formulation for the system integration of hydrogen are limited. There have been surveys of ESMs [32–35], comparisons of the various paradigms of ESMs and their modelling features [36,37], and discussions of specific modelling attributes [38,39]. However, these review papers covered a broad range of ESMs and did not specifically examine the models accounting for the hydrogen vector. Some of the review papers investigated the energy system models that include some hydrogen technologies, or the whole hydrogen sector. But these reviews only examined hydrogen's integration in certain sectors or certain types of energy system models, as summarised in Table 2. Reviews [40–45] examined the microgrid-level ESMs and did not cover regional or national level energy systems that reveal the role of hydrogen in large-scale energy systems. Some other reviews looked into hydrogen's applications in smart grids [46], residential buildings [47], or natural gas systems [22], which could only reveal partial sectoral coupling between other sectors. Some reviews examined the energy system models that studied specific research questions, such as system expansion planning [15] and market operation [48], so only a specific range of papers were reviewed. Some review papers have examined large-scale ESMs (regional and national levels) that are capable of investigating hydrogen's emergence within low-carbon pathways, but the detailed discussion of model formulation was still limited. A project report [49] compared the inputs and outputs of energy systems and the representations of hydrogen technologies in energy systems. But the review scope was within a range of TIMES models only. One recent paper [50] conducted a taxonomy study on the hydrogen energy system models. However, it focused more on the comparison of different model archetypes, with limited discussion of how different models were formulated to tackle hydrogen-related research questions.

None of the aforementioned review papers comprehensively covered the full spectrum of model types while summarising the detailed modelling of the hydrogen value chain, and successfully linked the existing modelling paradigms to the key research questions pertaining to the system integration of hydrogen. Consequently, no consensus has been achieved on the model approaches to tackle the challenges under this topic, and the modelling capabilities gaps of existing studies. Therefore, there is a need for a comprehensive review of all types of ESMs investigating the system integration of hydrogen and targeting the key research questions, while discussing the modelling formulation in detail.

[1] Currently, hydrogen supply and demand levels remain relatively low, accompanied by a limited scale of hydrogen infrastructure. The cost of hydrogen is still relatively high and this hinders the growth of demand. In turn, the lack of demand discourages investment in hydrogen infrastructure, which potentially impedes the cost reduction. The high infrastructure cost is expected to decrease once hydrogen demand increases.

Table 1
The sectoral coverage and scope of review papers regarding hydrogen applications in the whole energy system.

Previous reviews	Sectoral coverage					Review scopes				
	Electricity	Gas	Heat	Transport	Industry	Technical characteristics	Economic assessment	Environmental assessment	Policy & regulation	Projection of future development
[15]	✓					✓	✓			
[16]	✓					✓	✓	✓		
[17,18]	✓					✓	✓			✓
[19]	✓					✓	✓			✓
[20]	✓					✓	✓		✓	✓
[21]	✓			✓		✓	✓	✓	✓	✓
[22]		✓				✓	✓	✓		✓
[23,24]				✓		✓	✓	✓		✓
[25–27]				✓		✓	✓	✓	✓	✓
[28]	✓	✓				✓	✓	✓		
[13,29]	✓	✓	✓	✓		✓	✓	✓		✓
[30,31]	✓	✓	✓	✓	✓	✓	✓	✓		

1.3. Contribution and organisation of this paper

In line with the trend toward the system integration of hydrogen, more and more energy system models have been developed to answer the research questions related to hydrogen infrastructure expansion planning, stakeholder decision-making and evaluating hydrogen's impact on the whole energy system from economic, technical and environmental perspectives. To reveal how the energy system models have been developed to address these hydrogen-related research questions, and to identify the potential modelling capability gaps, this paper presents a systematic review of the modelling methods that have been used to study hydrogen's integration into energy systems. The main contributions of this paper are 1) a summary of hydrogen technologies linking hydrogen with other sectors, with statistics of publications and projects revealing the research trend in hydrogen system integration; 2) a summary of the representations of hydrogen technologies in energy system models and the interactions between different vectors and spatial and temporal scales, as well as the comparison of different types of models corresponding to various modelling goals; 3) discussions of the modelling capability gaps and future research questions related to modelling complexity, uncertainty in hydrogen pathways, the chicken-and-egg dilemma, and the interactions between hydrogen and other sectors.

The remainder of this paper is organised as follows. Section 2 summarises the features of hydrogen technologies with their interaction with the different sectors. Section 3 demonstrates the literature search and the screening procedures, as well as the statistics of relevant publications and projects. Section 4 reviews the modelling approaches that have been used to study the system integration of hydrogen in the energy system. Section 5 presents the gaps in the current modelling and suggests potential research topics. Finally, Section 6 concludes this paper.

2. Hydrogen techonologies in the energy system

There are multiple pathways for the supply, storage and consumption of hydrogen linking hydrogen with many other sectors (Fig. 1). This section presents some key hydrogen technologies that interact with the whole energy system.

2.1. Hydrogen production technologies

Almost all global hydrogen demand is currently satisfied by fossil-fuel based production, while low-carbon hydrogen production is still very low. The IEA's Global Hydrogen Review 2023 [51] showed that hydrogen production from fossil fuels with carbon capture, utilisation, and storage (CCUS) and from renewable electricity only accounted for 0.6 % and 0.1 % of the total generation, respectively. The rest of the hydrogen production came from natural gas without CCUS (62 %), coal (21 %), oil (0.5 %), and 16 % was produced as by-products at refineries. However, with strong policy and environmental drivers, low-emission hydrogen production is expected to increase substantially by the 2030s [52] (Table 3).

2.1.1. Steam methane reforming

Steam methane reforming (SMR) is a fossil-fuel based hydrogen production technology that consumes the methane in the natural gas and generates hydrogen using high-temperature steam. In 2022, SMR accounted for 62.6 % of the global hydrogen production mix, and many new SMR projects with CCUS have been announced since 2021 [52]. In the UK, SMR with CCUS is expected to be the main production method through the 2020s, and it is hoped that its bulk supply will kick-start the hydrogen economy [2]. The energy efficiency of SMR with/without carbon capture and storage (CCS) is around 69 % and 76 %, respectively [53]. For each kilogram of hydrogen produced, the SMR without CCS consumes 21.90 kg of water and 0.31 kWh of electricity, with the carbon emission of 9.26 kg, while the SMR with CCS consumes 23.70 kg of water and 1.11 kWh of electricity, with the carbon emission of 1.03 kg [54]. Natural gas accounts for around 70 % of the levelized cost of hydrogen production via SMR [55]. LCOH via SMR in Europe increased sharply in 2022 due to the shortage of natural gas supply, and gradually fell with the rebalancing of natural gas supply in 2023. By IEA's estimation, the LCOH of SMR with/without CCS were around € 2.3 and €2.7 per H_2 production in Northwest Europe [55].

2.1.2. Water electrolysis

Electrolysis is used to split water into hydrogen and oxygen using electricity or heat, and is expected to be one of the main hydrogen production methods by 2030. There are four main types of electrolysers: alkaline water electrolyser, proton exchange membrane (PEM) electrolyser, solid oxide electrolyser cell (SOEC), and anion exchange membrane (AEM) electrolyser. Electrolysers are viewed as flexible electricity consumers in the power grid. They can provide demand-side flexibility in the power grid, making use of the excess electricity generation from renewable energy source (RES) units such as wind farms, photovoltaic power plants, and geothermal sites, converting the surplus RES production to hydrogen for storage and electricity generation at a later time [56]. It is also possible for electrolysers to provide ancillary services, such as frequency support to the power grid [57–60]. Projects such as Demo4Grid [61] and QualyGridS [62] are working on the feasibility analysis or standardisation of electrolysers providing electrical grid services.

Although electrolysis is regarded as one of the core components of the hydrogen economy, the portion of electrolysis-based hydrogen production is still very low (0.1 % in 2022) [51] and has a higher cost than other hydrogen production options [63]. The insufficient demand

Table 2
The contents of review papers examining the energy system models with the system integration of hydrogen.

Previous reviews	Energy system type	H2 technology	Model review contents
[40]	Microgrid	Multiple hydrogen technologies	A summary of optimisation model formulation of micro-grid energy management and planning
[41]	Microgrid	electrolyser	A summary of mathematical modelling of HRES-H2 components and optimisation techniques
[42]	Microgrid	Multiple hydrogen technologies	A summary of micro-grid structure and control strategy
[43]	Microgrid	Fuel Cell	A comparison of non-isolated DC-DC converter topology for fuel cell applications, a summary of mathematical modelling
[44]	Microgrid	Multiple hydrogen technologies	A summary of system components, and a summary of models for system component sizing and component integration
[45]	Microgrid	Multiple hydrogen technologies	A summary of microgrid energy management models
[46]	Smart grid	Multiple hydrogen technologies	A summary of AI applications in smart grids with hydrogen integration, discussions of AI models and research challenges
[47]	Residential building	Multiple hydrogen technologies	A summary of modelling, simulation and optimisation of solar and hydrogen energy-based systems for residential applications
[15]	Various types of energy systems engaged with market activities	Electrolyser	A summary of electrolysers technical parameters and optimisation models
[22]	Natural gas system	Multiple hydrogen technologies	A technology overview, a summary of natural gas supply chain optimisation considering hydrogen integration
[48]	Regional/national energy system	Multiple hydrogen technologies	A summary of modelling formulation and characteristics of expansion planning models of integrated power, natural gas and hydrogen systems
[49]	Energy system models from the ETSAP community	Multiple hydrogen technologies	A summary of hydrogen technology coverage and model input & output, discussion of hydrogen technology representation in models
[50]	Various types of energy systems from 29 reviews	Multiple hydrogen technologies	A taxonomy of models investigating hydrogen energy systems, with a summary of model archetypes and research challenges

for low-carbon hydrogen has led to a lack of investors to deploy the infrastructure at a large enough scale to reduce cost, which positions RES-powered hydrogen as a costly option with relatively low market demands [64]. In terms of providing ancillary services to power systems, both alkaline electrolysers and PEM electrolysers are regarded as potential options for providing grid services, but the stack capacity of both technologies are not big enough to meet the minimum capacity requirements of some grid services. These two technologies have different operating characteristics and technical limitations. The alkaline electrolyser is a mature technology and also the cheapest electrolysis option, but its performance deteriorates during part-load operation, which makes the alkaline electrolysers powered by intermittent RES less competitive when compared with PEM electrolysers [65]. Meanwhile, PEM electrolyser is suitable for integration with RES power sources and ancillary service provision due to its quick start-up time [66] but uses costly raw materials during manufacture, which makes it difficult to lower the cost of PEM hydrogen production [67]. Finally, the efficiency of PEM electrolyser and alkaline electrolyser ranges from 50 to 68 %, AEM electrolyser's efficiency ranges from 52 % to 67 %, whereas SOEC could achieve 85 % efficiency [67]. However, the capacity factor (the ratio between actual hydrogen production and production at full capacity) for green hydrogen production is usually less than 60 % [51]. The LCOH of electrolytic hydrogen still remains high due to high capital cost and labour cost [51].

2.1.3. *Other hydrogen production technologies*

Autothermal Reforming (ATR) is a chemical process in which partial oxidation and steam reforming of hydrocarbon (such as natural gas) produce hydrogen and carbon monoxide that is then used to convert more water steam into hydrogen. ATR can operate with a lower supply of external heat than SMR but with a lower efficiency of around 60–75 % [68]. Currently ATR's technology readiness is still lower than electrolysis and SMR [51].

Methane pyrolysis technology uses heat (around 900 °C) to split methane into hydrogen and solid carbon. It can produce hydrogen with 75 % reduction in GHG emissions compared to the SMR process [69]. Additionally, the solid carbon byproduct can potentially generate additional revenues, which substantially reduce the LCOH of methane pyrolysis [55].

Biomass gasification is a thermochemical process that converts biomass materials into a combustible gas mixture known as "producer gas" or "syngas" (synthesis gas). Biomass gasification is considered a renewable energy technology as it utilises organic materials that can be replenished through sustainable forestry and agriculture practices, and the residual tar and ash can often be used as a soil conditioner, contributing to the sustainability of the process. Biomass gasification proposes an efficiency of around 48 % and hydrogen yield for biomass gasification is around 0.8 $Nm^3/kg_{biomass}$ [70].

Apart from the aforementioned hydrogen production technologies, there are also other technologies but with lower technology readiness levels, such as anaerobic digestion, chemical looping, thermochemical water splitting, electrolysis using waste water or sea water, and so on. These technologies are recognised by IEA as technology readiness level under 6 (only small or large prototype functional) [51].

2.2. *Hydrogen storage and transportation*

2.2.1. *Hydrogen storage*

Hydrogen can be stored in two forms. Physical storage includes gaseous hydrogen storage, liquid hydrogen storage and cryo-compressed hydrogen storage. Material-based storage is mainly in solid form via hydrides, with less concern about storage pressure and leakage [74]. Currently, physical storage in gas/liquid form through hydrogen vessels and in gas form through underground storage facilities are the most discussed options, and are expected to help the energy system sustain supply and demand balance in both the short and long term, as well as provide energy supply security. Storage tanks could reach MWh-level storage with a fast charge/discharge rate and would usually operate with a pressure range between 350 and 700 bar [75]. These could be used by industry plants and hydrogen refuelling stations to help maintain the on-site supply and demand balance. Underground hydrogen storage (UHS) technologies, such as salt caverns or depleted

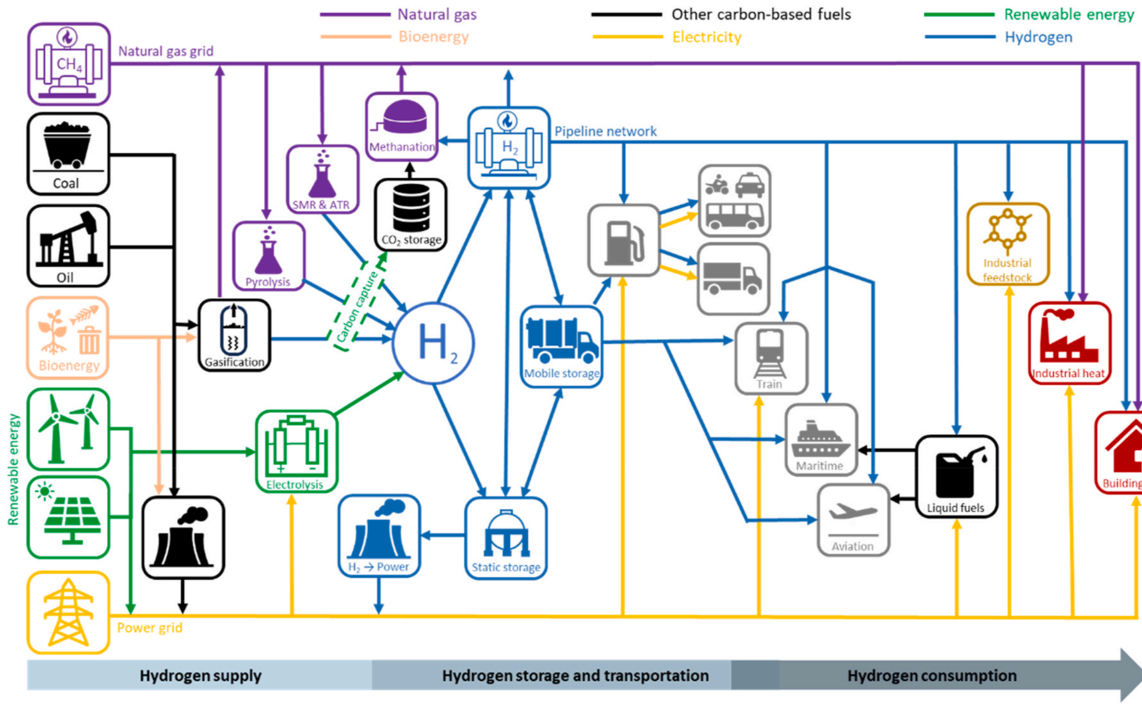


Fig. 1. Coupling the hydrogen sector with other sectors.

Table 3
Comparison of levelised cost of hydrogen, efficiency, emission and feedstock consumption of mainstream hydrogen production technologies [54,67,68,70–73].

Technology	Levelised cost of hydrogen (€/kg H_2)[a]	Energy efficiency	CO2 emission per kg H_2	Feedstock consumption per kg H_2
SMR	2.2–5.3 (without CCS); 2.9–4.9 (with CCS)	69 % (without CCS); 76 % (with CCS)	9.26 kg (without CCS); 1.03 kg (with CCS)	21.9 kg water, 0.31 kWh electricity, 3.36 kg natural gas (without CCS); 23.7 kg water, 1.11 kWh electricity, 3.76 kg natural gas (with CCS)
Electrolysis	8–10.2 (low-temperature electrolysis); 5.7–9.5 (high-temperature electrolysis)	Alkaline: 50–68 %; PEM: 50–68 %; SOEC: 75–85 %; AEM: 52–67 %	0 kg	10 kg water, 52.4 kWh electricity
ATR	2.7–4.9 (with CCS)	60–75 %	0.62 kg (with CCS)	3 kg natural gas
Methane pyrolysis	0.8–5.9	58 %	2.5 kg	8.08 kg water, 4.86 kg methane
Biomass gasification	4.3–5.8 (without CCS)	48 %	32.84 kg (without CCS)	47.48 kg water, 3.58 kWh electricity, 36.28 kg biomass feedstock (without CCS)

[a] The data of levelised cost of hydrogen production was retrieved from Ref. [72], where a series of price and technical specification assumptions were used.

gas fields, have larger storage volumes (usually over 500,000 m^3 [76, 77]) and lower pressure levels (usually within 200 bar [76]). These storage facilities have slower hydrogen release rates, which makes them more suitable for satisfying seasonal hydrogen demand swings. Currently, there are operating salt cavern storage sites in the United States, UK and Germany. In addition, decommissioned natural gas storage caverns are also a suitable option for hydrogen storage [78]. However, there are no established facilities in depleted gas fields, and further investigation is required for hydrogen storage capability and the competing relationship to CO_2 storage. The potential for underground storage is highly dependent on the geographical conditions, and the lead times for newly built infrastructure are considerable (e.g., five to ten years) [52]. As for the technical aspect, potential risks and challenges of UHS lie in the geochemical reactions, such as biochemical reaction, hydrogen fingering, diffusivity, and leakage [79]. Additionally, cushion gas is required in salt caverns, depleted gas fields and aquifers to sustain the pressure during injection and withdrawal stages [77], which usually takes up 33 %, 50 % and 80 % of the total volume of these three storage facilities respectively [80].

2.2.2. *Hydrogen transportation*

Hydrogen can be transported in various ways, such as pipelines, trucks, and ships, ensuring that hydrogen can reach a wide range of end users [2]. The costs of these approaches vary with the volume and distance of hydrogen to be transported, and pipelines are generally the most economical option when the transportation distance is within around 7500 km [81]. Apart from transporting hydrogen in the gaseous form, pipeline networks also store a certain amount of hydrogen within the pipelines, known as the 'linepack', which can be adjusted to provide flexibility. In GB, the within-day linepack of the National Transmission System (for natural gas) ranges between 3000 GWh and 4500 GWh [82]. In Europe, the construction of hydrogen pipelines will start from several major pipes connecting the existing hydrogen generation to industrial hydrogen demand. It will then gradually stretch to users in other sectors such as electricity, transport and heating [83,84]. The expansion of the pipeline infrastructure could be achieved by two routes: repurposing existing natural gas networks (slowing increasing the hydrogen injection); and the construction of new hydrogen assets (transporting pure hydrogen from the start). Given that repurposing is more cost-effective than new built, and with lower environmental impact [84], a large portion of the future hydrogen transportation backbone is planned to be based on repurposed natural gas pipelines [83,84]. In the Project Union led by National Grid, the energy networks operator in the UK, the hydrogen-natural gas (N2-NG) mixture will first be transported by repurposed natural gas pipelines, with a gradual increase of the hydrogen ratio to 100 % by around 2050 [84].

There are still a number of technical issues to be addressed in the pipeline transportation of hydrogen or H2-NG blend. Some countries, such as the UK, plan to transport the H2-NG blend in repurposed natural gas pipelines with a gradually increasing hydrogen ratio [85]. This requires further testing and investigation into the safety of hydrogen transportation in existing gas infrastructure, especially the hydrogen embrittlement issue of compressors, pipelines, welded joints and valves [86]. In addition, because some consumers are not hydrogen-ready or have specific requirements for hydrogen ratio, feasibility analyses of deblending technologies are being conducted to evaluate the feasibility of adopting gas separation facilities while managing the impact on network operation and market [87]. Because hydrogen has a lower energy density than natural gas, the volume of pure hydrogen or H2-NG mixture would be substantially greater than the natural gas with an equivalent amount of energy, which leads to higher pressure levels throughout the whole network. This requires transmission systems to be tested to examine their capability at higher pressure and to evolve by various solutions such as protective coating throughout the network, increase in network operating pressure, adjustment of the control system, adapted materials' thickness and characteristics, or novel gas detection and metering devices to deal with the lower density and viscosity of the blended gas [88]. In addition, the linepack in the hydrogen network is likely to be smaller, which may compromise the hydrogen network's ability to withstand demand and supply interruptions. This leads to the need for extra compressor capacity and a more complicated compression strategy to sustain the pressure level and linepack level of the pipeline network [80,88].

Trucks (e.g., liquid tank trucks and gaseous tube trailers) have been used to deliver hydrogen at the local level, supplying the demands of industry and the transport sector. They are more suitable to the current stage of hydrogen (i.e., low demand volumes from market, and clustering distribution of hydrogen suppliers and end users) than pipelines. Meanwhile, shipping is suitable for long distance transmission, supporting international trading. Hydrogen could be shipped in the form of liquefied hydrogen, ammonia, liquid organic hydrogen carrier, or synthetic hydrocarbon fuel [52].

Hydrogen refuelling stations (HRSs) are used to deliver hydrogen to hydrogen fuel cell vehicles. An HRS compresses and stores the hydrogen by high-pressure vessels and then quickly fills the FCEVs by hydrogen dispensers [89]. The location selection of hydrogen refuelling stations is determined by multiple factors, such as the hydrogen demand levels, the travelling patterns of FCEVs, the public acceptance, and safety requirements [90]. The number of refuelling stations experienced a rapid increase in the past five years and surpassed 1000 for the first time in 2022. Still the growth of HRSs is trapped by the hesitation of infrastructure investors due to the slow growth of FCEVs.

2.3. Hydrogen consumption

According to the IEA [51], consumption of hydrogen reached 95 Mt in 2022, mostly for industry usage (55 %) and refining (43 %). However, projections show that novel usage of hydrogen will rise over the next years. In the scenarios designed to achieve net zero in 2050, the 2030 hydrogen consumption is expected to reach 150 Mt, a 60 % increase driven by the growing industry usage, synfuels production, and power generation.

2.3.1. Industry

Almost all of the 95 Mt of hydrogen consumed in 2022 was used in refining or other industry applications [51]. 80 % of the hydrogen consumed by refineries is produced onsite by dedicated hydrogen production or as a by-product, while all industry-consumed hydrogen is produced from fossil fuels at the same location as where it is used [51]. The ratio of low-carbon hydrogen is still very low. Therefore, there is a need for industries to develop the production of green hydrogen and to ensure carbon storage throughout the whole process.

2.3.2. Transport

Hydrogen is expected to contribute to the replacement of fossil fuels or serve as a complement to electrification in the transport sector. Hydrogen applications such as buses, trains and heavy goods vehicles (HGVs) are expected to help reduce carbon emission in road transport, although for now, only some studies and trials have been conducted for non-road transport (rail, shipping, and aviation) [51]. Fuel cells are particularly suitable for HGVs thanks to the shorter refuelling time and long travelling distance compared with electric vehicles, recognised as an important decarbonisation approach by many countries or regions [3,91,92].

The application of hydrogen in the transport sector is still at an early stage. Hydrogen only takes up 0.003 % of the total transport energy [52], and most of the road transport trials are within one city or a multi-city region. The uptake of FCEVs was still low— around 72,000 in 2022 compared with 18 million battery electric vehicles [93]. The scale-up of hydrogen-powered vehicles relies on the expansion of hydrogen refuelling stations, storage facilities, and hydrogen distribution infrastructure. Many projects working on hydrogen-powered transport (especially on buses [94,95] and HGVs [96,97]) and hydrogen refuelling infrastructure [98] have been announced or launched to scale-up the utilisation of hydrogen in the transport sector.

Apart from the direct use of hydrogen in transport, other solutions based on hydrogen are being explored for maritime transport, such as ammonia and methanol. Green methanol comes from the reaction of hydrogen with water vapour and carbon dioxide that can come from biomass or direct air capture. On the other hand, ammonia is composed of nitrogen and hydrogen, and does not require any carbon source for its production as a fuel for shipping. However, the use of ammonia is not legal everywhere yet, which hinders the technology.

2.3.3. Power generation

Hydrogen could be utilised for power generation via fuel cells and turbines [99], although both approaches are still adopted in small-scale energy systems. A fuel cell (FC) converts the chemical energy of hydrogen into electricity. The mainstream types of fuel cells are proton exchange membrane fuel cells (PEMFC), alkaline fuel cells, solid oxide fuel cells (SOFC), and anion exchange membrane fuel cells (AEMFC). Stationary fuel cells could be regarded as a flexible source of electricity in integrated energy systems [100], especially in electricity distribution networks and microgrids [101]. So far, the lifespan of stationary fuel cells is usually 12 years with a generation capacity within 1 MW, while the industry is making efforts to improve the lifespan and increase the generation capacity beyond the MW level [102]. In addition, most fuel cells require high purity levels of hydrogen infeed with a low tolerance of contaminants [99]. And the typical electrical efficiency for fuel cells is about 60 % [103], whereas combined heat and power (CHP) systems can achieve overall efficiencies of 65–85 % [104].

Turbines (open cycle gas turbines, OCGTs, and combined-cycle gas turbines, CCGTs) can be powered by either pure hydrogen or H2-NG blend. They could help the system to meet short and long-term load peaks thanks to their flexible operation (Department for Energy Security and Net Zero, 2021). One of the challenges comes from nitrogen oxide emission during the high-temperature combustion process [105]. Another issue is the high cost of OCGT and CCGT due to the low load factor (the ratio of electricity produced to the generation capacity) [106]. With the low load factor, the levelised cost of electricity is very sensitive to the initial capital investment cost, therefore retrofitting the existing natural gas plants is more cost-effective than building new hydrogen power plants [106]. Still, retrofitted plants need new accessories to accommodate the high blend of hydrogen [107].

2.3.4. Heat supply

Hydrogen is a potential clean fuel for heat supply in industry and the building sector. For industrial heating, hydrogen, or H2-NG blend, could be used to fuel steam boilers, CHP units or furnaces. Although hydrogen for industrial heating is a promising option to decarbonise the industry sector, as of 2022 no hydrogen production had been dedicated to this application [99]. Hydrogen-ready boilers [108], CHP units with PEMFCs [109], and SOFCs [110], are potential options for the heat supply in residential and commercial buildings. The hydrogen demand for building heating is relatively low or unclear in the hydrogen roadmaps of many countries. Though the efficiency of hydrogen boilers is around 80 %, the electricity-hydrogen-heat efficiency of from electrolysers to hydrogen boilers is lower than heat pumps [111]. The economic viability of hydrogen for heating in both industry and building sectors highly depends on the price of green hydrogen [111]. Further evidence of the economic, technical, safety, and environmental aspects are still required [2,112].

3. Review methodology and statistics

3.1. Methodology

This literature review was conducted with the search, appraisal, synthesis, and analysis (SALSA) framework [113].

3.1.1. Search

The literature search process aims to identify research articles in academic literature databases or the non-academic reports from companies and other institutions that have conducted model-based studies related to the topic of “hydrogen integration in energy systems”. Two databases were used in the search for academic articles: the Web of Science and Scopus, which cover a wide variety of publishers including IEEE, Elsevier Science Ltd, Wiley, Springer, MDPI, and Frontiers. The following combination of keywords was used in the literature search: (“integrated energy system” OR “hybrid energy system” OR “market”) AND (“hydrogen” OR “power-to-gas” OR “electrolyzer” OR “fuel cell”). The literature search was carried out in June 2023, and the time range of the search was set as 2012 to 2022.

To identify non-academic publications, an additional search was conducted on the websites of government departments, research laboratories, industry alliances, utility companies, energy consultancy companies and other relevant organisations. The search process was mainly carried out in the “publication” or “document” list of these websites to identify relevant documents and reports. In addition, information about the related projects undertaken or managed by these organisations was also retrieved from project reports and other databases.

3.1.2. Appraisal

The appraisal process identified the relevant studies to be reviewed. This was conducted in compliance with the PRISMA 2020 flowchart [114], which consists of three parts: the “identification” record presenting the literature identified during search; the “screening” record of the literature excluded during each round of screening; and the “inclusion” record showing the number of studies included in the literature review.

The reference files of all the papers 7933 academic papers and 20 non-academic reports that have been collected from the initial search were first input into the automatic literature management software Mendeley, and the duplicate records of 3367 academic papers were removed. Both academic and non-academic papers were then screened. For academic papers, the titles or abstracts/overviews of 4566 articles were examined to check their relevance to the topic during the initial selection process. 4300 articles focusing on hydrogen-related chemical reactions or single hydrogen-related technologies were excluded during this process. The retrieval of the full-text files was then conducted for the remaining articles (266 papers). With one irretrievable paper excluded, 265 papers remained to be further evaluated in the third round of selection. 154 papers were further excluded due to one of the following reasons: (i) hydrogen is used for methanation only and the hydrogen vector does not interact with other vectors; (ii) focusing on specific hydrogen technologies with little consideration of their system integration; (iii) hydrogen technologies are integrated into small-size (building-level, community-level) or stand-alone energy systems; or, (iv) no models or modelling approaches were used in the studies.

For the non-academic publications, all of the documents were retrieved successfully and then evaluated, and 14 papers were excluded for the last three reasons above. The snowballing method [115] was then applied to find additional documents that are relevant to the review topic but were not identified during the literature search. From the snowballing method and the recommendation from coauthors, 15 more journal articles were added. Finally, 132 articles were reviewed. The number of papers included/excluded during each stage was recorded in Fig. 2.

3.1.3. Synthesis and analysis

The hydrogen technologies and other vectors that have been considered in the models, and the components or infrastructure through which hydrogen technologies interact with other vectors were summarised from the final selected articles. The details of model formulation, including the parameters, equations or constraints that representing represent the operating characteristics of hydrogen technologies, the model paradigms (optimisation, simulation, equilibrium and so on), the spatial and temporal scales and resolutions, the energy scenarios, and solving methods were also extracted from these articles. Based on this information, the key characteristics of the models used for studying the systems integration of hydrogen were presented and compared in Section 4, with a description of the research gaps and potential research topics in Section 5.

3.2. Statistics of publications and projects

3.2.1. Publications

126 journal articles from 32 journals were shortlisted. Among them, four journals are the main sources of shortlisted journal articles: International Journal of Hydrogen Energy (38), Applied Energy (16), Energy (10) and Energies (10). Six non-academic publications were shortlisted, which demonstrated the modelling of energy systems with different sectoral and geographical coverages. These six publications were released respectively by Aurora [116], National Grid ESO [106], the Department for Business Energy & Industrial Strategy [117], IRNEA [81], NREL [118], and the Carbon Trust [119].

A brief summary of the yearly publication number, the hydrogen technologies and sectors included by the publications, and the geographical coverage of case studies have been made as shown in Figs. 3–6. Fig. 3 presents the number of publications released between 2012 and 2022. The number grew slowly until 2020 and experienced a steep rise since then. This shows the growing interest in the system integration of hydrogen, possibly in response to the net-zero agenda proposed by many countries.

Fig. 4 demonstrates the distribution of publications with different sectoral coverage. Approximately 32 % of the existing publications focused solely on the interaction of hydrogen with one single sector (most are studies targeting electrolysers and FCEVs) while around one-third of the publications covered the electricity sector with another sector. Notably, less than one third of publications accounted for hydrogen’s interaction with more than three sectors. As for the summary of hydrogen technology coverage shown by Fig. 5, different technologies were grouped into three types: hydrogen production, transportation &

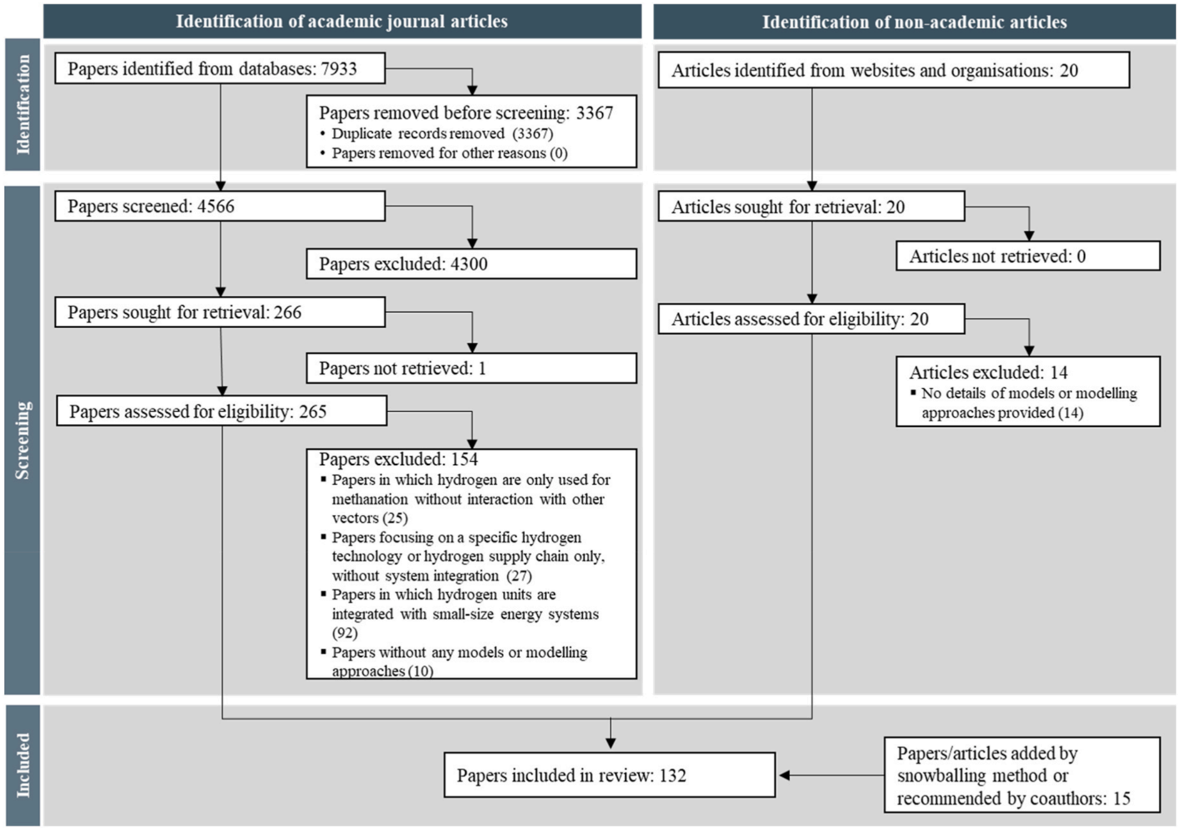


Fig. 2. The number of publications involved in the PRISMA procedures.

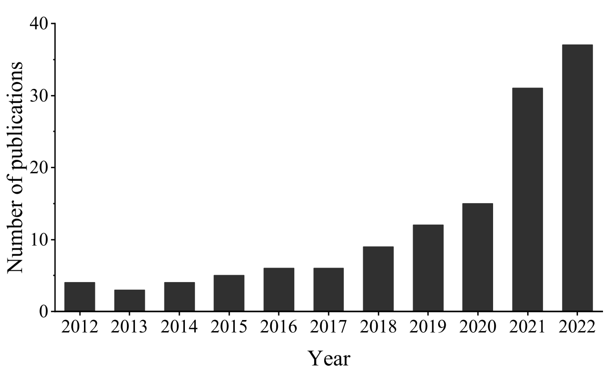


Fig. 3. The number of selected publications related to the topic "hydrogen's integration in the whole energy system" published between 2012 and 2022.

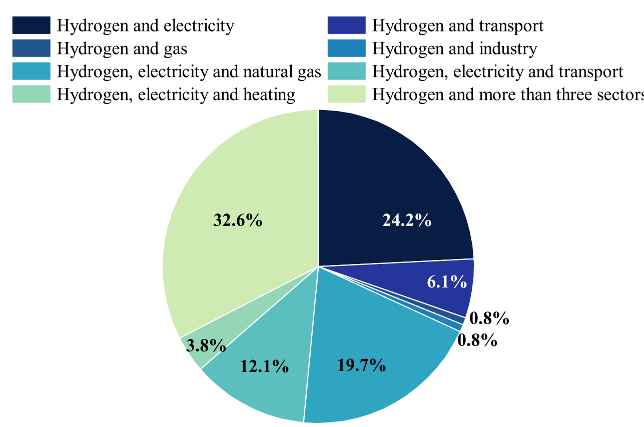


Fig. 4. The sector coverage of the existing publications.

storage, and end-use. 27.5 % of publications investigated only one type of technology. Approximately 24 % of the publications accounted for two types. Nearly half of the studies covered all three parts of the hydrogen value chain.

Fig. 6 shows the number of publications with case studies targeting specific geographical ranges. European countries, especially Germany and the UK, are the most popular objects to the existing studies. This could be linked to the proactive strategies of hydrogen economy development in Europe, and also corresponds to the ongoing projects of infrastructure expansion. Apart from Europe, multiple studies have been conducted targeting countries in North America and Asia.

3.2.2. Projects

The systems integration of hydrogen technologies has received increasing interest from both academia and industry. Fig. 7 presents the number of projects in the UK and the European Economic Area that are hydrogen-related or specifically working on the system integration of hydrogen. Information on the projects were collected from online databases, including the IEA hydrogen project database [120], ENTSO-G hydrogen project visualisation platform [121], ENTSO-G innovative project platform [122], HI-ACT expertise map [123], CORDIS database (HORIZON 2020 and HORIZON Europe grants) [124] and EPSRC grant database [125]. The academic projects are identified as projects led by higher education establishments or research organisations, and the industrial projects are identified as projects led by industrial organisations. During the project search, hydrogen-related projects were defined as projects related to any part of the hydrogen value chain. The projects specifically focusing on the system integration of hydrogen were selected based on the criteria of whether the project investigates "the

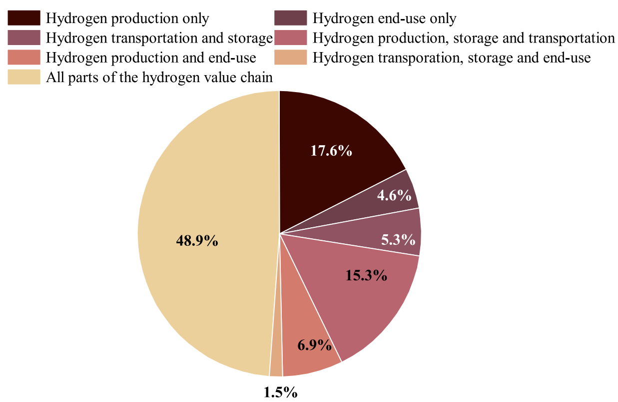


Fig. 5. The hydrogen technologies covered by the existing publications.

interaction of hydrogen technologies with other sectors".

It can be seen from Fig. 7 that Germany, the UK, Spain, France, Italy, and Netherlands have the most projects. The projects regarding the system integration of hydrogen are relatively low in number when compared with all the hydrogen-related projects. This is because some of hydrogen technologies are still low in technology readiness, with limited hydrogen demand. Therefore, a majority of the projects focus on the research and development of specific hydrogen technologies, with a limited number of projects investigating the system integration of hydrogen.

4. Review of the modelling approaches to studying the system integration of hydrogen

This section reviews modelling approaches for system integration of hydrogen. The focus is on: (1) formulation of the operating characteristics of hydrogen technologies; (2) modelling approaches accounting for the interactions across hydrogen and other energy vectors, and between multiple temporal/spatial scales; (3) modelling approaches for informing the infrastructure expansion plan, investment decision making and the assessment of the role of hydrogen in the whole energy system.

4.1. The formulation of the operating characteristics of hydrogen technologies

Many existing models, especially bottom-up optimisation models (models including detailed description of technologies [126]) and short-term simulation models, considered the operation details of part or all activities of the hydrogen value chain. The modelling of operating characteristics in the shortlisted literatures are as below.

4.1.1. Hydrogen production technologies

4.1.1.1. Electrolysers. To study how electrolysers would operate in the whole energy system and interact with other vectors by consuming input energy, the operation status of electrolysers has been modelled with reasonable levels of detail. For all types of electrolysers, the key feature is the energy conversion of electrolysers. The energy conversion equation is used by both simulation and optimisation models to link the consumption of input energy from the electricity vector (and potentially heat vector for some electrolysers) and the hydrogen production of the hydrogen vector.

Most studies assumed that when the electrolysers are active, they are operating near the nominal capacity and the energy conversion ratio is a known fixed value. Therefore, the hydrogen production is proportional to the electricity consumption. One study considered the variation of energy conversion ratio by curve-fitting the varying energy conversion ratio [127]. For SOECs, the thermal energy consumption and hydrogen production were linked by a linear energy conversion equation with a constant power-heat ratio [127]. As for the water consumption and oxygen production, one reference utilised linear equations to calculate the water consumption and oxygen production of electrolysers [128]. In most of the studies, the hydrogen generation rate was limited by setting an inequality constraint with the installed capacity. One study considered a temporarily overloaded condition of electrolysers, using a separate variable to represent the hydrogen production under overloaded condition [129]. For two studies that considered the flexibility provided by electrolysers [129,130], the fluctuation of electrolyser power consumption was constrained by adding inequality constraint limiting the ramping rates (input power change rate) of electrolysers.

Some studies assumed that hydrogen production is only involved in the power-hydrogen-methane route (i.e., used as the feedstock for methanation plants). These studies focused on power-to-gas units where

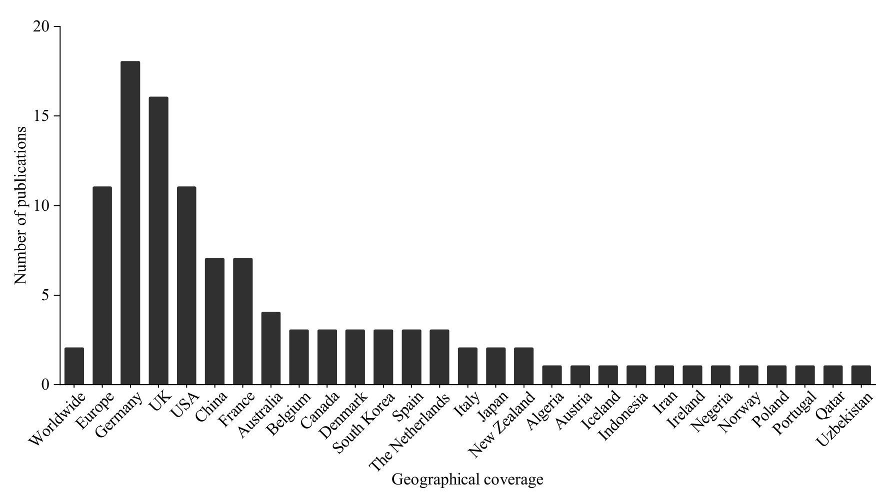
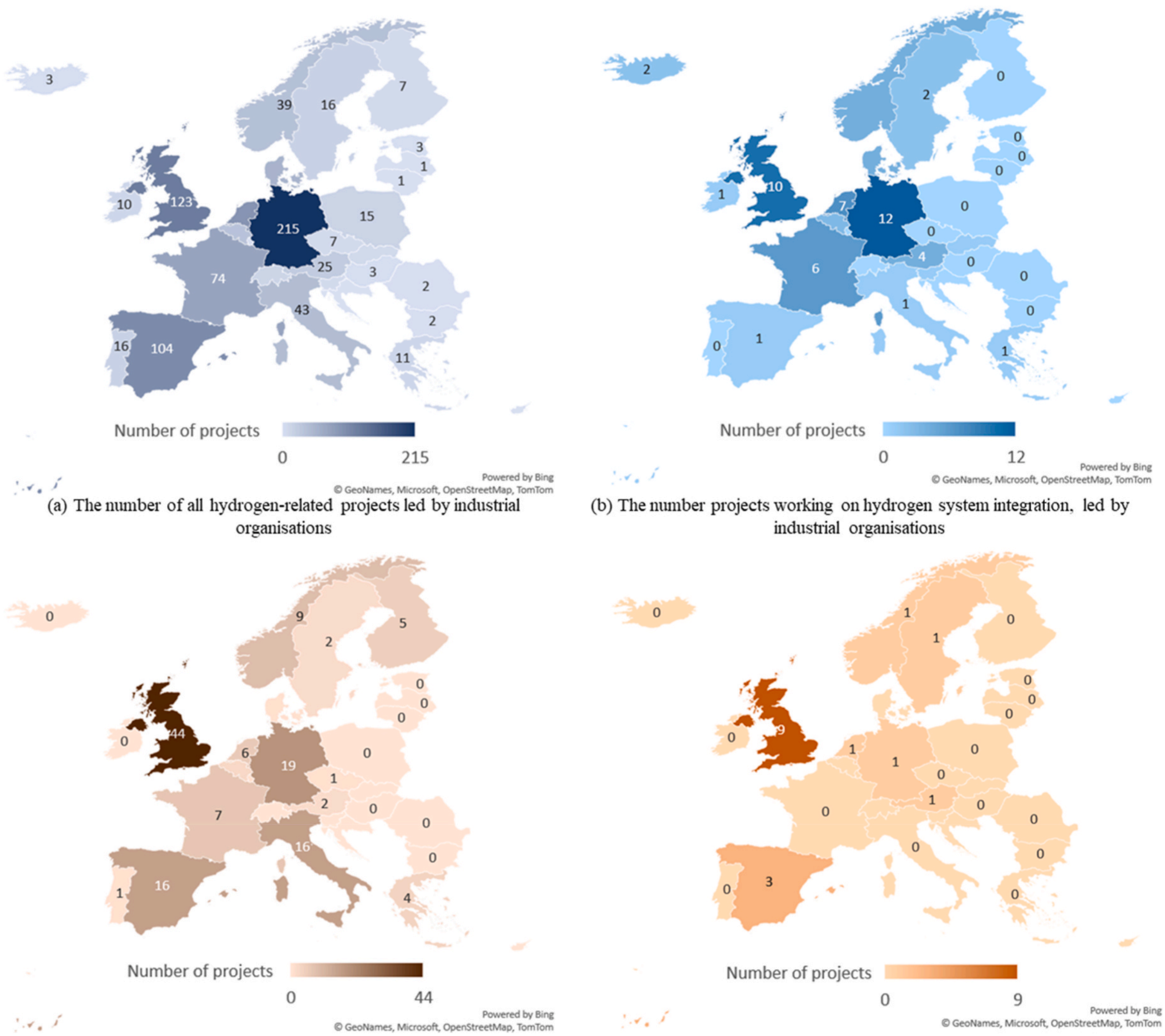


Fig. 6. The geographical coverage of the existing publications.
Most of the papers included by Fig. 6 are long-term models investigating the hydrogen economy development or the whole energy system development. The first two columns represent the number of publications with case studies including multiple countries around the world or within Europe, respectively. Apart from the first two columns, each column represents the number of publications that use case studies of a specific country, or a region within this country. The papers that utilised benchmark cases (such as IEEE power grid test cases) or the combination of these test cases as an integrated energy system, were excluded from the summary, as they provided limited analysis and conclusion to the specific country or region that these test cases originally derived from.



(a) The number of all hydrogen-related projects led by industrial organisations

(b) The number projects working on hydrogen system integration, led by industrial organisations

(c) The number of all hydrogen-related projects led by academic/research organisations

(d) The number projects working on hydrogen system integration, led by academic/research organisations

Fig. 7. The number of hydrogen-relative projects in the UK and EEA.
The information was collected from IEA hydrogen project database [120], ENTSO-G hydrogen project visualisation platform [121], ENTSO-G innovative project platform [122], HI-ACT expertise map [123], CORDIS database (HORIZON 2020 and HORIZON Europe grants) [124] and EPSRC grant database [125].

all the electrolyser-generated hydrogen is transformed into synthetic methane [131,132]. Other models considered multiple energy conversion paths simultaneously: while hydrogen could be the feedstock of the methanation, it could be directly injected into the natural gas network [133,134] or used for electricity generation [135]. Both options rely on a linear energy conversion equation to link methane production and hydrogen consumption.

4.1.1.2. Other hydrogen production technologies. In the existing literature, SMR plants were regarded as a continuously-running hydrogen source that consumes natural gas. SMR plants were modelled by two linear equations to link the natural gas consumption, the power consumption, and hydrogen production rate, based on known energy conversion coefficients [128]. For the studies accounting for the carbon emission of SMR plants, the carbon emission of SMRs with/without CCS was defined as a continuous variable and calculated by multiplying the natural gas consumption rate with the carbon intensity factor [136]. The SMR's carbon emission variables were either capped by inequality constraints or incorporated into the objective functions in the form of carbon emission penalty. Though SMR's energy efficiency decreases at part-load, this feature was not considered by the aforementioned works.

The biomass gasification is modelled in one reference [137], with the hydrogen production calculated based on the higher heating value of biomass, mass/water consumption, energy efficiency, parasitic factor of biomass gasification facility and power consumption. Other hydrogen production technologies were included by a few studies that targeted the whole hydrogen value chain [138–140] which did not account for their operating status or did not disclose the detailed modelling approaches.

4.1.2. Hydrogen storage technologies

The operation status of gaseous hydrogen storage facilities is modelled by the hydrogen level of the storage equipment and the amount of hydrogen charge or discharge per period. For hydrogen storage tanks or other relatively small-size facilities, the charging and discharging modes could be switched instantly, which are usually modelled by binary variables and inequality constraints in a 30-min or hourly time resolution. To ensure the repeatability of operation, some of the studies required the hydrogen storage levels at the first and last time periods of operation to stay the same [141,142]. Additional inequality constraints were used to control the pressure of the hydrogen tank [143].

For underground hydrogen storage sites, some works additionally considered the self-release and hydrogen loss due to the methanation of methanogenic bacteria [144]. The UHS storage level is bounded by inequality constraint similar as small-size storage facilities, with the minimal storage level were set based on the UHS's cushion gas requirements [141,144].

Some studies included liquid hydrogen storage and transportation in the models. The storage or release of hydrogen was represented in the form of hydrogen consumption or supply in the model [145], sometimes constrained by upper limit of liquid hydrogen storage capacity [146]. As hydrogen conditioning is needed for liquid hydrogen storage, the efficiency of hydrogen conditioning was considered in the assessment of liquid hydrogen as a hydrogen carrier [147].

4.1.3. Hydrogen transportation technologies

4.1.3.1. Pipeline transmission network. Pipeline network models are used to describe the topology, pressures, flow rates, temperatures and gas composition of hydrogen transmission networks. Many studies employed pipeline models to examine whether the existing or newly built infrastructure could handle the hydrogen injection or pure hydrogen transportation, and to account for the technical requirements in expansion planning or operation scheduling. The modelling of pipelines can be categorised into transient models [134,148–152] and steady-state models [133,142,153–155].

Transient models could reflect the variation of pressure, velocity, and density with time and distance, which are commonly used in short-term optimisation and simulation studies. Transient models (1-D isothermal pipe) are based on a set of partial differential equations (PDEs), including the continuity and momentum equations. The boundary conditions are usually set up based on the nodal pressure and mass flow rate. PDEs can be transformed into algebraic form by discretization based on space and time [134,148,149,152], or by Laplace transformation-based method [150,151]. The whole transmission network models consist of PDEs representing pipeline dynamics, the equations for non-pipe components, and the flow balance or energy balance equations. In simulation models, these equations could be converted to a set of linear equations and solved easily. For optimisation models, these constraints are usually simplified into linear forms as well.

Steady-state models come from the integral form of pipeline PDEs and assume the inlet and outlet flows of one pipe are equal. The steady-state models provide the relationship between pressure and mass flow rate in nonlinear algebraic equations. Among the reviewed works, the Weymouth Equation has been used most frequently. For optimisation models, the nonlinear constraints between gas flow rate and nodal pressures make the models nonlinear and nonconvex. This could be directly solved by certain solvers (e.g., IPOPT [155]) or by an intelligent search algorithm such as particle swarm optimisation algorithm [133]. In other studies, these nonlinear constraints are transformed into a linear form by piecewise linearisation method [142,153,156]. In simulation models, the steady-state gas flow equations are usually solved by the Newton Raphson method.

In terms of the linepack level of the network, one transient model-based study [148] modelled the linepack of the pipe based on average pressure. Two additional studies [133,141] calculated the linepack based on the linepack at previous time period and the pipeline inflow/outflow.

Most of the industrial reports and academic studies assumed that the injection of hydrogen in the natural gas networks will stay relatively low by the 2030s. Studies such as [133,142,150,155] set an upper limit on hydrogen volumetric ratio of H2-NG blend, from 3 % to 40 %. Two approaches have been used to maintain the energy or gas flow balance while considering the volume and gas composition variation due to hydrogen injection. Studies including [142,153,157] converted the amount of injected hydrogen into a volume of equivalent natural gas without consideration of gas properties variation. Other studies evaluated the gas properties change due to the hydrogen injection by calculating the molar fraction of hydrogen in the H2-NG blend, tracking the change of higher heating value [134,142,151,154,155], Wobbe Index and combustion potential [150]. As the hydrogen injection profiles are likely to be geographically dispersed and time-varying and cause an uneven distribution of hydrogen within the pipeline network, some studies included component tracking (tracing and analysis of gas composition) to guarantee the gas quality and to contain hydrogen blend ratio within an acceptable range. A clear trend could be seen that rather than assuming a uniform distribution of gas composition over the whole network, researchers started to conduct component tracking by formulating their models with detailed pipeline physical constraints. Some of the studies evaluate the gas qualities at each node by calculating the molar fraction of each component [133,134,144,150,152,154]. Another approach is to segment the hydrogen pipelines and monitor the transportation of each segment [151].

In most of the studies including gas transportation network at mid/high-pressure levels, compressors were included, and the power consumption of compressors was calculated based on gas flow through the compressor and inlet/outlet pressures [133,157].

4.1.3.2. Road-transport. Hydrogen transportation via road-transport applications (e.g., tube trailers and tank trucks) is regarded as an important approach of hydrogen transportation for local or regional energy systems. In one hydrogen supply chain optimisation model [138], hydrogen delivery via both approaches were presented by the number of available/in-use transportation units, hydrogen capacity of each transportation unit, the amount of hydrogen loaded from hydrogen generation sites and the amount of hydrogen delivered to end users or hydrogen refuelling stations. Two other studies [158,159] modelled the transportation via tube trailer in regional models, where routing constraints were used to track the geographical location of each trailer or truck and to assure that it is driving via the pre-fixed path.

4.1.3.3. Hydrogen refuelling station. The modelling of hydrogen refuelling stations is made up of the hydrogen flow balance within the refuelling station and the range limit of hydrogen storage level. Though HRSs request gas conditioning units to satisfy the pressure and purity requirements, very few HRS-related works included the installation or operation of these gas conditioning devices.

4.1.4. Hydrogen consumption technologies

Although the projected electricity generation by hydrogen-fired turbines will remain low in the next decade, a number of studies such as references [142,144,160,161] considered the option that generators powered by H2-NG blend or pure hydrogen offer flexible electricity generation to the power grid. The operation of hydrogen turbines that consumes either pure hydrogen or H2-NG blend is usually modelled by a linear energy conversion equation linking gas consumption and power output [142,144]. The power output of turbines is limited within the installed capacity by inequality constraints. Compared with natural gas-fired turbines, the ramping rate limits, as well as the start-up and shutdown of hydrogen-fired turbines, have been scarcely considered by the existing studies.

The operation of a fuel cell has been modelled based on an energy conversion equation that calculates the hydrogen consumption and power output, along with the inequality constraint to bind the maximal power output [128,141,144]. Some studies added inequality constraints to limit the ramp rate of fuel cells [141,144]. In Refs. [162–164], electrolysers and FCs (sometimes with hydrogen storage units) were aggregated as a "hydrogen energy storage system". Binary variables were utilised to indicate the operation of the components and additional constraints were set to avoid the simultaneous operation of electrolysers and FCs [162].

The most common road-transport application in the reviewed papers is FCEV. Though plenty of reviewed papers included the transport sector and FCEV, the detailed modelling of individual FCEVs was not utilised by these reviews. The operation of FCEVs has been represented by the total hydrogen demand FCEV during energy system operation [165]. Some other models only used the demand profiles of FCEVs [166] (specifically light-duty vehicles [167] or very heavy vehicles [168]) to represent the hydrogen consumption of the transport sector, while the constraints did not include the detailed model of vehicle driving. The hydrogen demand profiles of FCEVs can be generated by energy supply and demand profiles [166], generated by scenario production methods such as the Monte Carlo method [156], or be estimated based on consumption projections released by reports [167–169].

For heating, the operation of hydrogen-fuelled boilers and CHP units are both modelled based on a constant coefficient of energy conversion [130,160,170]. For the gas boilers using H2-NG blend as feedstock, the heat power output is calculated based on the heating value of the infeed gas mixture [141]. The heat production of FCs has been included in two studies [141,144], and was calculated based on the thermal energy conversion ratio (known parameter) and power generation.

The industrial usage of hydrogen has been considered by long-term operation models investigating the techno-economic performance of hydrogen system integration, such as Refs. [166,171,172]. However, the industrial usage is only described as hydrogen demand profiles in possible energy scenarios [171,173], sometimes regarded as a flat base load [161]. The industrial hydrogen demand could be estimated based on current hydrogen demand or industry yields [140,174]. The operation characteristics were not modelled by the reviewed works. A brief summary of basic modelling formulations of mainstream hydrogen technologies is provided in the supplementary material.

4.2. The modelling approaches accounting for the cross-vector and cross-scale interactions

4.2.1. Interactions across vectors

To investigate how hydrogen would evolve in a coordinated way with other vectors, and to evaluate the economic and environmental benefits of hydrogen to the wider energy system, a large number of ESM-based studies included hydrogen's interactions across vectors. The hydrogen technologies included by these studies were set to operate in coordination with other vectors to maintain the energy supply and demand balance of the whole energy system. Additionally, the environmental requirements and technical requirements were included by formulating constraints (e.g., the total CO_2 emission cap constraint [165] and the constraint for the frequency response requirement of the power grid [175]) or adding corresponding terms in the objective functions of the optimisation models. These constraints and objective functions also make the operation/investment of hydrogen technologies coordinate with other vectors.

Hydrogen technologies also interact with other vectors in energy markets via energy trading Such interactions have been captured by optimisation and equilibrium models, such as the procurement of electricity to produce hydrogen through an electrolyser [176], or the procurement of ancillary services [177], or the hydrogen purchase by HRSs from a hydrogen market [178]. The behaviour of hydrogen-based participants influences the market price or social welfare of the whole system, while the energy price variation and market trading mechanism impact the revenue of hydrogen-based participants.

The following indicators have been used to evaluate the impact of the integration of hydrogen into the whole energy system: the improvement of economic value (reduction of cost in generation and maintenance, load shedding penalty, renewable energy curtailment, and increase in system revenue, social welfare), the improvement of the environmental contribution (carbon emission reduction), and the system's resilience or reliability. Interaction could also be studied by direct quantification of the flexible provision from hydrogen technologies, such as the frequency response service from electrolysers [57] and operating reserves from hydrogen providers [178]. The impact of hydrogen's interaction with other vectors has also been revealed by the outcomes of market operation models, especially how power-to-gas installation could maintain or increase the electricity price [138,179].

4.2.2. Interactions between different time scales

To evaluate the role of hydrogen in both the short and long term, many long-term optimisation models have been formulated in an intertemporal way. Long-term optimisation models are formulated based on objective functions containing yearly cost or revenue, as well as long-term constraints, such as the steady change of system configuration and seasonal profiles of energy generation and demand. Some models consist of constraints or equations in hourly resolution, accounting for the short-term operation characteristics of hydrogen technologies at each time step. To reduce the computational burden, some model-based analyses were carried out in several typical days to emulate the operation during the whole horizon [128,129,144,172,180,181].

For optimisation models working on infrastructure expansion with a duration longer than 20 years, multi-period optimisation models have been used to divide the whole planning period into smaller parts (usually 10 years) [137,138,145,182,183]. The expansion plan in each period was optimised and then used as a known input in the next period's optimisation. These models focused on a shorter-term gain rather than studying long-term strategic investment decisions.

4.2.3. Interactions between different spatial scales

To evaluate how hydrogen could contribute to the energy transitioning of a region or a country, the large-scale deployment of hydrogen infrastructure has been studied through models of regional or national energy systems. Nevertheless, because many hydrogen facilities are involved in the operation of local energy systems, such as microgrids [184], some studies have included the operation of smaller-scale energy systems and considered the interaction between energy systems at different scales. Bi-level/tri-level models have been adopted to combine the operation of energy networks or entities at different scales, or even over different energy vectors. Some bi-level models looked into the interaction between service providers or microgrids and the energy market [154,185]; another bi-level model used upper and lower levels for the operation of electricity distribution network and transmission network respectively [162]. One tri-level model took hydrogen production stations, electricity and natural gas networks, and the hydrogen network as three levels [136]. These models were transformed into an equivalent single-level model to be solved, or solved using an iterative algorithm that transmits the variables between different levels.

Some studies have targeted the interactions between national and cross-border energy systems. For example, a pan-EU energy system model has integrated the models of Germany [186], accounting for the difference in the spatial distribution of RES sources and energy demands. In contrast, there are studies targeting one European country that interacts with the neighbouring countries or the European energy market via cross-border energy trade, which brings extra flexibility to the national energy system [187,188]. Another kind of interaction is between national and regional systems, such as the national energy system combining regional hybrid renewable energy systems in 16 different regions of South Korea [140].

4.3. Models to inform the hydrogen development strategy

Diverse model types have been used to inform the design of hydrogen development strategies, including the expansion planning of energy systems with integration of hydrogen infrastructure, the investment decision making and interactions between stakeholders, and evaluation of hydrogen technology contributions to and impact on the whole energy system. A summary of these models is given in the following subsections.

4.3.1. Expansion planning models of hydrogen infrastructure

Many studies have developed expansion planning models to design the most cost-effective expansion plan for the deployment of hydrogen infrastructure in the future energy system. These models targeted either the expansion of the whole hydrogen supply chain, or the deployment of specific types of hydrogen infrastructure, such as the sizing and location of electrolyser and hydrogen storage facilities. The majority of optimal expansion planning models use cost oriented objective functions, such as cost minimisation and profit maximisation, accounting for the investment cost, operation, and maintenance cost and energy trade revenue. Two studies [145,189] formulated expansion planning models as multi-objective optimisation problems combining economic, environmental, and technical factors. The inputs to these models usually include: economic parameters, such as capital cost and maintenance cost; technical parameters, such as energy conversion ratio and capacity limit; geographical parameters, such as local energy demand, availability of natural resources, distances to other energy infrastructure. The decision variables in the expansion planning models could be the capacity of hydrogen production, storage, or consumption technologies, the location of hydrogen facilities or the topology of future pipeline network, and the timing of installing new facilities. There are three types of core constraints in the planning models: the constraints indicating the location or installation capacity of hydrogen facilities during each time step, which describe the timeline of hydrogen infrastructure expansion; the capacity limits of the components that restrain the maximal energy supply and demand ranges by the hydrogen infrastructure; the energy balance constraints ensuring that the demand will be satisfied, which include the energy flow within/across energy vectors. In recent years, hourly energy balance constraints [128,129,136,141,144,165,170,180,188–194] and constraints representing hydrogen technology operating characteristics [129,138,141,144] have been incorporated into the expansion planning models, which leads to intertemporal interactions between the short-term operation and long-term hydrogen infrastructure expansion. This may bring a substantial increase in the number of constraints and variables, leaving the expansion models faced with a great computation burden. Two common solutions are to simplify the modelling constraints (such as using the energy flow constraints only rather than using pipeline models) and to use representative days over the long planning periods. The original optimal planning model could also be decomposed into several sub-problems that were then tackled separately by different models or software, with data exchange between them. This approach has been adopted by three studies [139,140,192] where planning problems consisted of the simulation of local energy system operation or energy trading, the long-term optimal dispatch or planning of energy systems or decision-making methods. The expansion planning models reviewed in this paragraph are summarised in Table 3 in Appendix.

Most of the published studies were conducted on a country or region (e.g., Europe, Germany, South Korea, etc), with accessible hydrogen development strategies and future energy scenarios. Because the deployment of hydrogen infrastructure relies greatly on location-specific resources and demands, the geographical features have also been considered by these national or regional models. The geographical features include: distribution of resources (water, raw materials, RESs, etc), hydrogen demand (collected from regional forecast data or estimated based on population and traffic flow) and cost of transportation hydrogen (calculated based on distance to hydrogen supplier points). These data are usually the inputs or parameters in the optimisation models [138,144,195,196], or used for the ranking of potential sites by multi-criteria decision-making method in terms of technical, economic, social, and environmental factors [197,198].

As uncertainty lies in the market share of hydrogen and the hydrogen-related policies, nearly all the models adopted different scenarios to include these uncertainties. In these papers, multiple test runs are carried out on the same models using a "business as usual" scenario, with some more ambitious scenarios representing different hydrogen ratios in energy generation, future energy demand, market share of hydrogen technologies, hydrogen unit life span or energy price. Many studies added sensitivity analysis to predict the potential fluctuations caused by uncertain factors, such as RES generation capacity, wind speed, carbon tax, energy cost, and demand. Mathematical approaches accounting for uncertainty, such as robust optimisation and stochastic programming, have rarely been used in the reviewed expansion planning models.

4.3.2. Investment-related models simulating the decision making of different stakeholders

During the long-term development of the hydrogen economy, stakeholders will make investment decisions or take actions that could potentially impact investment decision making. In contrast to centralised optimisation models where the total system cost or revenue is optimised while not considering the impacts on or influences of stakeholders, game theory-based models and system dynamics models are better suited to account for the different economic goals of stakeholders and to simulate the interactions between them. The outcomes of these models present the investment decisions and profitability of each stakeholder, which could be used to emulate and analyse the behaviour of investors and end-users in the "chicken and egg" problem. The impact of government subsidy strategy on the market diffusion of FCEVs has been studied by Refs. [199,200]. [199] utilised a tripartite evolutionary game model to simulate the strategy evolution of central government, local government, and enterprises. [200] used an agent-based model to simulate the interaction between the government, the HRS planning department and consumers, in which the subsidy choice process of the government was described by an experience weighted attraction learning algorithm. In Ref. [201], a system dynamics model was used to depict the investment decisions for PEM electrolysis and SMR technologies, consisting of five feedback loops representing capacity acquisition, market overview, resource depletion, technological learning, and support scheme. Because most of the suppliers or consumers will be trading under market mechanisms, many studies [179,202–204] formulated a long-term investment equilibrium model that simultaneously accounted for investment decision making and energy market trading. Reference [204] established an investment equilibrium model between EPS, NGS, and hydrogen fuelling system while including the energy trading, which was transformed into a MILP form based on Karush–Kuhn–Tucker conditions. In studies [176,179,202,203,205], the investment decision and operation strategy of hydrogen storage and electrolysers were investigated in the energy market, modelled as a mixed complementarity problem. In the aforementioned studies, the main metrics to evaluate the investment decision were the cost and revenues of the hydrogen infrastructure, and the associated carbon emission mitigation. The impact of hydrogen infrastructure's investment and operation on the electricity market was evaluated by comparing the whole system's welfare and renewable energy market values under the scenarios with/without the integration of hydrogen infrastructure [176,205].

4.3.3. Evaluation of hydrogen's role and competitiveness in the energy transition

In addition to models working on optimal expansion planning and stakeholders' investment decision making, various model paradigms have been employed to evaluate the impact and contribution of the hydrogen technologies in the whole energy system. These model paradigms encompass optimisation models for the energy system's long-term/short-term operation planning and daily energy market operation, and simulation models which conducted the transient simulation of gas pipelines or calculated the energy flow across different vectors.

In contrast to expansion planning models, the system configuration of short-term/long-term operation models is predetermined. The input of the optimisation models usually consists of the energy generation and demand profiles, the price of fuels and renewable energy curtailment, and the system configuration and capacities of each device. These models generate the optimal energy supply mix for the economic goal, the portfolios of hydrogen production and consumption, the operation cost or revenue of hydrogen infrastructure, the overall system cost, and the total CO_2 emission. Optimisation models can be categorised by the level of aggregation: one group is multi-node models, which account for the energy flow between regions and the operating status of each component [167,181,187]; the other group is the aggregated models that use one node to represent the whole energy system and only consider the energy balance between vectors [171–173,206]. The optimisation models targeting ESM's long-term and short-term operation are summarised by Tables 4 and 5 in Appendix.

Simulation models could be categorised as the transient simulation model of H2-NG transportation pipelines [151,152], or the long-term models that calculated the hydrogen generation or consumption values by calculating the gap between energy supply and demand [166, 168,207–209]. Many studies utilised published modelling tools to assess different future energy scenarios of the large-scale deployment of hydrogen infrastructure, such as PRIMES [173], MARKAL/TIMES [171, 172,210], LEAP [211] or a combination of multiple tools [206,212, 213]. The role of hydrogen has been evaluated based on the modelling outcomes from these models, including the economic indicators for both the whole energy system and hydrogen facilities (e.g., total annual cost, net present value, pay-back time, internal rate of return, and levelised cost of energy); the environmental impact evaluation, which is usually total CO_2 emission; and the penetration level of hydrogen technologies (e.g., the installed capacity and power consumption of hydrogen facilities).

Some studies have focused on the market competitiveness of specific hydrogen technologies, such as the market penetration level, cost development, and profit analysis. The market potential of specific hydrogen technology has been forecast by a Bass diffusion model or logistic functions that simulate the gradual adoption of hydrogen technology, or has been estimated by the potential capacity needed for hydrogen generation and storage [146,214–216]. The cost development has been modelled by Wright's Law [214] and learning curves [217]. The impacting factors of HRS cost have been studied by conducting simulation with varying parameters, which could further used in the cost reduction of HRS and FCEV development [218]. The economic feasibility of hydrogen technology, especially the business case in an individual country, has been assessed based on the estimation of the levelised cost of hydrogen production, future cost degression or other economic-related indicators [214,217–232]. Three studies considered technology competition [214,221,232]. The environmental performance can be evaluated by the life-cycle analysis [233].

The long-term uncertainty regarding the market share development, policy and regulation implementation, renewable energy capacity, and so on have been included in these models via scenario analysis [146,168, 221,229,234] or Monte Carlo trials [214,226]. Sensitivity analysis has been frequently used to analyse how the market would respond to uncertain factors, such as energy price, technology's efficiency or lifetime, and so on [146,219,222,229,234–236]. Several optimisation models used stochastic modelling techniques, such as stochastic programming [156,158,164,175,237] and robust optimisation [149,150].

5. Research gaps

5.1. Models' resolutions and complexity

In all ESM-based studies, energy supply and demand should be balanced in each time period. To account for RES fluctuations and potential grid services that hydrogen-related technologies could provide, many studies have adopted a half-hourly or hourly temporal resolution (as demonstrated by Tables 2, 3 and 4). Some long-term models even incorporated the optimal dispatch model, such as [129,136,148,165, 238]. Although a finer temporal resolution could provide more details on system operation, the computational burden that it causes remains challenging. Balancing the details of the system operation represented by models and the computation burden would be one of the most challenging issues.

Many of the reviewed models, including all short-term operation models, adopted a "multi-node" structure partitioning national or regional energy systems into multiple geographical zones. These models were formulated with spatial constraints, such as the energy flow between different zones by the energy transportation constraints, and the geographical features of each zone (e.g., energy supply, demand, capacity of natural resources, etc.). On the other side, some of the long-term operation models used "single-node" models, such as [128,189, 239]. As each node represents the aggregation of energy supply and demand from multiple sources, it is inevitable that a certain amount of data details within the coverage of the node would be neglected. For example, the estimated capacity of hydrogen infrastructure in different regions of Germany is uneven, which leads to regionally-different costs of hydrogen generation and transportation that could not be reflected if Germany is represented by one aggregated node in the model. Choosing the most suitable spatial resolution is an essential issue for modellers who wish to account for the different features of each zone, while maintaining a relatively low computation burden.

Apart from the computation burden raised by finer resolutions, the challenge of increasing modelling complexity arises with the consideration of more operating characteristics of existing or emerging hydrogen technologies. For example, the varying energy conversion ratio and the start-up time delay of electrolysers that had not been considered in energy system models until recently [240], introduce more binary variables and nonlinear constraints. Another example is adding constraints that represent emerging hydrogen technologies with their operating characteristics, such as ATR or liquid organic hydrogen carriers.

The modelling complexity is particularly important to the models including pipeline networks. In optimisation models, solving PDE-form constraints remains challenging due to a substantial increase in the number of variables and constraints caused by linearising the PDE-based constraints. Even with the steady-state pipeline models, the nonlinearity and nonconvexity brought by them often require an extra linearisation approach to facilitate the solving process. Though many approaches used in natural gas pipeline modelling could be applied to the pipeline transportation of pure hydrogen, greater challenges arise with the H2-NG blend transportation. Many research outputs regarding the detailed modelling of H2-NG blend transportation in short-term operation models have just been released recently [241–250] with more to come in the future. Still, most existing models considering the variation of H2-NG blend composition have been mainly conducted in test cases with no more than 20 nodes. Both the industry and the academia will face more challenges when looking into larger networks with more components, more hydrogen injection nodes, and more complicated topologies. In addition, the need of modelling pipeline's physical constraints in the expansion planning models considering hydrogen blend is imperative as omitting such constraints may compromise the practicability of modelling outcomes [251]. This again requests more effort towards model development.

Furthermore, the modelling scale and complexity substantially increase when multiple energy vectors or stakeholders are included in the model. Many studies have partitioned the original problem into several sub-problems to reduce the computation burden, or to satisfy the data privacy requirement and independent operation of each network or stakeholder [134,136,150,154,158,162,185,252]. One way is to decompose the original optimisation model with techniques such as Benders decomposition method [252] and alternating direction method of multipliers [158]. Another approach is to formulate a sequential or parallel computation framework consisting of separate models corresponding to each sub-problem [134,150]. It is likely that both approaches will be adopted more frequently by future research. With the pursuit for higher accuracy, another trend is to utilise various models or tools that work on one specific energy vector only, and combine them into one overall modelling framework, such as [139,192,212,213]. The partitioning criteria in existing studies are based on energy vectors, regulation authorities, or geographical coverage. With the development of the hydrogen economy, the model partitioning is likely to change with the expansion of the hydrogen network (from district-level industrial clusters to national/international networks), and the development in the hydrogen market.

5.2. Uncertainty of hydrogen pathways

The uncertainty of the techno-economic performance of hydrogen technologies, as well as the development of supply and demand has been recognised as major barriers to the growth of the hydrogen economy [2]. Nearly all models accounted for uncertain factors to forecast the development of hydrogen economy and energy systems in potential pathways, and also to investigate how the energy system would react to the variations of uncertain factors. As more energy technologies join the energy system operation, there will be more uncertain factors to be considered by the models in terms of market share, cost, and technological development. This works for both the nascent hydrogen technologies and competing technologies. So far, only the commercially available hydrogen technologies and some of the competing technologies (e.g., the fuel cell and li-ion battery [221]) have been included in the scenarios, while the nascent technologies (e.g., hydrogen aviation, low-temperature hydrogen storage) were neglected. In addition, the uncertain meteorological features in future decades, which would not only impact RES generations but also potential water sources supporting hydrogen production, should be added to the long-term planning models.

The selection of future energy scenarios requires attention from modellers to guarantee that the model-based studies cover various hydrogen development pathways. Some studies utilised the future energy scenarios issued by organisations or companies such as ENTSO [186,207] and National Grid [154]. Many other modellers generated their own sets of scenarios based on the projection of future energy data, which were sometimes facilitated by scenario reduction methods. Given that energy profile projections and relevant regulations will be updated, modellers need to be aware of how up-to-date the scenarios used by their studies are.

5.3. The chicken and egg problem in hydrogen economy development

To address the chicken and egg dilemma in hydrogen economy development, it's crucial to simulate the stakeholders' behaviour, and to analyse the factors that could potentially affect the stakeholders' investment decision. Many types of models have been applied, such as agent-based models, game theory models, and partial equilibrium models. All have been proved to be useful to study the interactions between different stakeholders. However, the scopes of the existing studies were limited. Only two studies have explored the interaction between government and consumers, with a specific focus on hydrogen refuelling stations [199,200]. Other studies concentrated on the interaction of hydrogen technologies with other market participants [179,202,203] or regarded one energy vector as a stakeholder [201,204], which did not address hydrogen suppliers' interactions with hydrogen consumers or government entities. Furthermore, there is a gap in research regarding stakeholder coordination for other hydrogen technologies, such as SMR with CCS, hydrogen storage and pipelines, which have not yet been thoroughly investigated. A wider coverage of hydrogen technologies and stakeholders is needed.

As the chicken and egg problem depends on the scale-up of supply and demand, as well as the variation of cost, model-based studies should consider the gradual changes in the value of supply, demand, and cost. In some of the optimisation models, the prospected values of hydrogen generation capacity, demand, and cost were obtained from reports or other models, usually staying fixed for years, which did not reflect the gradual change due to the technology advancement and hydrogen economy development. Though existing studies have investigated the cost correlation between hydrogen production price and renewable electricity price, other external factors that may potentially affect the hydrogen price, such as carbon price, the scarcity of raw materials and natural resources, and the development of competing technologies should also be considered in the modelling of hydrogen technologies' cost development.

5.4. Hydrogen interaction with other sectors

Compared with natural gas, which usually interacts with electricity in an uni-directional way that can be easily quantified, hydrogen could establish the bidirectional interactions with electricity through various applications including electrolysers, fuel cells, turbines, and so on. These interaction pathways could potentially offer more types of flexibility services to the electric power system. Therefore, the evaluation of the flexibility provision of a hydrogen energy storage system or a specific hydrogen technology, should take all potentially available services into consideration. Most of the existing studies that investigated hydrogen's flexibility provision chose to quantify the electricity supply/demand by hydrogen technologies, with only a few additionally evaluated the frequency response potential of electrolysers [60,160]. The technical and economic performance of hydrogen technologies providing other types of flexibility service, or stacking different services, have not been thoroughly investigated by far.

Hydrogen could also facilitate the balancing of energy systems on a seasonal basis. Some models have included long-term hydrogen storage facilities [144,154,159,186,213,216]. For UHS, its storage capacity is substantially larger than common battery storage systems and the time scale of it is much longer than battery, with one injection-withdrawal cycle lasting for weeks. This makes UHS more suitable to address the seasonal fluctuations in energy supply rather than hourly regulation. Apart from UHS, hydrogen turbines coordinated with hydrogen suppliers, could potentially be another cost-effective way to sustain the power system's long-term balance [232].

In addition to hydrogen turbines, other hydrogen technologies, such as electrolysers and fuel cells that have a quicker response time, could be technically capable of delivering some grid services similar as battery storage. Therefore, it's important to consider multiple energy storage routes when evaluating hydrogen's impact on energy systems. In many studies, the calculation of the needed hydrogen storage volume was conducted by calculating the gap between energy supply and demand without consideration of other flexibility resources, or the flexibility provision was calculated under one certain scenario and with limited sectoral coverage. More sophisticated models, which could include the flexibility provision from all potential providers and consider different energy scenarios within the whole energy system, are in need.

On the other hand, hydrogen infrastructure could provide flexibility to the gas pipeline network, which could indirectly influence the operation of the whole system. Hydrogen storage could be used as a back-up supply during pipeline failures, which has hardly been considered in energy system studies. In the case of transporting H2-NG blend, the hydrogen blend ratio along the pipeline network is unevenly distributed and varies with the hydrogen injection fluctuation. Hydrogen storage and deblending facilities could regulate hydrogen blend ratio to some extent. In return, the blend ratio of H2-NG gas would affect the operation of end users in other sectors, such as boilers and turbines. More and more researchers started investigating the impact of hydrogen storage or other components on the variation of H2-NG blend and the operation of the whole system [248,249,253].

The research on the system integration of hydrogen should be extended to other sectors, especially the hard-to-abate sectors. Research on hydrogen's interaction with industry and heating is relatively limited and requires further investigation. Only a limited number of long-term operating models considered the industrial hydrogen demand [116,140,166,171–174,216] while none of the reviewed articles included the detailed modelling of industrial plant operation and the consumption of all types of feedstocks. Though industry has been and will be the mainstream hydrogen consumer, scarcely any studies have looked into the decision making by industrial plant investors and the relevant government policy in this area. As for heating, the number of studies accounting for hydrogen-powered heating technologies is substantially lower than that of electric heating technologies. More calculation on the energy efficiency and cost of hydrogen-powered heating is needed to justify whether hydrogen is suitable for heating and to assess whether hydrogen is competitive with other heating technologies.

6. Conclusion

This paper conducted a review of the modelling approaches that have been used to investigate the system integration of hydrogen and has identified four research challenges to be tackled in the future. A total of 132 publications have been shortlisted for their relevance to the hydrogen infrastructure expansion plan, hydrogen-related stakeholder decision making, and the evaluation of hydrogen's impact on the whole energy system regarding the economic, technical, and environmental aspects. The models demonstrated by the shortlisted publications were examined with their modelling formulation of hydrogen technologies' operating characteristics, and the modelling approaches accounting for the interactions across vectors and between different temporal/spatial scales. It can be seen that electrolysers, hydrogen gaseous storage facilities, hydrogen transportation via pipeline, and fuel cell electric vehicles are the most frequently-included hydrogen technologies in existing studies. Other hydrogen technologies were less considered due to low technology readiness or their small share in the hydrogen generation/consumption mix. Many studies investigated hydrogen's interactions with more than one vector or constructed the models with energy systems at different temporal and spatial scales. More and more long-term models have been formulated in an intertemporal way by incorporating hourly operation details. A discussion of how different model paradigms have been developed to inform the strategy making in different aspects of hydrogen development was also conducted. To address different research questions related to the system integration of hydrogen, each model paradigm was developed using different resolutions, durations, and equations or constraints that represented the status and operation of hydrogen infrastructure, along with modelling approaches accounting for uncertainty.

This review also identified some modelling capability gaps of the existing studies and potential research topics in four aspects. (1) Modelling complexity will still be critical to the model-based studies in this area. The careful selection of temporal and spatial resolutions to maintain the model details while restricting the computation burden is a necessity to all works. As the research on the system integration of hydrogen goes further, more hydrogen technologies and operating characteristics, energy vectors and stakeholders will be included. This along with the need for composition tracking in the H2-NG blend transportation, calls for advanced modelling approaches to ensure the solvability of the models. (2) There will be more uncertain factors to be considered due to the introduction of new energy technologies. Future research should consider the nascent hydrogen technologies and competing technologies to hydrogen. Researchers should keep updating their energy scenario projections and include a broader source of uncertain elements as needed. (3) The number of current studies regarding stakeholders' decision making is low, with only a few studies working on electrolysers, hydrogen refuelling stations and fuel cell electric vehicles. The need to address the chicken and egg dilemma requests a broader research scope covering various hydrogen technologies and different stakeholder groups, with consideration of the factors potentially affecting the supply, demand and price of hydrogen. (4) The evaluation of hydrogen's flexibility provision to power grid should consider all potentially viable options, both electricity supply and grid service provision. Future research efforts should be directed to hydrogen's long-term energy storage capability and hydrogen's interactions with industry and heating sectors.

This review provides some insights into the modelling methods employed to study hydrogen's system integration. Still this work is carried out based on the information disclosed in the literature, subject to the level of information availability. It is foreseeable that more and more studies will investigate hydrogen's interactions with other sectors (especially industry), include emerging hydrogen technologies, and adopt more advanced modelling methods. Future research will benefit from incorporating these new modelling approaches and research trends.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.rser.2024.114964.

Appendix

Table 3
The summary of articles proposing expansion planning model of energy systems considering the deployment of hydrogen infrastructure

Ref	Year	Hydrogen technologies*	Other involved vectors**	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
[138]	2022	Electrolysis (L), SMR (L), CG (L),	E, G, T	Economic	Formulated as a MILP,	N	N	N	N	1 year	30 years (2020–2050)

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Table 3 (*continued*)

Ref	Year	Hydrogen technologies*	Other involved vectors**	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
		BG (L), byproduct (L), hydrogen conditioning & reconditioning (M), hydrogen storage tank, pipeline transportation (M), truck transportation (M), HRS (L), FCEV (L)			solved by CPLEX						
[129]	2022	Electrolysis (H)	E	Economic	Formulated as a LP, solved by Gurobi	N	Y	Y	N	1 h	4 typical days (representing 1 year)
[165]	2022	Electrolysis (L), HRS (M), FCEV (L), fuel cell (L)	E, T	Economic	Formulated as a LP, solved by YALMIP and Gurobi	Y	Y	N	N	1 h	1 year
[189]	2022	Electrolysis (M)	E, T	Economic, environmental	Formulated as a MILP	N	Y	N	N	1 h	30 years (2020–2050)
[136]	2022	Electrolysis (M), SMR w/wo CCS (M), HRS (M), hydrogen vehicle (L)	E, G, T	Economic	Formulated as a tri-level optimisation problem, solved by genetic algorithm	Y	Y	N	Y	1 h	5 years
[192]	2022	Electrolysis (L), SMR (L), cavern storage (L), hydrogen transportation via pipeline (L), compression (L), hydrogen vehicle (L)	E, G, H, T	Economic	Built based on REMIX and MuGriFlex	N	Y	N	N	1 h	1 year (2020, 2030, 2040, 2050)
[139]	2022	Electrolysis, SMR with CCS, hydrogen form gasification with CCS	E, G, H, T, I	***	Built based on MIRET-EU, Integrate Europe, Hype	Y	Y	N	Y	/	1 year (2020, 2030, 2040, 2050)
[193]	2022	Various hydrogen production technologies	E, G, H, T, I	Economic	Built based on SCOPE SD solved by CPLEX	Y	Y	N	N	1 h	1 year (2050)

Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
[141]	2022	Electrolysis (M), blending/deblending device, UHS (M), hydrogen storage tank (M), transportation and compression (M), fuel cell (M), H2-NG turbine (M)	E, G	Economic	Formulated as a MILP, solved by YALMIP and GUROBI	Y	Y	N	N	1 h	8 typical days (representing 1 year)
[186]	2022	Electrolysis (L), hydrogen storage (M), hydrogen transportation	E, G	Economic	Formulated as an optimisation model solved with a nested decomposition approach	Y	Y	N	Y	1 h	1 year (2040)
[81]	2022	The hydrogen value chain	E, G, H, T, I	/	/	/	/	/	/	/	1 year (2050)
[254]	2022	The hydrogen value chain	E, G	Economic	Combined Resource Technology	N	Y	N	N	RTN: 6 h;	RTN: 4 days; WeSIM: 1 year (2050)

(*continued on next page*)

Table 3 (*continued*)

Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
					Network (RTN) and Whole-electricity System Investment Model (WeSIM)					WeSIM: 1 h	
[180]	2021	Electrolysis, SMR w/wo CCS, hydrogen transportation via truck and pipeline, hydrogen storage tank, FCEV, hydrogen turbine	E, T	Economic	/	Y	Y	N	N	1 h	1 year (30 representative weeks in 2050)
[119]	2021	The hydrogen value chain	E, G, H, T, I	Economic	Formulated as a LP (known as integrated whole energy systems model, IWES model)	Y	Y	N	N	1 h	1 year (2040)
[188]	2021	Electrolysis, SMR, hydrogen compression, cavern storage, chemical methanation	E, G, H, T, I	Economic	formulated based on REMix solved by CPLEX	N	Y	N	N	1 h	1 year (2020, 2030, 2040, 2050)
[194]	2021	Electrolysis (M), tube trailer (M), cascade storage (L), HRS (M), FCEV (M)	T	Economic	Formulated as a MILP, solved by CPLEX solver	N	N	N	N	1 h	1 year
[159]	2020	Electrolysis (M), hydrogen transportation via tube trailer (M), hydrogen storage (M)	E	Economic	Formulated as a MILP, solved by CPLEX	N	Y	N	N	1 h	80, 640 h
[144]	2020	Electrolysis (M), hydrogen compressor (M), UHS (H), fuel cell (M)	E, G, H	Economic	Formulated as a MILP, solved by Yalmip and Gurobi	N	Y	N	N	1 h	4 typical days (representing 10 years)
[140]	2020	Electrolyser, SMR with CCS, ammonia synthesis	E, G, I	Economic	Simulation model using HOMERPRO, optimisation model formulated as a MILP, analysis model using TOPISIS	Y	N	N	N	1 year	20 years
[128]	2020	Electrolysis (M), SMR, hydrogen storage (M), fuel cell (M), methanation (M)	E, G, H, T, I	Economic	Formulated as a MILP, solved by CPLEX	Y	Y	N	N	1 h	5 years (representing full horizon of 20 years)
[170]	2020	Electrolysis (M), hydrogen boiler (M)	E, H, T, I	Economic	Formulated based on Enertile	N	Y	N	N	1 h	1 year (2050)
[181]	2020	The hydrogen value chain	E, G, H	Economic	formulated as a MILP using the Value Web Model, solved by CPLEX solver	Y	Y	N	N	1 h	40 years (2017–2056, 4 planning periods)

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Table 3 (*continued*)

Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
[60]	2020	Electrolysis (M), hydrogen storage (M), FCEV (L)	E, G, T	Economic	Formulated as a MILP	Y	Y	N	N	1 h	1 year (2040)
[160]	2020	Electrolysis (L), SMR with CCS (L), hydrogen storage (M), hydrogen boiler (M), hydrogen-powered electricity generation (L)	E, G, H, T	Economic	Formulated as a MILP	Y	Y	N	N	1 h	1 year (2040)
[190]	2019	Electrolysis, hydrogen transportation via pipeline, hydrogen compressor (M), hydrogen storage (M), HRS (M), hydrogen turbine, FCEV (L)	E, T	Economic	Formulated as a LP	N	Y	N	Y	1 h	1 year (2050)
[174]	2018	Electrolysis, UHS, hydrogen storage vessel, compressor, hydrogen transportation via pipeline, FCEV, refinery, steel making	E, G, T, I	Economic	Formulated as a MILP and solved by Pyomo	N	Y	N	N	1 h	1 year (2040)
[209]	2018	HRS	T	Economic	/	N	N	N	N	/	/
[255]	2018	Electrolysis, underground hydrogen storage, hydrogen transportation via pipeline, fuel cell, hydrogen turbine	E	Economic	/	Y	N	N	N	1 h	1 year (2050)
[256]	2018	The hydrogen value chain	/	Economic	Formulated as MILP, solved by Gurobi solver	N	N	N	N	/	30 years (2020–2050)
Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
[182]	2017	The hydrogen value chain (M)	E, G, T	Economic	Formulated as a MILP, solved by CPLEX solver	Y	Y	N	N	1 day	5 years (Total duration: 2020–2070)
[137]	2016	Electrolysis (M), biomass gasification (M), hydrogen storage (M), tank truck (L)	E	Economic	Formulated as a MILP, solved by CPLEX solver	N	Y	N	N	1 month	1 year (2044)
[191]	2015	Electrolysis (M), hydrogen storage (M), hydrogen-powered electricity generation (L)	E, G	Economic	Formulated as a LP	Y	Y	N	N	10 min	1 year
[145]	2014	Electrolysis, hydrogen conditioning, tanker truck, liquid hydrogen storage, HRS (M)	E, G	Economic, technical, environmental	Formulated as MILP, solved by CPLEX solver	Y	Y	N	N	1 day	1 year (2020, 2030, 2040, 2050)
[257]	2014	Electrolysis, SMR, integrated gasification combine cycle,	E, G, T	Economic	Formulated as a LP and solved by CPLEX	Y	N	N	N	1 year	40 years (2010–2050)

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Table 3 (*continued*)

Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
		hydrogen storage, FCEV									
[225]	2013	Electrolysis, lignite gasification plant, hydrogen transportation via pipe, HRS, FCEV	E, G, T	Economic	/	N	Y	N	N	/	/
[183]	2013	The hydrogen value chain (M)	E, G, T	Economic	Formulated as a MILP, solved by CPLEX solver	Y	Y	N	N	1 day	/

* The detailed level of hydrogen technology modelling is marked by the (L), (M) and (L) in the Hydrogen technologies column. “(L)” means lower level of details as the technologies are only represented by known demand or supply profiles. “(M)” means middle level of details as the hourly/daily energy conversion or the energy transfer of the technologies was modelled via constraints. “(H)” means high level of details as the dynamic characteristics of the technologies was modelled via constraints. Some rows were not marked as the corresponding information was not given in the paper.

** Abbreviations of sectors: E for electricity; G for natural gas; H for heating; T for transport; I for industry.

*** /means the paper doesn’t contain corresponding information, or not applicable for this blank.

Table 4

The summary of articles using long-term operation planning models

Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
[192]	2022	Electrolysis, SMR, hydrogen storage and transportation, compression	E, G, H, T	Economic	Built based on REMIX and MuGriFlex models	N	Y	N	N	1 h	1 year (2020, 2030, 2040, 2050)
[148]	2022	Electrolysis (M), methanation (M), hydrogen transportation via pipeline (H)	E, G	Economic	Formulated as a nonlinear optimisation model, solved by Gurobi	N	Y	N	Y	1 h	52 weeks
[172]	2022	Electrolysis (L), SMR (L)	E, G, H, T, I	Economic	Modelled using a calibrated MARKAL-TIMES model	Y	N	N	N	1 h	2 typical days (representing 1 year)
[238]	2022	Electrolysis (M), hydrogen storage (M), fuel cell (M)	E	Economic	Formulated as a LP-form optimisation model	Y	Y	N	N	1 h	1 year (2019)
[239]	2022	Hydrogen boiler (H), hydrogen-driven absorption heat pump (H)	E, H	Economic	Formulated as a single-node optimisation model (WeSIM)	N	N	N	N	1 h	1 year (2035)
[212]	2021	The hydrogen value chain	E, T, I	Economic	A model package combining REMES, EMPS and TIMES	N	Y	N	N	/	1 year (2030, 2050)
[166]	2021	Electrolysis (M), hydrogen storage (M), FCEV (M)	E, G, H, T, I	Economic	Formulated as a simulation model based on energy supply/demand balance	N	Y	N	N	1 h	1 year (2050)
[168]	2021	Heavy-duty FCEV (M)	E, T	Economic	Formulated as an assessment model based on energy supply/demand balance	N	Y	N	N	1 year	/
[116]	2020	The hydrogen value chain	E, G, H, T, I	/	/	N	Y	N	N	30 min	/

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Table 4 (*continued*)

Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
[167]	2019	Electrolysis (M), FCEV (M)	E, T	Economic	Formulated as a LP-form optimisation model, solved with CPLEX solver	N	Y	N	N	1 h	1 year (2015)
[173]	2019	The hydrogen value chain	E, G, H, T, I	Economic	Modelled using PRIMES	Y	N	Y	N	1 year	20 years (2031–2050)
Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
[171]	2018	The hydrogen value chain	E, G, H, T, I	Economic	Modelled using a MARKAL model	Y	N	N	N	/	40 years (2010–2050), 9 periods
[258]	2018	The hydrogen value chain	E, G, H, T, I	Economic	Modelled using TIMES	Y	Y	N	N	/	/
[213]	2017	Electrolysis, FCEV, hydrogen storage, hydrogen pipeline, HRS	E, T	Economic	A model package combining multiple models	N	Y	N	N	1 h	1 year (2050)
[154]	2016	Electrolysis (M), hydrogen transportation via pipeline (M)	E, G, H	Economic	Formulated as a two-stage optimisation problem	N	Y	N	Y	30 min	1 year (2030)
[206]	2016	The hydrogen value chain	E, G, H, T, I	Economic	Combining the TIMES-based models (built as a LP), solved by Simplex algorithm	N	N	N	N	1 year	25 years (2015–2040)
[118]	2016	Electrolysis, SMR, fuel cell	E	Economic	/	N	N	N	N	1 h	1 year
[187]	2015	Electrolysis	E	Economic	Combining a yearly dynamic programming model and an hourly dispatch model	Y	Y	N	N	1 h	1 year
[211]	2014	The hydrogen value chain	E, T	Economic	Modelled using LEAP	Y	/	N	–	1 year	50 years (1990–2030)
[210]	2014	The hydrogen value chain	E, G, H, T	Economic	Modelled based on UK MARKAL model	Y	/	N	N	/	/
[259]	2013	The hydrogen value chain	E, T	Economic	Modelled using TIAM-UCL model	Y	–	N	–	1 year	2015–2050

Table 5
The summary of articles using short-term operation planning models

Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
[130]	2022	Electrolysis (M), hydrogen storage (M), hydrogen gas turbine (M)	E, H	Economic	Formulated as MIP, solved by particle swarm algorithm	N	Y	N	N	1 h	1day
[162]	2022	Electrolysis (M), hydrogen storage (M), fuel cell (M)	E	Economic	Formulated as a bilevel rolling horizon optimisation problem solved by Gurobi	N	Y	N	Y	1 h	1 week (rolling horizon 48 h)
[142]	2022	Electrolysis (M), hydrogen storage (M), hydrogen transportation via pipeline (M), fuel cell (M)	E, G	Economic, environmental	Formulated as a MILP, solved by CPLEX	Y	Y	N	N	1 h	1day

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Table 5 (*continued*)

Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
[149]	2022	Electrolysis (M), hydrogen blending (M), hydrogen transportation via pipeline (H)	E, G	Economic	Formulated as a robust optimisation problem	Y	Y	Y	N	1 h	1day
[152]	2022	Electrolysis (M), hydrogen blending (M), hydrogen transportation via pipeline (H)	E, G	Economic	Formulated as a MILP, solved by GAMS	Y	Y	N	N	1 h	1day
[260]	2021	Electrolysis (M), hydrogen storage (M), micro gas turbine generator (M)	E, H	Economic	/	N	Y	N	N	1 h	1day
[163]	2021	Electrolysis (M), hydrogen storage (M), fuel cell (M)	E, G, H	Economic	Formulated as MILP, solved with CPLEX	N	Y	Y	N	1 h	1day
[155]	2021	Electrolysis (M), hydrogen blending (M), hydrogen transportation via pipeline (H)	E, G	Economic	UC Formulated as a MILP, solved by Gurobi; OGF formulated as MINLP, solved by IPOPT	N	Y	N	N	30 min/ 1 day	1 week
[158]	2021	Electrolysis (M), compressor (M), hydrogen transportation via tube trailer (M), HRS (M)	E	Economic	Formulated as a MILP, solved by Gurobi	N	Y	Y	Y	1 h	1 day
[127]	2021	Electrolysis (H)	E, H	Economic	Formulated as MIQP problem, solved by Gurobi solver	N	Y	N	N	1 h	1 day
[164]	202	Hydrogen storage (M)	E, G, H, T, I	Economic	Formulated as a stochastic optimisation problem in MINLP form, solved by DICOPT	N	Y	Y	N	1 h	1day
Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
[156]	2021	Electrolysis (M), hydrogen storage (M), fuel cell (M), hydrogen-based vehicles (L)	E, G, T	Economic	Formulated as MILP	Y	Y	Y	N	1 h	1day
[261]	2021	Electrolysis (H), hydrogen storage (M)	E	Economic	Formulated as a NLP, solved by CONOPT4	N	Y	N	N	15 min	1 day
[133]	2020	Electrolysis (M), hydrogen blending (M), hydrogen transportation via pipeline (M), compressor (M)	E, G	Economic	Formulated as a MINLP, solved by Newton Raphson method and black-hole particle swarm algorithm	Y	Y	N	N	1 h	1 day
[143]	2020	Electrolysis (M), hydrogen storage (M)	E, H	Economic	Formulated as a MILP	N	Y	N	N	1 h	1 day
[150]	2019	Electrolysis (M), hydrogen transportation via pipeline (H), hydrogen blend (M)	E, G	Technical	Formulated as a robust optimisation problem	Y	N	Y	Y	30 min	1day

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Table 5 (*continued*)

Ref	Year	Hydrogen technologies	Other involved vectors	Optimisation objective	Modelling features	Carbon-related constraint	Consider RES	Stochasticity modelling	Model decomposition	Time step	Horizon
[237]	2019	Electrolysis (M), hydrogen storage (M), fuel cell (M)	E	Economic	/	N	Y	Y	N	1 h	1day
[175]	2019	Electrolysis (M), hydrogen storage (M), hydrogen-based turbine (M)	E, G	Economic	Formulated as a MINLP, solved DICOPT	N	Y	Y	N	1 h	1 day
[262]	2019	Electrolysis (M), SMR (M)	E, G	Economic	/	Y	Y	N	N	1 h	1 day
[252]	2017	Electrolysis (M), hydrogen storage (M), hydrogen turbine (M)	E, G	Economic	Formulated as MILP solved by CPLEX	N	Y	N	Y	1 h	1 day
[157]	2015	Electrolysis (M), compressor (M)	E, G	Economic	/	Y	Y	N	N	1 h	1 day
[134]	2015	Electrolysis (M), gas transportation via pipeline (H), methanation (M)	E, G	Economic	Formulated as MILP	Y	Y	N	Y	30 min	1 month

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