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The representation of hydrogen in open-source capacity expansion models

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ABSTRACT

The intermittent nature of wind and solar power has led to a scientific consensus in the international energy research community that a mix of energy sources and carriers is necessary to achieve carbon neutrality. The search for alternatives has sparked renewed interest in Hydrogen (H_2) and its derivatives, such as ammonia and methane. It has also motivated researchers to expand their models to study H_2 investments in future energy systems. However, despite years of well-motivated research, a single scalable model that captures the unique characteristics of H_2 does not yet exist. It is a consequence of the limitations imposed by computational resources and the availability of data. With the above motivation, we review the current literature on relevant aspects for H_2. We find that temporal resolution, seasonal storage, spatial resolution and grid representation, uncertainty, and sector-coupling are important to accurately model H_2. We then analyze 18 case studies based on 11 open-source Capacity Expansion Models (CEMs) applied to study power or energy systems in developed countries that include H_2 and evaluate which models capture these idiosyncrasies best. Although no model covers all aspects simultaneously, some models tend to be more efficient in certain aspects, which ultimately depends on the underlying research questions they aim to address. We also outline potential research directions in this area.

1. Introduction

Combating climate change and mitigating its adverse impacts on the environment are among the greatest challenges of today's world [1]. In response to the urgent need for action, more than 190 countries came together at the 2015 United Nations Climate Change Conference to limit global warming to below 2°C [2]. The transition from fossil fuels to renewable energy sources has become the focus of political discourse and has led to increased investments in renewable capacity. Variable Renewable Energy Sources (VRES), such as wind and solar power, have contributed significantly to this growth. In contrast to fossil fuels, renewable energy sources come from naturally replenished resources, they do not produce direct greenhouse gas emissions, and they can be technologically and geographically diversified [3]. However, their power generation technologies rely more heavily on critical minerals [4], and VRES power output varies across space and time [5].

To address these risks and uncertainties [3], various energy carriers have been explored. H_2 has come to the forefront of the discussion due to its natural abundance on Earth, its high energy content per unit of weight [6,7], its carbon-free nature at its point of use [8], and long-duration energy storage potential [9]. These properties make H_2 well-suited to support the integration of VRES [10], and to provide a renewable feedstock where the direct use of electricity is not feasible [11,12]. However, in 2021, renewable energy sources accounted for less than 1% of H_2 production [13], and only ten underground H_2 storage sites were operated worldwide [14]. Also, in 2020, the H_2 pipeline system spanned over 5,000 km, compared to 3 million km for natural gas [15,16].

Understanding the potential role of H_2 in highly renewable energy systems is crucial for making informed investment decisions. In this regard, CEMs have become increasingly popular within the international energy research community. CEMs are based on mathematical optimization to determine cost-efficient investments in generation, storage, and transmission. However, due to the simplifications required to make such models computationally feasible [17], it is difficult to accurately capture the intermittent nature of VRES. Modeling H_2 adds another layer of complexity due to its complementary role to electrification and its sector-coupling potential [18]. Another challenge that arises is to address the uncertainty that surrounds H_2, e.g. cost and performance improvements of electrolyzers and fuel cells [19], demand for low-emission H_2, or regulatory uncertainty [20].

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Acronyms

CEM	Capacity Expansion Model
ED	Euclidean Distance
GIS	Geographic Information System
H_2	Hydrogen
LOPF	Linear Optimal Power Flow
TP	Transport Approach
VRES	Variable Renewable Energy Sources

The literature concludes that a coherent framework is needed to capture these idiosyncrasies. At the same time, there is a general understanding that no single model is able to address all aspects [18,21–27], which is why models with different purposes and varying levels of detail have been developed [28]. In this review, we limit our scope to open-source CEMs. First, mathematical optimization is well established in the international energy research community and therefore offers a wide range of possible applications. We focus on central planning and exclude models that simulate competitive markets, where multiple players interact and make decisions based on market dynamics. Second, we only consider models with open-source character, as these come with increased transparency, peer review, reproducibility, and traceability [29,30]. The code of open-source models is openly available, free to the public [31], and accessible through the web [23]. Third, we focus on CEMs applied to developed countries since H_2 projects are currently mainly driven by industrialized nations [32] and their energy systems and corresponding modeling needs differ from those of developing countries [33].

A significant body of literature has already dealt with model simplifications and modeling needs of highly renewable energy systems. More specifically, the main thrust of research effort in this area [5,17,23,34–39] studied aspects, requirements, and challenges of modeling energy systems with high shares of VRES. However, the difficulties associated with H_2 modeling are only briefly addressed. More recent reviews have sought to address this research gap [18,26,40–42]. For example, the authors in [18] proposed a taxonomy to classify modeling frameworks and highlighted specific modeling challenges with respect to H_2. Another work [26] defined guidelines to promote a more consistent representation of H_2 in energy scenarios. Both studies identified important aspects for H_2 modeling but did not investigate how these are currently considered in CEMs. A more in-depth study was carried out in [40], where the focus was on CEMs for planning power, natural gas, and H_2 systems. Based on the existing modeling landscape, the authors identified several modeling research needs. They argued that a holistic framework is needed to capture those unique characteristics of H_2 and natural gas. Finally, the authors in [42] provided a comprehensive review of H_2 within low-carbon pathways from different integrated energy system models. However, they focused on drivers and policy scenarios instead of specific modeling tools. To this end, the bibliographic review has revealed some serious research gaps that have led to the following research questions:

Research Question 1: What aspects are important in CEMs to accurately capture the idiosyncrasies of H_2 in renewable energy systems?

Research Question 2: Which models in the current modeling landscape handle these various aspects best?

For the first research question, we synthesize the literature to identify relevant aspects for modeling H_2 in highly renewable energy systems. For the second research question, we perform an in-depth analysis of different methods applied in CEMs to address these aspects. To tackle these issues systematically, this paper is structured as follows: Section 2 presents the methodology to identify reviews that propose requirements for modeling H_2 in highly renewable energy systems in CEMs. We also present the strategy to find all open-source CEMs applied to study energy systems in developed countries that include H_2. In Section 3, we describe each aspect and analyze how each is considered in those models. We give a conclusion in Section 4.

2. Methodology for the literature search

First, we performed a citation-based and a keyword-based literature search in ScienceDirect and Google Scholar. The purpose was to collect timely research on relevant aspects for H_2 modeling. Given that VRES play an important role for low-carbon H_2 production, aspects for modeling H_2 and VRES are included using the search strings "energy system modeling" and "energy system modeling hydrogen". We then applied several criteria to refine the results, such as being a peer-reviewed journal review article, written in English and published within the last 10 years. These criteria excluded conference papers, unpublished studies, working papers, government documents, or white papers. However, a considerable amount of literature remained. Thus, another criterion was that these either had a high citation score (>100) or included H_2. This is because the literature on H_2 is relatively recent and scarce, whereas modeling VRES in CEMs has been actively researched for several years. Based on their titles and abstracts, we manually filtered the remaining papers to ensure that these cover CEMs in developed countries. In this process, we found 14 reviews (see Appendix A).

In the next step, we identified specific CEMs applied to developed countries that have studied H_2. Here, we followed the process as shown in Fig. 1. We found that the representation of H_2 is highly dependent on the underlying model configuration and case study. We therefore focused on specific applications of the model published in a scientific journal article. First, we created a database of available models and mapped related H_2 articles to the model. For this purpose, we used the platform for open-source models Openmod, which lists models published under open-source licenses. In this process, 70 open-source modeling tools were found and manually filtered according to the following criteria: (1) based on mathematical optimization, (2) including investments in generation and transmission, and (3) applied at a national or international level in developed countries. However, not all of them included H_2 or conducted studies using H_2. Therefore, we used the article for the model publication and screened all cross-referenced articles. We then performed a manual selection process

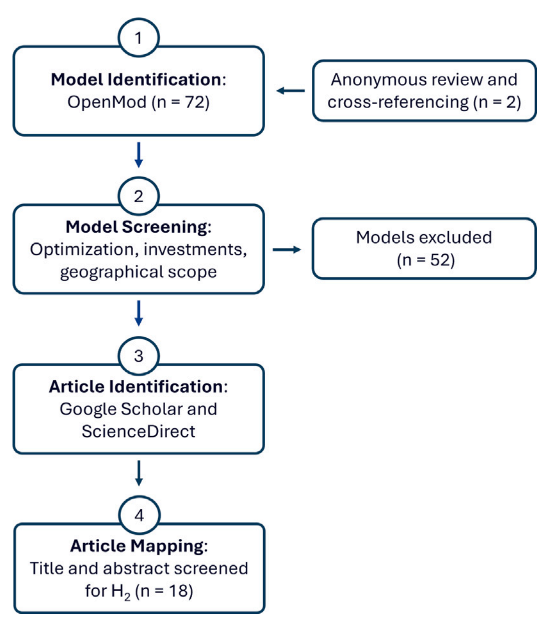

Fig. 1. Search strategy to identify 11 open-source CEMs and 18 related research articles.

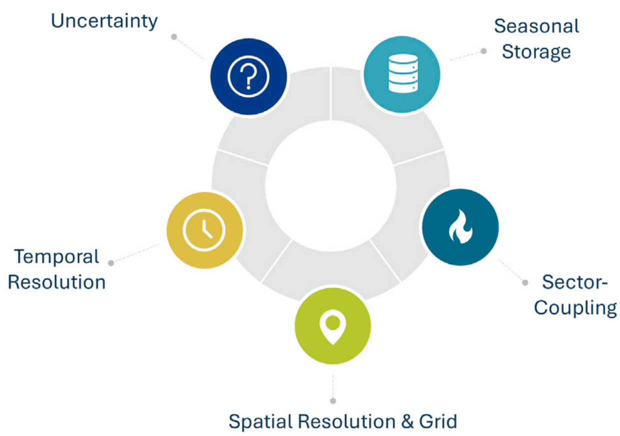

Fig. 2. Relevant aspects for modeling H_2 in renewable energy systems [45]: temporal resolution, seasonal storage, spatial resolution and grid representation, uncertainty, and sector-coupling.

based on abstracts and titles. We acknowledge that this approach leaves out models that have H_2 in their topology but have not been used for H_2 studies (e.g. Calliope [43] or Switch [44]). Another exception was made for the open-source TIMES ecosystem, which is a model generator with multiple branches, many of which are not open-source. Due to its availability and previous relevance in politics and academia, the model JRC-EU-TIMES was included, although it is no longer maintained. In total, we limited our analysis to 18 case studies using the following 11 models: Balmorel, DOLPHyN, EMMA, EMPIRE, FINE, GENeSYS-MOD, GenX, JRC-EU-TIMES, PyPSA-Eur, urbs, and SpineOpt. These are presented in Table 1. In Appendix A, all models are listed, including those recommended by anonymous reviewers and found through cross-referencing.

3. Modeling hydrogen in highly renewable energy systems

To tackle the first research question, we collected relevant aspects for modeling H_2 in highly renewable energy systems from the literature [5,17,18,23,26,34–40,42]. Instead of including all aspects, we only focused on the most frequently mentioned ones: temporal resolution, seasonal storage, spatial resolution and grid representation, uncertainty, and sector-coupling (see Fig. 2).

This rigorous process leaves out specific aspects that are not as often discussed or researched as others. For example, some authors [26] argued that individual technologies or plants should be modeled in more detail to accurately account for their flexibility constraints. Others found that the complexity of consumer behavior [26] and other sociological aspects are not adequately represented in CEMs [46]. However, we leave these and others to future research and focus on the aforementioned aspects. In the following, we briefly describe these and emphasize their importance in the context of modeling H_2 in highly renewable energy systems. Afterward, we investigate how each model considered these aspects and assess which models handle these idiosyncrasies best.

3.1. Temporal detail for operation and investment decisions

The planning horizon in CEMs is split into one or more years in which cost-optimal investments are determined. Each year is further subdivided into a number of operational time-steps to optimize the dispatch of the renewable energy system. The literature [5,23,26,35–38,40] argues that sufficiently temporally resolved data is important to capture hourly variations of VRES. Unlike their dispatchable fossil fuel-based counterparts, VRES depend on time-varying weather conditions [5] and therefore exhibit hourly, daily, or seasonal patterns. Temporally resolved data helps to capture such variations and provides better flexibility signals for H_2 technologies [26]. At the same time, some research [47,48] suggests that the transition from a fossil fuel-dominated energy system to a sustainable H_2 economy may require bridge technologies that are based on natural gas or fossil methane. To include these in the modeling, it is also necessary to have a sufficient number of investment years.

Although decisions for operation and investment are made on two different temporal dimensions, their resolution is inherently intertwined, as both compete for limited computational resources. We illustrate this trade-off in Fig. 3, where the number of hourly operational time-steps in each investment year (x-axis) and the number of investment years (y-axis) are shown. Each data point refers to a specific case study from Table 1. The size of each data point corresponds to the product of both dimensions and thus yields the total number of time-steps (hours) considered.

Accordingly, each data point is positioned along the x-axis or y-axis. We can distinct these into models based on brownfield (brown color code) or greenfield optimization (green color code). Models like Balmorel [49], EMPIRE [50,51], GENeSYS-MOD [52,53], JRC-EU-TIMES [54–56], PyPSA-Eur [57], and SpineOpt [58] used less than 1,000 time-steps to optimize the dispatch of each investment year. In particular, the planning horizon was split and optimized in intervals with a historical start year to account for the current capital stock and power grid. In the literature, this approach is known as brownfield optimization. By contrast, models like DOLPHyN [59,60], EMMA [61], FINE [62,63], GenX [64], urbs [65], and PyPSA-Eur [66] used between 2,000 to 8,760 time-steps but only considered one investment year. These models were greenfield-optimized from scratch, irrespective of existing capacities (see Table 1).

Although both aspects are important, none of our models covered both equally. Instead, we found that the priority depends on the underlying research question. For example, greenfield studies mainly focused on the role of H_2 as flexible demand response and grid-scale energy storage in a low-carbon power sector [59–61,63–65]. To model the operation of electrolyzers, H_2 storage, and fuel cells, it is essential to have highly resolved operational data as it better captures hourly and intra-annual variability in supply and demand [26]. Brownfield studies, by contrast, focused on the transition and competition of different technologies and energy carriers. In particular, they emphasized the temporal aspect of medium- to long-term H_2 production and transport methods, e.g. H_2 blending [52], or low-carbon H_2 production processes [50,58].

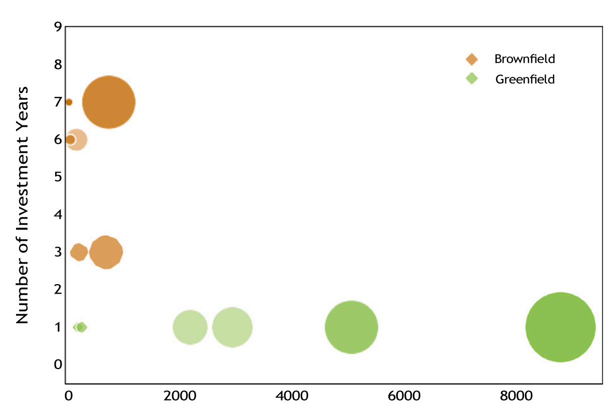

Fig. 3. Number of investment years versus the number of hours in each investment year. The size of each observation refers to the total number of considered time-steps in the optimization problem.

Table 1
Overview of CEMs considering H_2 systems.

#	Model	Applied in	Use Case for H_2	Temporal Resolution			Seasonal	Spatial Resolution & Grid		# Sectors	Uncertainty
				Investment	Operation	TSA	Storage	# Nodes	TP/LOPF		
1	Balmorel [67]	[49]	Socio-economic value of offshore H_2 generation in the North-central European energy system	Multi	192	DS	✓	~40	TP	3	Deterministic
2	DOLPHyN [60]	[60]	Flexible demand response and grid-scale energy storage for the power sector in the U.S. Northeast	Single	5,040	CL	✓	7	TP	1	Deterministic
		[59]	Economic value of liquid H_2 storage options for energy system decarbonization								
3	EMMA [68]	[61]	Impact of electrolytic H_2 production on wind and solar market values in the North-western European power market	Single	8,760	–	✓	5	TP	1	Deterministic
4	EMPIRE [69]	[50]	The impact of H_2 investments on the European grid infrastructure and power prices	Multi	720	ST	–	50	TP	1	Stochastic
		[51]	Competition between blue and green H_2 deployment in the European power sector								
5	FINE [63]	[63]	Role of H_2 technologies for Northern Germany	Single	168	CL	✓	13	TP	1	Deterministic
		[62]	Routing and sizing of a pan-European H_2 pipeline network		2,168			96			
6	GENeSYS-MOD [70,71]	[53]	Role of H_2 imports for the Japanese energy system	Multi	144	ST	–	8	TP	4	Stochastic
		[52]	Impact of H_2 blending on the European energy system		36	H&O	✓	30			Deterministic
7	GenX [72]	[64]	Flexible demand response and grid-scale energy storage for the power sector in Texas	Single	8,760	–	✓	1	TP	1	Deterministic
8	JRC-EU-TIMES [73]	[56]	Role of H_2 in the European energy system	Multi	12	TS	–	31	TP	4	Deterministic
		[54]	Potential for H_2 and Power-to-Liquid in a low-carbon EU energy system								
		[55]	Role of H_2 for cars in the European energy system								
9	PyPSA-Eur [74]	[66]	The potential role of a H_2 network in Europe	Single	2,920	DS	✓	181	LOPF	4	Deterministic
		[57]	Scale-up of electrolysis and renewable capacities in Europe		240	CL	–	1	TP		
10	urbs [75]	[65]	Flexibility potential for the European power sector	Single	8,760	–	✓	36	TP	1	Deterministic
11	SpineOpt [76] & Balmorel	[58]	Impact of different production pathways on H_2 investments in the Nordic energy system	Multi	672	MS	✓	11	TP	4	Deterministic

CL (Clustering), DS (Downsampling), H&O (Heuristics and Optimization), MS (Manual Selection), TS (Time-Slicing), TSA (Time-Series Aggregation), ST (Stochastic Sampling).

3.2. Seasonal storage modeling

Balancing seasonal variations of VRES generation and energy demand (e.g. heating and cooling) is one of the main challenges faced by highly renewable energy systems [23]. Consequently, there is great interest in long-term (seasonal) energy storage to provide such flexibility [23,28,35,40]. Energy storage with weekly to monthly cycling is also where H_2 is expected to play an important role [26,77–79]. However, modeling the operation of seasonal storage with a reduced temporal scope is a daunting task. Although the literature on methods to aggregate time-series data (e.g. VRES capacity factors, electricity demand) is rich and actively researched, a widely accepted method that efficiently reduces hourly data while preserving the most relevant information for the optimization problem does not yet exist [80,81]. A difficulty that often arises with aggregated data is to preserve the chronological order of the original time-series [23]. Nonetheless, this information is important to simulate realistic charge and discharge cycles for seasonal storage.

In this study, only EMMA [61], GenX [64], and urbs [65] applied a full hourly resolution, whereas all other models used a reduced data set. In the following, we describe the methods used to aggregate time-series data and investigate how well the value of seasonal storage is captured. To draw such a conclusion, we evaluate if the chronological order is preserved. In addition, we discuss the underlying assumptions and resulting drawbacks of each method.

3.2.1. Time-series aggregation methods

In this study, clustering algorithms (FINE [62,63], DOLPHyN [59,60] and PyPSA-Eur [57]), stochastic sampling (EMPIRE [50,51] and GENeSYS-MOD [53]), downsampling (Balmorel [49] and PyPSA-Eur [66]), time-slicing (JRC-EU-TIMES [54–56]), and methods based on heuristics and optimization (GENeSYS-MOD [52]) were used to aggregate the input data. Methods that only rely on the modelers' expertise were not considered here, because they are often not reproducible (e.g. SpineOpt [58]).

Clustering algorithms. Clustering algorithms group similar periods (e.g., hours, days, or weeks) into subgroups (clusters) [82–84]. For this purpose, the time-series data is transformed into a matrix, where one dimension represents periods, and the other one represents features (e.g. VRES capacity factors, electricity demand). The algorithm then compares the dissimilarity of each feature across different periods [85]. The Euclidean Distance (ED) is often used as a distance metric [80]. The data matrix is then split in a single partition (partitional clustering) or in a sequence of partitions (hierarchical clustering) [82]. Agglomerative hierarchical clustering in combination with Ward's algorithm was used in FINE [62,63], whereas partitional clustering algorithms such as K-MEANS and K-MEDOID were applied in DOLPHyN [59,60] and PyPSA-Eur [57]. In the academic literature, there is no consensus with respect to which clustering algorithm performs better for aggregating time-series data in CEMs. Instead, it is more important how the representative period is specified [86]. The cluster representative is selected once the clusters have been identified. In this paper, either the centroid (DOLPHyN [59,60]) or the medoid (FINE [62,63], PyPSA-Eur [57]) were used and weighted by the relative size of the cluster. Due to the statistical features of the centroid, there is evidence in the literature that it smooths out the variability of the original data. According to [86], this effect is less pronounced when using the medoid, the data point closest to the cluster's centroid [87].

The dissimilarity between different periods is typically measured with the ED, irrespective of their occurrence in the original time-series. Therefore, the chronological order within days (FINE [62,63] and PyPSA-Eur [57]) or weeks (DOLPHyN [59,60]) was preserved but not necessarily between them. Since seasonal storage covers longer cycles [79], the literature [23,88] argues that the modeling of seasonal storage cannot be adequately considered in investment decisions. This issue is widely acknowledged, and several solution methods have been proposed [88–90]. One of the most referenced methods is the seasonal storage coupling approach as described in [88]. This formulation is based on the general algebraic state space model, which has been successfully applied in different energy system configurations [88]. It was implemented in DOLPHyN [59,60] and FINE [62,63] to restore some of the original chronological information. Due to its significance in the academic literature, we consider both models suitable for modeling seasonal storage.

Stochastic sampling. Stochastic sampling was used to aggregate the input data for GENeSYS-MOD [53] and EMPIRE [50,51]. Here, a customized random algorithm was initialized to select a year from available historical data and then to collect hourly data for a day [53] or week [50,51]. As this is done for each of the four seasons, the chronological order within each season was preserved, but not necessarily between seasons. Note also that the randomness of the algorithm raises doubts as to how accurately these days or weeks can describe the statistical properties of the original data. More specifically, the underlying assumption is that each season can be represented by an arbitrary observation, although there is also considerable variation within seasons [91]. It is, amongst others, for these reasons that seasonal storage was not considered in these models.

Downsampling. Downsampling refers to the process of grouping and averaging consecutive time-steps [81]. It was applied in PyPSA-Eur [66] and Balmorel [49]. With respect to seasonal storage modeling, the advantage is that the chronological order of the original time-series can be preserved. However, we want to stress that hour-to-hour variations can be smoothed out [86], particularly for coarser time resolutions.

Time-slicing. Time-slices are constructed by sequentially averaging and grouping time-steps. This method was applied in JRC-EU-TIMES [54–56], where morning, night, and peak time-slices were defined for each season. However, this approach also suffers from the smoothing effect due to averaging. In addition, the chronological information between morning, night, and peak blocks is lost.

Heuristic and optimization-based methods. A non-linear optimization problem to aggregate time-series data was applied in GENeSYS-MOD [52]. Here, a reduced time-series was created by manual selection. The resulting time-series was then smoothed and scaled up such that the minima, maxima, and full-load hours of the original time-series were met [92]. This method can preserve chronology but also partly relies on manual pre-processing steps. If these are not well-documented, the results of the non-linear optimization problem may become inconsistent and difficult to replicate.

3.2.2. Summary

We conclude that clustering algorithms, in combination with the seasonal storage coupling approach, downsampling, and the heuristics and optimization-based approach described in [92] are able to preserve the chronological order of the original time-series. These have been used in PyPSA-Eur [66], DOLPHyN [59,60], FINE [62,63], Balmorel [49], and GENeSYS-MOD [52]. However, we found that each method comes with its specific drawbacks. Downsampling or clustering algorithms that use the centroid as representative suffer from the smoothing effect, which becomes particularly critical at low resolutions. To mitigate this effect, a high number of time-steps has been used in DOLPHyN [59,60] (5,040 time-steps), PyPSA-Eur [66] (2,920 time-steps), and FINE [62] (2,168 time-steps). The heuristics and optimization-based approach [92] does not suffer from the smoothing effect but requires manual pre-processing steps, which are dependent on the modeler's expertise and knowledge of the data set.

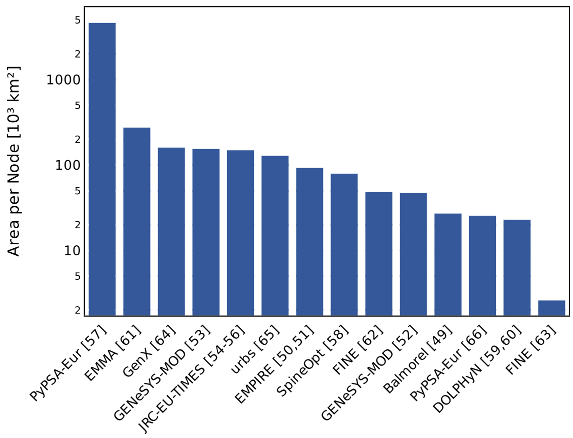

Fig. 4. Geographical area in 10^3 km^2 described by a single node.

3.3. Spatial resolution and grid modeling

The spatial resolution refers to the number of modeled spatial units or nodes [5,17,93]. In CEMs, nodes typically represent regions or countries, assuming that they have similar energy system-related characteristics. Given that VRES vary not only in time but also in space [5,23], the need for spatial data with sufficient resolution was raised in the academic literature [5,17,23,26,34,36–38]. Another point to consider is that spatial disparities result from synoptic-scale weather differences (∼600 – 1,000 km) [94], rather than from political boundaries. Accounting for these variations would better identify potential locations for H_2 technologies and represent the flexibility that H_2 offers with respect to different transportation modes [26].

The geographical scope and the number of nodes (n) among all models reviewed varies significantly; from Europe (n=11), Northeast U.S. (n=2), Nordic countries (n=2), single regions within Germany (n=1), hypothetical states (n=1) to Japan (n=1). Comparing how these models account for spatial variation is not straightforward. To this end, we divided the geographical area, measured in km^2, by the number of spatial nodes. In Fig. 4, this metric is plotted on a logarithmic scale and describes how many km^2 are contained in a single node. Accordingly, the lower this metric, the more spatial detail the model includes.

Except for PyPSA-Eur [57], where an entire continent was aggregated, a single node typically covered an area of ∼3,000 to 200,000 km^2, which is comparable in size to that of Luxembourg or Portugal. Interestingly, only DOLPHyN [59,60], which is among the most spatially detailed models, considered different H_2 transport options, e.g. H_2 trailers and pipelines, while all other models did not permit a regional analysis and thus limited H_2 transport to pipelines.

The spatial resolution is closely related to grid modeling, as it describes how spatial units are connected. Traditionally, the centroid of each continent, country, or region is used to quantify the trade between different energy carriers and sources. This method is known as Transport Approach (TP), as it provides a rather generalized framework for energy systems with multiple commodities [95]. However, these simplifications have been criticized in the literature and more detailed modeling of power and gas flows to account for the synergistic and complementary uses of electricity and H_2 has been encouraged [40].

Of all models reviewed, only PyPSA-Eur [66] provided an alternative to the TP and used a Linear Optimal Power Flow (LOPF) formulation according to [96]. In the literature, LOPF is accepted as a good approximation of the network's real behavior and can therefore provide a more accurate estimation of overloaded lines [97–99]. The partitioning of the grid was done with K-MEANS clustering, which reduced the number of buses and lines in the European power grid. This method was initially proposed in [94], where the authors proved its ability to capture major transmission corridors even with a small number of clusters. This grid reduction method accounts for electrical parameters of the grid and also indirectly region-specific renewable potentials. However, the modeling of gas flows was still based on the TP.

We found that PyPSA-Eur [66] provided the most sophisticated approach to include details of the power grid and region-specific renewable potentials. While we recognize the benefits of detailed network modeling [100,101], there are also several limiting factors [102]. Examples include data availability and the computational complexity involved with considering detailed network constraints and gas flow equations [102]. Therefore, more detailed H_2 transport concepts have not yet been explored by the models reviewed. Since CEMs focus on large-scale network analysis and thus adopt a central planning perspective, we argue that alternative models based on Geographic Information Systems (GISs) may prove more appropriate for such purposes.

3.4. Uncertainty

Traditionally, CEMs are based on a deterministic formulation, where an omniscient agent knows what has happened in the past and what will happen in the future [103]. Optimal decisions are made subject to the underlying weather data and load profiles, ignoring their uncertain nature [104] with respect to different weather years [69]. However, limited information is available behind the driving forces that shape renewable energy systems [34,105]. The literature argues that uncertainty should be adequately assessed to provide a sound basis for decision-making [5,23,34] and refers to two types of uncertainty [106–108]: Short-term uncertainties describe the variability and unpredictability of input parameters [107] (e.g. VRES forecasting errors, yearly demand, or fuel prices [17,35,107]). They have a direct effect on H_2 systems, as they influence operational decisions and market prices in the short-term. Long-term uncertainty is realized only once but has an impact over many years (e.g. demand growth, climate variability [107], or cost development of electrolyzers, fuel cells [109], and new or repurposed H_2 pipelines [110]). These factors impact the overall development of H_2 systems, including infrastructure investments, technology development, and policy planning. In the following, we examine both separately and evaluate how these have been considered.

Short-term uncertainty. Out of all the selected models, only EMPIRE [50,51] and GENeSYS-MOD [53] applied a stochastic formulation to capture the stochastic nature of uncertain input variables. In stochastic optimization problems, a central planner makes optimal decisions over a horizon with incomplete information while taking into account that some parameters are revealed after a decision has been made [17]. In the literature, these uncertain parameters can be described as a finite set of realizations or scenarios for which a single optimal solution must be found [111]. EMPIRE [50,51] and GENeSYS-MOD [53] are based on a two-stage stochastic linear optimization problem. Their system design was optimized in the first stage and operated under uncertain demand and VRES output in the second stage. Data from historical years was used to define a finite set of stochastic scenarios that could materialize with equal probability. Yet, despite decades of dedicated research, stochastic problems are still more difficult to solve than their deterministic counterpart but are more robust with respect to weather uncertainty [27,34,112]. Furthermore, as acknowledged by [53], decomposition methods could have been applied to exploit computational resources [107,111]. Also, there is a lack of a more sophisticated approximation to the real probability distributions of stochastic scenarios.

Long-term uncertainty. The majority of models sought to address the long-term uncertainty of H_2 by employing a scenario analysis or sensitivity analysis. In scenario analysis, a base case scenario is defined and compared against a range of different alternative scenarios, where each has different values for a set of uncertain assumptions [112,113]. JRC-EU-TIMES [56], EMPIRE [51], PyPSA-Eur [66], DOLPHyN [60], Balmorel [49], GenX [64], and urbs [65] used this method to analyze different renewable energy policies and H_2 cost technology developments. Sensitivity analysis, on the other hand, specifically addresses those input parameters that have the most impact on the model results. For this purpose, these are varied while all other assumptions are held constant [113]. This method was applied in PyPSA-Eur [66], EMPIRE [50], and JRC-EU-TIMES [54] to analyze the impact of different techno-economic parameters (e.g. investment, O&M costs, lifetime, or efficiency). However, both methods were criticized in the academic literature as they rely on a deterministic formulation. Specifically, the authors in [114] argued that these methods cannot cope with complex and multi-faceted problems with inherent uncertainties [114], and therefore do not classify as formal techniques to describe uncertainty [113]. We found that the lack of formal techniques to address the long-term uncertainty component of H_2 is a rather general issue, as it is more common to apply short-term uncertainty methods [107].

3.5. Sector-coupling

Apart from the power sector, there are also other energy sectors (e.g. heating, cooling, transport) that still rely on fossil fuels [115]. The main idea of sector-coupling is to account for interactions between these sectors. This can improve cost and resource efficiency savings [26] and increase the flexibility of the energy system [116], which, in turn, is beneficial for the integration of VRES [12]. H_2 is a central sector-coupling component in this regard, with applications for power-to-gas [117], power-to-heat [118], power-to-liquid [54], and power-to-ammonia [119]. The literature [23,26,40,116] therefore emphasizes the importance of co-optimization and integrated energy system planning.

The degree of interaction and interconnection of H_2 varies greatly across models, as evidenced by the number of different energy carriers and sector-coupling technologies. However, with respect to the number of endogenously optimized energy sectors, we can differentiate between traditional power sector models that have been extended to include H_2 and those that already cover multiple energy sectors. Both are discussed, and their implications for modeling H_2 investments are outlined.

Out of all models reviewed, DOLPHyN [59,60], EMMA [61], EMPIRE [50,51], FINE [62,63], GenX [64], and urbs [65] focused on optimizing dispatch and investment decisions for the power sector. In these case studies, the main application for H_2 was to provide flexibility to the power sector using gas turbines, electrolyzers, underground storage, and storage vessels. However, except for GenX [64], these models acknowledged that H_2 will also play an important role in the decarbonization of the transport and industry sector. The demand for H_2 from these sectors was therefore given exogenously. We note that this places strong assumptions with regards to the uncertainty of future H_2 demand [120].

On the other hand, cross-sectoral interactions between the power, heat, industry and transport were modeled in Balmorel [49], GENeSYS-MOD [52,53], JRC-EU-TIMES [54–56], PyPSA-Eur [57,66], and SpineOpt [58]. We found that most models endogenously optimized the use of H_2 in the heating sector through H_2 boilers or fuel cells. Also, synergies between methane and ammonia were considered. Only in JRC-EU-TIMES [54–56], and GENeSYS-MOD [52,53] transport and industry was not fixed as exogenous demand. Instead, different H_2 technologies were modeled to endogenously determine the optimal use of H_2 across all sectors.

In Fig. 5, we illustrate the various pathways for H_2 production, conversion, and application. In particular, we highlight with a solid line the pathways that are endogenously optimized by all models. The dashed line, by contrast, illustrates the pathways modeled by GENeSYS-MOD [52,53], and JRC-EU-TIMES [54–56]. We argue that an endogenous optimization leads to a more cost-efficient use of H_2 from a system perspective. Yet, this increases the number of variables and constraints in the optimization problem and, thus, the computational burden.

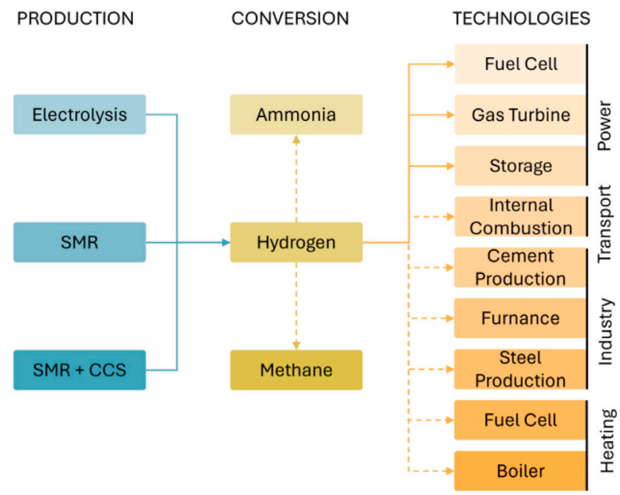

Fig. 5. Scheme of H_2 supply and delivery chain. The typical pathway is represented with a solid line. The dashed line refers to the endogenous optimization of H_2 across different sectors.

4. Conclusion

Due to data limitations and computational constraints, real-world dynamics are often modeled in a simplified manner. While this has been accepted for energy systems based on dispatchable generators, there are concerns that the full complexity of highly renewable energy systems with electricity and H_2 as main energy carriers may not be adequately captured [36]. In this study, we focused on relevant aspects for modeling H_2 in CEMs and investigated how these have been addressed by current models.

In line with the literature [18,21–27], we found that no single model can fully capture all the complexities of H_2, particularly when it comes to simultaneously addressing spatio-temporal detail, sector-coupling synergies, seasonal storage potentials, and accounting for uncertainty. Instead, some models tend to be more efficient in certain aspects, which ultimately depends on the underlying research questions they aim to address.

In this respect, we found that it is challenging to consider both short-term operational details and long-term transitional dynamics of H_2. The models reviewed focused on either one aspect or the other, which leaves a research gap in capturing both temporal scales simultaneously. Modeling seasonal storage, on the other hand, is a quite established topic in the energy research community. Our research suggests that the methods used in PyPSA-Eur [66], DOLPHyN [59,60], and FINE [62,63] provide a sound foundation for modeling seasonal storage with a reduced temporal scope. However, we stress the need for high temporal resolution to capture hour-to-hour variations. Spatial variability and grid features were best captured with the grid partitioning method and LOPF approach applied in PyPSA-Eur [66]. Moreover, short-term uncertainty is only explicitly addressed in GENeSYS-MOD [53] and EMPIRE [50,51] that relied on a two-stage stochastic formulation. However, no formal methodology addressed the long-term uncertainty in H_2 energy systems. Also, only few models (e.g. GENeSYS-MOD [52], JRC-EU-TIMES [54–56]) accounted for endogenous H_2 demand, which we identified as a critical gap given the uncertain H_2 demand in renewable energy systems.

Although a systematic manner has been adopted to identify relevant aspects for modeling H_2 in highly renewable energy systems, the evolution of H_2 and its most influential parameters remains uncertain. Instead of focusing on the most relevant aspects discussed in the academic literature, it would be valuable to examine the full range of modeling aspects. This limitation is also related to the fact that this review is not a comprehensive one. In particular, it is important to note that there may be more efficient methods in the academic literature that have not yet been applied in the context of H_2. Also, this study did not exhaustively map all CEMs, as it relied on a single database. Therefore, some studies might have been overlooked. In addition, a critical discussion would be valuable to analyze the benefits of model coupling. Furthermore, all of our analyses are based on the existing literature. To gain a more comprehensive understanding, it would be valuable to run each model individually. This approach could provide deeper insights into their relative strengths and limitations.

CRediT authorship contribution statement

Dana Reulein: Writing – original draft, Methodology, Formal analysis, Conceptualization. **Herib Blanco:** Writing – review & editing, Conceptualization. **Dimitri Pinel:** Writing – review & editing, Conceptualization. **Hossein Farahmand:** Writing – review & editing, Methodology, Conceptualization. **Christian Andre Andresen:** Writing – review & editing, Conceptualization.

Declaration of Generative AI and AI-assisted technologies in the writing process

The authors used Grammarly [121], and ChatGPT [122] to improve the readability of this paper. The suggested improvements have been manually reviewed so that the authors can take full responsibility for the content of the publication.

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.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.ijhydene.2024.11.436.

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