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Hydrogen supply chain modelling at energy system scale: a review

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Abstract

Hydrogen is going to play an important role in future decarbonized energy systems and understanding its interaction with other energy vectors is crucial to create adequate policies. In this review, the green hydrogen production literature was classified and analysed to unveil the gaps that avoid a proper integration of hydrogen production in energy system models. Production-side supply chain (PSSC) and systems side impact (SSI) models were analysed. Based on site-specific models, the former showed detail on the optimization of the supply chain, whereas the latter on the impact of hydrogen deployment in an energy system. The first challenge identified is the variables considered, where inherent endogenous variables of one type of model were exogenized in their counterpart model. This is relevant because of the unique geographical characteristics of the sites and the effect of the large-scale production of hydrogen on the energy system. Further, PSSC models tend to consider a profit maximization approach and SSI model, cost minimization. The first normally does not consider social externalities in their investment decisions and the latter neglects the effect of competition between different players in the market. Moreover, the computational requirements of a cost minimization approach are less demanding and complex than a profit maximization approach at a large-scale. Other gaps found included; a lack of life-cycle assessment and the effect of large-scale hydrogen facilities integrated into SSI. This study reveals gaps in the current hydrogen modelling literature that need to be addressed for defining the future of energy systems' decarbonization.

Keywords: Hydrogen, Energy Systems, Supply chain, Optimization, Modelling, Integration, Renewable

Nomenclature

aFRR	Automatic frequency restoration reserves
CSP	Concentrated solar power
FCR	Frequency rontainment reserves
LCOE	Levelized cost of electricity
LCOH	Levelized cost of hydrogen
mFRR	Manual frequency restoration reserves
PEM	Polymer electrolyte membrane
PPA	Power purchase agreement
PSSC	Production-side supply chain
PV	Photovoltaic
SMR	Steam methane reforming
SOEC	Solid oxide electrolytic cell
SOEL	Solid oxide electrolysis
SSI	Systems side impact
TES	Thermal energy storage
UC	Ultracapacitor
WACC	Weighted average cost of capital

1 Introduction

Concerns about climate change have motivated many countries to prioritize the decarbonization of the energy system. The decarbonization strategies from the majority of states have focused on the integration of renewable sources of electricity such as onshore and offshore wind farms, photovoltaic (PV) and concentrated solar plants, geothermal power, and others Zachmann (2021); Miniard et al. (2020). Renewable energy has many advantages: in addition to the evident lower carbon footprint per MWh than fossil fuels, there have been significant declines in the capital cost of many sources of renewable electricity, such that those with high capacity factors (eg, onshore wind in northwest Europe and PV in the Middle East, Australia or southern USA) have lower unit electricity costs than conventional gas or coal plants Way et al. (2022).

Renewable energy also has some drawbacks related mainly to the variability of the underlying energy supply. Capacity factors of renewable generation depend strongly on the location and weather conditions, with values normally under 50%, versus conventional units that could theoretically reach up to 100%. Furthermore, the seasonal difference in output is tremendous, producing a surplus of energy in some moments and a deficit in others. This makes direct dependence on wind or solar power without any backup or long-duration storage system unfeasible. Batteries can play an important role in energy security in systems with high variable renewable electricity penetration, but for the foreseeable future, they will be limited to delivering storage over short time scales on the order of hours to a few days J. Liu et al. (2023).

Hydrogen, produced from electrolysis powered by renewable energy, is a promising energy carrier which can be stored for long periods and serve as backup for electricity generation IEA (2019) There is also a potential market for hydrogen in the ”hard-to-abate” sectors, those sectors that are more difficult to electrify, including heavy-duty industrial heat, heavy-duty transport, fertilizer, chemical production, and aviation fuels.

The different end uses of hydrogen have been evaluated in several papers. For instance, Gunawan & Monaghan (2021) evaluated under a techno-econo-environmental analysis different options to decarbonize the heavy-duty trucks, where hydrogen fuelcell trucks were one of the options evaluated. The decarbonization of fertilizers production was studied by Mostafaeipour & Sedeh (2019), where hydrogen is a key input for the process. In addition, Shahriar & Khanal (2022) shows how every single sustainable aviation fuel approved by the ASTM includes hydrogen as a crucial feedstock. On the other side, the production of hydrogen has also been extensively studied and within the large literature related to hydrogen production, we classify papers into two main categories, depending on the aim of the research:

1) Production-side supply chain (PSSC)
2) Systems side impact (SSI)

Those two categories are not mutually exclusive; furthermore, if integrated, PSSC could be embedded inside an SSI (see Figure 1). Nonetheless, the extant research tends to focus on one category or another when analysing hydrogen production systems. The first category is far more expansive in the extant literature. Typically, researchers try to optimize the production of hydrogen by using different types of algorithms and different supply chain configurations to meet the demand for the specific end use of hydrogen or to optimize equipment size, and try to maximize profit or minimise production cost in favour of the investor. In the second category, the literature mostly focuses on how hydrogen will be integrated into an energy systems level. An energy system model considers the interaction of different supply chains of energy vectors such as gas, electricity or hydrogen, usually on a national or regional scale. Those models evaluate the impact hydrogen will have on the energy system, by minimizing the system cost under a least-cost approach, sometimes only considering the electric system, and others a multi-energy system, i.e. that includes not only electricity but other energy vectors such as natural gas, biogas and/or oil. Both approaches are complementary, but they typically consider the outputs of one approach as inputs for the other. For instance, electricity demand and price are often outputs of an SSI approach and are considered an input for a PSSC, where normally, due to the small scale of production, the site's influence on the market can be considered negligible. The latter assumption is not accurate when bigger PSSC models are considered within an energy system, because they will have a significant effect on the energy system. Conversely, the size of the hydrogen production facility and equipment like electrolysers and storage are outputs of the PSSC, and are considered a fixed input in the SSI approach and not a variable due to the lack of technical detail in the production process in a system model. On the PSSC side, sometimes a disconnection with an SSI approach renders the modelling less accurate due to only considering one end use of hydrogen rather than considering hydrogen as a multi-purpose feedstock, under or overestimating the production of hydrogen.

Since hydrogen is projected to be produced at a large scale in several countries and regions, the effect that industrial-size renewable hydrogen facilities will have on the energy system is likely to be non-negligible. Some effects from hydrogen production may manifest in the power sector, by increasing power demand and supply and by replacing natural gas and or/electricity usage, consequently affecting the gas, heating and power prices. These effects have repercussions on the accuracy of the PSSC and SSI models. Since policymakers often use model outputs in designing policy, inaccurate integration of hydrogen production within energy system models could lead to suboptimal policies for the development of a net-zero energy system, making the integration of both systems an important issue to be addressed.

In this review, we analyse the existing literature to find the gaps in the knowledge related to the integration of SSI and PSSC models towards a more precise modelling approach. The original contributions of this study are:

- A comprehensive analysis of the different approaches taken on the energy systems modelling regarding hydrogen systems.
- Identification of the capabilities and gaps of existing models to answer future problems related to hydrogen being integrated into the energy system.
- Evaluation of the compatibility issues of different hydrogen models' approaches for future integration.
- Unveiling whether any research has addressed the marginal effect of big-scale hydrogen facilities over the energy system.

This research will only focus on literature dealing with hydrogen produced by means of electrolysis, primarily via renewable electricity, with some exceptions that consider grid electricity and non-renewable hydrogen production for the sake of comparison.

The objective of this paper is to identify the critical challenges in the different approaches reported in the literature that do not allow the generation of more accurate SSI and PSSC-integrated models. By being aware of the different approaches, in the next sections, the PSSC and SSI papers reported in the literature are presented and analyzed to understand how they could be better integrated into future optimization models. Further, a discussion about the main difficulties related to the integration of both approaches and some solutions proposed for these issues are presented followed by the conclusions.

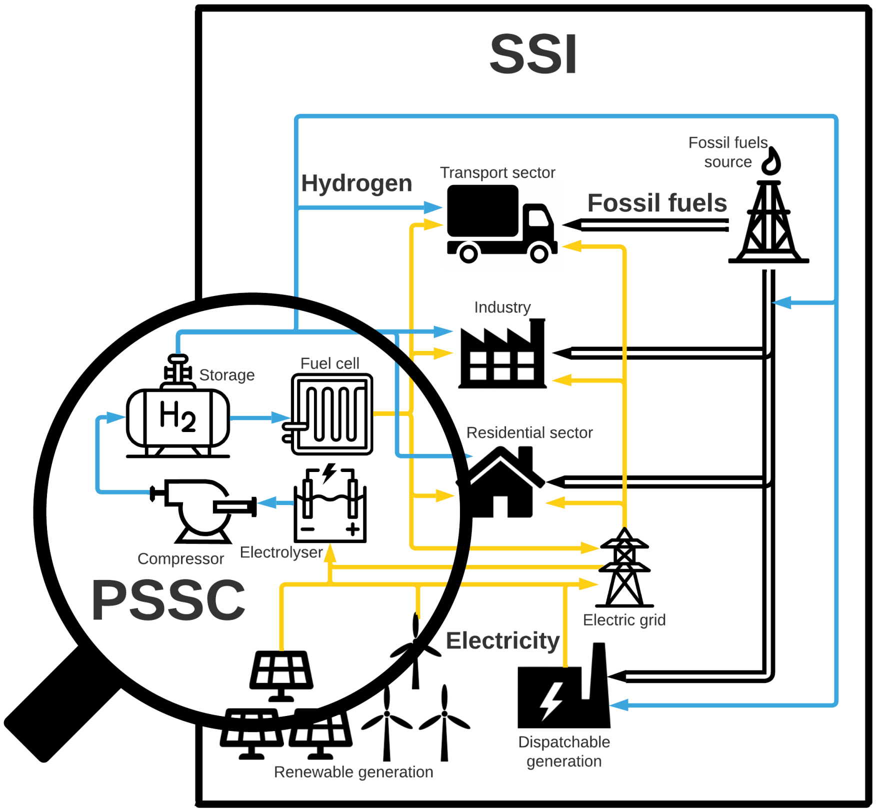

Figure 1: Graphical separation of hydrogen production models classification. Production side supply chain models are a more detailed version of the hydrogen production models but without considering other energy system elements. The systems side impact models consider hydrogen production but with less granularity and include all the other elements of the energy system.

2 Production-side supply chain literature

A Production-Side Supply Chain model usually aims to optimize the production of hydrogen or another energy vector by minimizing the operational and/or investment costs, or by maximizing the profit of the supply chain system. This is done by varying the size of the equipment involved or the energy flow towards the different unitary operations.

Typically, PSSC research includes detailed technical descriptions of the operation of the different supply chain elements. The most common setting of a PSSC considers a renewable source of electricity, which is usually of a variable nature. An energy management unit is also considered, which is the element that decides where and when the energy goes to each one of the elements of the system. The central part of every hydrogen production facility is the electrolytic system which usually is either an alkaline, a polymer electrolyte membrane (PEM) or a solid oxide electrolyser. Moreover, the systems consider compressors for the gaseous outputs of the electrolyser, or in less usual cases, a liquefaction plant or an ammonia production plant. Also, a storage system for the hydrogen, which could be of geological nature, compressed tanks or liquefied if a liquefaction plant is considered. A distribution system and sometimes a reconverting unit are also sometimes considered if energy is produced from hydrogen, that can be a hydrogen turbine or a fuel cell (see Figure 2). Some models also include alternative equipment, e.g. secondary electricity storage systems such as lithium-ion batteries or ultracapacitors, oxygen storage systems, and water purification units.

According to the aim of each study, the economic analysis will include or exclude some elements of the supply chain. For example, the renewable energy plant can be either inside or outside the boundaries of the study. When inside, the renewable energy plant's CAPEX and OPEX are included in the analysis (Figure 2D). When outside, renewable energy is considered an input at a certain price (Figure 2A). The same distinction can be made for hydrogen distribution equipment (Figure 2C). The boundaries and parameters of the study depend strongly on its aim: if the hydrogen system aims to produce electricity, as in Hernández-Torres et al. (2019); Singlitico et al. (2021), part of the electric system will be included and it is most likely that the economic results are expressed as the Levelized cost of electricity (Figure 2A). If the aim is to produce hydrogen, such as in Olateju et al. (2016); He, Mallapragada, Bose, Heuberger, & Gencer (2021), the boundaries may include a pipeline or a hydrogen transmission system, and the results might be expressed as a Levelized cost of hydrogen (Figure 2B).

Another important issue is the level of detail in the operation of the hydrogen system in the model. The novelties presented in hydrogen system operation models are different levels of detail in the dynamics of the electrolyser operation (e.g. ramp-up, shut down, cold and warm start), limits and leakage in the storage system, transportation pressures, and stack degradation and replacement.

Depending on the aim of the study the formulated problem can be classified into supply chain configuration optimization with or without investment optimization, or as an operation optimization problem. We define and discuss each below, with emphasis on the variables and parameters that determine the differences between the models, as well as the novelties of different systems presented in the literature.

2.1 Supply chain configuration optimization

2.1.1 Basic concepts of supply chain configuration optimization

Normally, research focused on optimizing the supply chain configuration aims to decrease the hydrogen or power production cost by changing the size of one or multiple pieces of equipment from the investor's point of view, usually including investment optimization algorithms. The given framework of each system, e.g. a fixed demand or a given renewable source available, defines the variables and parameters of the optimization problem (see Table 1).

2.1.2 Variables, parameters and scenarios commonly used

As mentioned, a significant number of studies usually use the size of the equipment as a decision variable to optimize the supply chain configuration. Within those equipment considered are the electrolyser Olateju et al. (2016); Scolaro & Kittner (2022); Glenk & Reichelstein (2019); Schnuelle et al. (2020); Armijo & Philibert (2020); Moran et al. (2023); He, Mallapragada, Bose, Heuberger, & Gencer (2021); Gunawan et al. (2020) and the storage Hernández-Torres et al. (2019); Eichman et al. (2016); He, Mallapragada, Bose, Heuberger, & Gencer (2021). There are also some studies that evaluate the type of storage in different scenarios Mallapragada et al. (2020); Moran et al. (2023), and in other cases, the technical specifications of the equipment are used as scenario parameters, such as efficiency Mallapragada et al. (2020); Vartiainen et al. (2022). In some cases, the supply chain configuration is given and an evaluation on other external factors is performed, for example by including or excluding energy system services revenues Eichman et al. (2016); Scolaro & Kittner (2022), different configurations for hydrogen export Gallardo et al. (2021), or the participation of grid electricity Raab et al. (2022); Jørgensen & Ropenus (2008); Eichman et al. (2016); Moran et al. (2023); Gunawan et al. (2020) which end up being different evaluated scenarios and not PSCC optimization models. The vast majority of models consider single sites as case examples, but in some cases, regional systems are considered and optimized following the approach of least cost optimization of power systems but without any effect over the power market He, Mallapragada, Bose, Heuberger, & Gencer (2021); Olateju et al. (2016). Some studies are more focused on the economic parameters of the projects and perform sensitivity analysis on the hydrogen production cost by varying the values of elements like variance factor, rebate, and annual inflation Rezaei et al. (2021); Vartiainen et al. (2022); Glenk & Reichelstein (2019); Scolaro & Kittner (2022). The different parameters and variables considered in every study reviewed are presented in table 2.

2.1.3 Main gaps

An important difference among these types of models is the size of the project. From a couple of kW of electrolysis capacity Glenk & Reichelstein (2019) to hundreds or thousands of MW Olateju et al. (2016); Scolaro & Kittner (2022); Raab et al. (2022); Vartiainen et al. (2022); Schnuelle et al. (2020); Singlitico et al. (2021); Moran et al. (2023); Gallardo et al. (2021). Due to economies of scale and the configurations and locations assumed in each study, the range of hydrogen production levelized costs, without considering hydrogen storage or distribution, is very wide and has been reported to go from 0.3 €/kgH_2 up to 12.38 €/kgH_2, as shown in Table 4.

Another important issue with the different scales of the projects are the assumptions made. In modelling small hydrogen systems, it is reasonable to assume that the effect produced by the project over the system is negligible. In the opposite case, when hundreds of MW of installed capacity are part of a supply chain, it is necessary to consider the effects the hydrogen system has on the energy system, and this aspect has not been addressed by mentioned studies.

This co-dependency with the energy system, if compared with off-grid hydrogen production, increases with supply chains that are connected to the grid, generating demand and/or supply of power. Several studies argue that connecting electrolysers to the grid could increase the capacity factors and produce cheaper hydrogen Raab et al. (2022); Vartiainen et al. (2022); Moran et al. (2023); Glenk & Reichelstein (2019). In some cases, considering connecting the hydrogen system to the power market allows to increase the revenues due to the ancillary services that these systems could supply Eichman et al. (2016); Scolaro & Kittner (2022). The participation of electrolysers and hydrogen storage in the energy services market will tighten even more the relationship between hydrogen systems and energy systems. From the supply chain configuration optimization models, will be essential to consider the optimization process of the size, location, and configuration, as well as the sensitivity analysis for further research that includes the effect on the energy system.

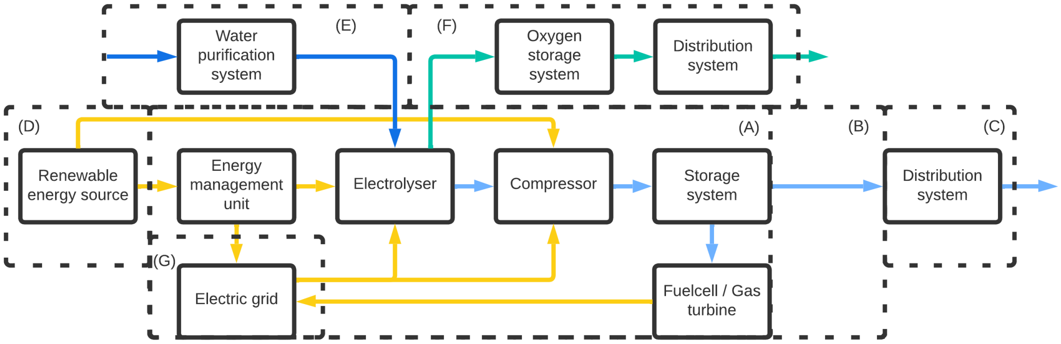

Figure 2: General hydrogen production supply chain elements with some example model boundaries. yellow arrows represent electricity, blue arrows represent a water flow, turquoise arrows show oxygen streams, and light blue arrows represent hydrogen streams. (A) Boundaries of a model that focuses on producing only electricity. (B) Boundaries of a model that produces electricity and hydrogen. (C) Hydrogen distribution system included. (D) Renewable generation plant included. (E) Water supply chain included. (F) Oxygen system included. (G) Electricity grid included

2.2 Operation optimization

2.2.1 Basic concepts of operation optimization models

Other PSSCs are focused only on the operation of the supply chain and try to optimize it, hence, only attend to the operational expenses of the system, neglecting the capital expenditures. The decision variables of these types of models are usually the working times of each equipment and the flows of energy or mass provided to each node. The parameters are the given system specifications and the energy system inputs, like power prices, hydrogen and power demand, etc (see Table 1)

2.2.2 Configuration examples

This literature aims to consider multiple operational modes and/or end-uses for hydrogen, including backup generation and selling hydrogen as a fuel or feedstock to demonstrate the capacity of the system for supplying multiple demands Korpås & Holen (2006); Proietto et al. (2014); Mansour-Saatloo et al. (2020); Agabalaye-Rahvar et al. (2021); Utomo et al. (2021); Mansour-Satloo et al. (2021). As in the Supply chain configuration optimization, in some cases, the innovation is on the production configuration side. New elements are added and the algorithm proves how the operation could supply the demand requested. For example, González-Rivera et al. (2020) explore the possibility of a hybrid storage system with hydrogen and an ultracapacitor, while Proietto et al. (2014) and Mansour-Satloo et al. (2021) consider solid-state hydrogen storage systems as part of their energy hub and optimize its operation. Similarly, there are other papers in which the innovation is on the algorithm side, where more detail on the operation is included, such as avoiding the excessive discharging or overcharging of the storage tank, limiting the power rate to protect the fuel cell and the electrolyzer Shehzad et al. (2019), cold and warm starts differentiation, minimizing the switching between different operating states Abdelghany et al. (2021), and adding financial risk evaluation Xiao et al. (2020). All the different approaches and novelties presented by the operation optimization models can be found in table 3.

2.2.3 Main gaps

Normally these evaluated systems have a size that goes up to a couple of MW of electrolysis, which can be easily assumed as negligible on a national or regional-wide energy system, but in some cases, these systems are located in places that are more isolated from the rest of the system, which could mean they are more constrained to obtain power supply due to a lack of infrastructure Korpås & Holen (2006). Hence, the relation between the energy system and the supply chain model cannot be always avoided, especially if the grid connection is assumed to be endlessly capable to provide or absorb power from the supply chain under study in places with restrictive transmission infrastructure Utomo et al. (2021); Abdelghany et al. (2021), or if ancillary services Proietto et al. (2014) or demand response programs

Mansour-Saatloo et al. (2020); Mansour-Satloo et al. (2021) are considered. The major contributions of the operation optimization models are the technical level of detail of the operation and dynamics of the hydrogen systems, which will be very important to consider in further research that includes the active relationship between the supply chain and the energy system.

Table 1.

Type of model	Typical parameters	Typical Variables	Typical scenarios
Supply chain configuration optimization	Equipment specification, renewable power generation, hourly electricity price, economic parameters.	Equipment size (mainly electrolyser and storage), mass flow to the different equipment, power purchased from the grid.	Location, operation modes (only electricity, only hydrogen, both), variation on the economic indicators, grid participation, year, sensitivity on CAPEX, type of hydrogen storage (geological, tanks, etc), type of electrolyser (Alkaline, PEM, etc).
Operation optimization	Equipment specification, renewable power generation, hourly electricity price, ancillary services revenue, demand (of hydrogen, electricity and/or heat).	Mass flow to the different equipment and operation, power purchased from the grid.	Adding demand response, year, adding novel equipment to the system, renewable generation (low or high), sensitivity on electricity prices.

Table 2.

Reference	Approach	Systems description	Novelty	Techno-economic assessment	Objective function	Energy market inputs	Variables & scenarios	Parameters
Olateju et al. (2016)	Supply chain optimization (investment optimization).	Wind capacity: 563 MW. Electrolysis: 283 MW. Located in Alberta, Canada.	Operational and techno-economic model for H2 production from a wind farm.	Yes.	Minimizing H2 production cost.	Hourly wholesale electricity price.	Variables: Electrolyser and battery size, operation of equipment. Scenarios: modes of operation (only hydrogen, only electricity, etc).	Parameters: Equipment specification data, hourly average wind energy data, hourly grid electricity price.
Scolaro & Kittner (2022)	Supply chain optimization (investment optimization).	Electrolyser: 131 MW (optimized), offshore wind farm: 150 MW. Located in Rostock, Northern Germany.	Optimize the size of an electrolyzer in a wind farm by considering the selling of hydrogen and electricity with possible backup generation from hydrogen and the optimized revenues of ancillary services showing higher costs if a fuel cell is involved. Also, carbon abatement costs were discussed.	Yes (simplified revenues of ancillary services and cost of power).	Yearly revenues maximized.	Hourly wholesale day-ahead power prices, Frequency Containment Reserves (FCR), Automatic Frequency Restoration Reserves (aFRR), and Manual Frequency Restoration Reserves (mFRR).	Variables: Energy bid, capacity bid, hydrogen price, electrolyser size, equipment operation. Scenarios: Sensibility analysis based on different economic parameters.	Parameters: Equipment specification data, grid electricity prices, frequency regulation services remuneration.
Glenk & Reichelstein (2019)	Supply chain optimization (investment optimization).	Electrolyser: 0.01 - 0.29 kW. Located in Texas & Germany.	Development of an analytical framework for general hybrid energy systems from the perspective of an investor.	Yes.	Maximize NPV	hourly wholesale electricity price.	Variables: equipment size. Scenarios: alternative hydrogen prices, adjustment rate of electricity price, rebate, and variance factor.	Parameters: Equipment specification data and cost, wind capacity factor, electricity price, the selling price of electricity, the conversion rate of Power-to-Gas.
Raab et al. (2022)	Supply chain optimization (investment optimization).	Electrolyser: 1.8 – 3.7 GW. Various locations.	Effect of grid electricity in the production of renewable hydrogen costs.	Yes.	Minimize annual costs	Fixed grid electricity prices.	Variables: equipment size. Scenarios: Location, allowed grid participation. Sensibility analysis regarding PV and electrolyser costs and data.	Parameters: Required hydrogen flow, constraints added by the user, equipment specification data and cost, weather data, and grid energy cost.
Jørgensen & Ropenus (2008)	Supply chain optimization.	Located in West Denmark.	Hydrogen production from grid electricity with high penetration of renewable sources. Inclusion of hourly grid prices. Peak shaving and part-time operation do not bring a great benefit to the economy of the process.	Yes.	Minimize hydrogen production price.	Hourly grid electricity prices.	Variables: Operation hours. Scenarios: wind power penetration, sensitivity analysis on Annual fixed capital cost.	Parameters: hourly electricity price (parametrized based on wind power, consumption and power price evolution).
Eichman et al. (2016)	Supply chain optimization.	Electrolyser: 1 MW. Located in California, USA.	Hydrogen production from grid electricity with a focus on ancillary services revenues. Hydrogen produces more revenue if sold and not for producing electricity (no mechanisms are available). The tightest the electricity market with hydrogen production, the better for both systems.	Yes.	Maximize the operational profits.	Hourly day-ahead electricity prices and 4 ancillary services: Regulation up and down, spinning reserve and non-spinning reserve.	Variables: Operation of the equipment, selling and buying power. Scenarios: supply chain configuration (fuel cell, batteries, energy market participation, ancillary services, etc), energy storage duration.	Parameters: hydrogen daily production, equipment size, supply chain cost and technical data (range), hydrogen selling price (range).

Hernández-Torres et al. (2019)	Supply chain optimization.	Wind farm: 8 MW Located in French islands (Guadalupe and Reunion)	Optimize the size of Li-ion batteries and/or H2 system for energy storage using techno-economic oriented modelling with day-ahead commitment.	Yes, but LCOE is the main result.	Multi-objective Optimization: Minimize LCOE and Failure of commitment. Obtains a Pareto front.	Two ancillary services: Day-ahead commitment with power production smoothing, and Primary energy reserve.	Variables: storage size. Scenarios: configurations of the supply chain (hydrogen storage and fuel cell and/or Li-ion batteries) Sensitivity analysis on the CAPEX.	Parameters: Equipment specification data, degradation curve, ancillary services, electric power availability profile from the wind farm.
Mallapragada et al. (2020)	Supply chain optimization (investment optimization).	36,500 tonneH2/year (different electrolyser sizes). Located in the USA.	Cost-effectiveness examination of PV-based hydrogen at an industrial scale with different storage options along the USA. Comparison between batteries and natural gas with CCS.	Yes.	Minimize hydrogen production costs.	Gas prices.	Variables: equipment size. Scenarios: location, storage type (geological or pressure vessel), different meteorological years, electrolyser efficiency, storage fixed operating and maintenance cost, minimum annual plant availability, and storage CAPEX.	Parameters: specific hourly production of hydrogen, electric power availability, equipment specification and operation data.
Vartiainen et al. (2022)	Supply chain optimization.	Electrolyser: 100 MW. Various locations	Estimation of hydrogen production costs from PV in 10 different locations around the globe.	Yes.	No optimization, calculation of LCOH based on assumptions and sensitivity analysis.	No energy market inputs are considered.	Variables: none. Scenarios: sensitivity analysis on location, nominal WACC, annual inflation, PV volume growth, electrolyzer LR, FLH, CAPEX, volume growth, OPEX, efficiency, lifetime, and stack replacement.	Parameters: Equipment specification and operation data.
Armijo & Philibert (2020)	Supply chain optimization (investment optimization).	Electrolyser: 60.2 MW. Located in Chile & Argentina.	Hydrogen and ammonia production from renewable hydrogen is produced in Chile & Argentina. Hybridization of wind and solar power decreases costs. The flexible operation of Haber-Bosch process effects is evaluated.	Yes.	Minimize LCOH.	No energy market inputs are considered.	Variables: the ratio between solar capacity and electrolysis capacity, the ratio between wind capacity and electrolysis capacity. Scenarios: location, hybridization of solar and wind power, flexible operation of Haber-Bosch process.	Parameters: Equipment specification and cost data, power generation profiles.
Schnuelle et al. (2020)	Supply chain optimization (investment optimization).	Electrolyser: 4.8 – 320.1 MW. Located in Northwest Germany.	Techno-economic analysis of dynamic hydrogen production with a detailed electrolysis model and policies considerations for renewable sources.	Yes.	Operation of the electrolyser follows a dynamic behaviour model and once the operation fed by the renewable electricity is defined, a techno-economic analysis is performed to obtain the LCOH.	No energy market inputs are considered, but fixed subsidization tariffs are assumed.	Variables: Electrolyser capacity (% of maximum power input according to the energy source). Scenarios: renewable electricity power source, type of electrolyser (Alkaline or PEM).	Parameters: Equipment specification and cost data, power generation profiles, fixed subsidization tariffs.
Rezaei et al. (2021)	Supply chain optimization.	4.09-5.49 tonneH2/year. Located in Lutak, Iran.	Hydrogen and renewable electricity are generated from a wind farm in Iran. Consideration of environmental penalty and degradation factor of the wind farm.	Yes.	Arithmetical method for LCOH and LCOE calculation.	No energy market inputs considered.	Variables: none. Scenarios: degradation rate of the wind power plant, difference between interest rate and inflation, selling price of hydrogen.	Parameters: Equipment specification and cost data, the capacity factor of the wind farm.

Singlitico et al. (2021)	Supply chain optimization.	Electrolyser: up to 12 GW, Wind farm: 12 GW. Located in the northern sea in front of Denmark.	Evaluates different scenarios of hydrogen production and supply chain configurations. Offshore, onshore and in-turbine electrolyser. Different electrolysers types. Electricity or hydrogen-driven production.	Yes.	Arithmetical method for LCOH and LCOE calculation.	No energy market inputs are considered.	Variables: None. Scenarios: electrolysers types (PEM, Alkaline, SOEL), hydrogen or electricity driven, electrolyser location (offshore, onshore or in-turbine), sensitivity analysis on the distance to shore and equipment cost.	Parameters: equipment specification and operation data, wind data.
Moran et al. (2023)	Supply chain Optimization (investment optimization).	Electrolyser: 2.5 – 138 MW. Located in Ireland.	Flexible techno-economic model that calculates optimal electrolyser capacity, LCOH, and equivalent CO2 emissions savings. It considers storage, different technological options, and different possible scenarios for hydrogen production.	Yes.	Minimize LCOH.	Hourly wholesale market electricity price and curtailment considered.	Variables: Electrolyser size, maximum bid price. Scenarios: The model allowed to change the type of electrolyser, type of storage, distribution method, end-uses, source of electricity, etc.	Parameters: hourly wind, solar, and electricity market price data, hourly demand profile for Hydrogen, storage capacity, specific CAPEX and OPEX, downtime for maintenance.
Gallardo et al. (2021)	Supply chain Optimization.	Electrolyser: 105.8-400.2 MW. Production from direct PPA and/or with PV or concentrated solar power (CSP) with thermal energy storage (TES). Located in the Atacama desert, Chile.	Production, exporting and reconversion techno-economic model of hydrogen (ammonia and liquefied hydrogen for export) from Chile to Japan.	Yes.	No optimization, calculation of LCOH based on assumptions and sensitivity analysis.	Power purchase agreements costs based on historic values.	Variables: None. Scenarios: Alkaline or PEM electrolysis, direct connection to a PV, CSP plant or using a PPA (PV or CSP), the year (2018 or 2025), different types of exporting. Sensitivity analysis was done with water cost, CAPEX variation, and electricity cost.	Parameters: Equipment CAPEX, OPEX and specifications, transport technical and economic characteristics, electricity cost, hydrogen demand, renewable generation profiles.
He, Mallapragada, Bose, Heuberger, & Gencer (2021)	Supply chain optimization (investment optimization).	Different zones with different demands, being the highest 40 tonne/hour of hydrogen. Located in the U.S. Northeast region.	Detailed optimization model with a focus on production, storage, and transmission. It considers detailed flexible truck scheduling, a wide range of production and storage technologies, and decreased computational requirements by simplifying key equations in the transmission model. Considers emissions costs as part of the objective function.	Yes.	Minimize hydrogen cost.	Hourly price of electricity.	Variables: capacities & numbers of units for production, storage, compression, and transmission, hourly operational schedules of the resources. Scenarios: different carbon prices, electrolyser CAPEX, 50% pipeline cost, truck travel time.	Parameters: Electricity cost, equipment and transmission infrastructure specification and costs, distance between zones, hourly hydrogen demand.
Gunawan et al. (2020)	Supply chain optimization (investment optimization).	Electrolyser: less than 500 kW up to 8 MW. Located in different wind farms in Ireland.	Evaluates the economics of different electricity profiles to produce hydrogen at different wind farms in Ireland and deliver it to the existing gas network.	Yes.	Minimizes the levelized cost of hydrogen production, a sub-model minimizes the levelized cost of hydrogen transportation.	fixed grid electricity price (high and low values).	Variables: Electrolyser size and all the equipment depending on the size of the electrolyser. Scenarios: Electrolyser electricity supply (curtailment, available wind, full capacity), electricity prices, year.	Parameters: Equipment cost, location, distance from each wind farm to the injection nodes, equipment specification, wind generation data.

Table 3.

Reference	Approach	Systems description	Novelty	Techno-economic assessment	Objective function	Energy market inputs	Variables & scenarios	Parameters
Korpås & Holen (2006)	Optimal operation.	Wind farm: 600 kW Electrolysis: 300 kW. Located in Norway, an Isolated system	Hydrogen production system for electricity back-up and selling. Optimization of operation for maximization of profits.	No, only OPEX and replacement of stacks.	Maximize profits in an online modelling scheme.	Day ahead spot market (price and demand).	Variables: Operation of the electrolyser and fuel cell. Scenarios: 3 case examples of different power systems (thermal-based, Norwegian system, isolated system)	Parameters: Day ahead spot market (price and demand), size and specification of equipment, wind power profile, hydrogen price.
Proietto et al. (2014)	Optimal operation.	Electrolysis: 1.15 MW. Fuel cell: 1 MW. Located in Troia, Italy.	Energy management algorithm with non-linear optimization for hydrogen solid-state storage in a multi-carrier energy hub.	No, only OPEX.	Maximize operational revenues.	Hourly prices of electricity and ancillary services.	Variables: hydrogen delivered to the fuel cell, the power delivered to the electrolyser (for electricity generation or selling). Scenarios: none.	Parameters: hydrogen price, hourly electricity price, specific ancillary services revenues, fuel cell and electrolyser efficiencies.
Mansour-Saatloo et al. (2020)	Optimal operation.	Electrolysis: 30 kW. Fuel cell: 30 kW.	A robust Optimization method was applied to a smart micro-energy hub scheduling model to address power price uncertainty.	No, only OPEX.	Minimize the total cost of the system over the time horizon.	Hourly electricity and gas price	Variables: equipment operation. Scenarios: Adding demand response, adding hydrogen storage system, solving method.	Parameters: size and specification of equipment, wind profile, hourly electricity and gas prices.
Agabalaye-Rahvar et al. (2021)	Optimal operation.	Wind farm: 50 kW. Electrolyser: 20-80 kW.	A Multicarrier energy hub with hydrogen generation was optimized by considering a bi-objective scenario-based stochastic approach that minimizes emissions and operational cost.	No, only OPEX.	Minimize the total amount of emissions and total operational cost minimized as a bi-objective function.	Hourly wholesale day ahead electricity and natural gas prices with stochastic normal distribution probability function. Prices are an input. Integrated demand response program.	Variables: equipment operation. Scenarios: case studies (only thermal and electric storage system, adding hydrogen system storage, and adding integrated demand response program	Parameters: Electricity and natural gas prices scenarios, electric and thermal demands, CO2 emissions factors, specification of equipment, wind speed and solar irradiation, cost of electrical and thermal curtailed and shifted demand.
Utomo et al. (2021)	Optimal operation.	Wind farm: 750 kW. Electrolyser: 370 kW. Located in Levenmouth, Scottland.	Hydrogen storage and fuel cell system are managed optimally to meet electric and FCV demand by considering forecasts.	No, only OPEX.	Minimize the operational cost of the system.	Electricity prices and demand profiles.	Variables: equipment operation, high or low renewables scenario.	Parameters: Equipment size and specifications, electricity prices and demand profiles, renewables generation profile.
Mansour-Satloo et al. (2021)	Optimal operation.	Electrolysis: 30 kW, Fuel cell: 30 kW.	A hybrid robust/stochastic approach was used to alleviate the uncertainty of wind power, energy demands, and electricity prices on an energy hub. Considers solid state hydrogen storage.	No, only OPEX.	Minimize total operating costs.	Hourly electricity and gas price. Adds a demand response program.	Variables: equipment operation. Scenarios: adding demand response, adding hydrogen storage system, sensitivity on price deviation and uncertainty budget impact.	Parameters: size and specification of equipment, wind profile, hourly electricity and gas prices, electrical, gas and thermal demand.
González-Rivera et al. (2020)	Optimal operation.	Wind capacity: 1.5 MW. Electrolyser: 350 kW, Fuelcell: 450 kW	Development of a supervisory control system for a hybrid energy storage system that considers a hydrogen storage system and an ultracapacitor (UC) driven by a wind farm.	No.	Optimize the operation to satisfy demand by protecting the state of charge of the ultracapacitor.	Day ahead electricity prices	Variables: Equipment operation. Scenarios: study cases (constant regulation of the state of charge of the ultracapacitor, change in the state of charge of the ultracapacitor).	Parameters: Wind turbine generation, Day-ahead estimation of the wind turbine power generation, power requested by the grid, power exchange between hydrogen system and UC, day-ahead electricity prices.

Shehzad et al. (2019)	Optimal operation.	Electrolyser: 3 MW, Fuel cell: 132 kW. Located in Raggovidda, Norway.	A model-Based Predictive Controller is used to minimize the degradation of the hydrogen storage system and the load tracking error. It considers operational constraints and dynamics.	No, only OPEX and replacement of stacks.	Minimize the operational costs of the electrolyser and fuel cell, and also the error between the delivered power and the forecasted demand.	Bid price and forecasted demand	Variables: Equipment operation. Scenarios: two examples of operation.	Parameters: Power demand reference, wind power profile, electricity price, equipment specification data.
Abdelghany et al. (2021)	Optimal operation.	Electrolyser: 3 MW, Fuel cell: 132 kW. Located in Norway	Implements a model-based predictive controller for a hydrogen energy storage system that considers degradation, cold and warm starts, minimization of switching among operational states, and revenue maximization.	No, only OPEX and replacement of stacks.	Minimize a cost function that includes: error between the delivered power and the forecasted demand, cost of selling/buying energy, and operational costs of the hydrogen storage system.	Bid price and forecasted demand	Variables: Equipment operation, power purchased from the grid. Scenarios: only one operation example.	Parameters: Power demand reference, wind power profile, electricity price, equipment specification data.
Xiao et al. (2020)	Optimal operation.	Wind farm: 1400 kW Electrolyser: 1000-1300 kW. Located in Denmark.	Proposes a wind-electrolytic system with electricity/hydrogen market-oriented operation optimization with risk consideration.	No, only OPEX.	Maximize revenues and considers Conditional Value at Risk.	Electricity prices	Variables: equipment operation. Scenarios: risk factor, hydrogen selling price, the maximum size of the electrolyser, system with or without power and/or hydrogen market.	Parameters: wind power and electricity prices stochastic scenarios, equipment specification data.

Table 4: Levelized Cost of Hydrogen in different Production-Side Supply Chain models reported in the literature.

Study	Location	Year	Electricity supply	Capacity	LCOH (not adjusted for inflation)
Schnuelle et al. (2020)	Northern Germany	2020	Wind & PV	252.1-21,044.6 tonne/year (around 4 tonne/year for PV)	4.33-12.38 €/kg (no storage & no distribution of H_2)
Mallapragada et al. (2020)	USA	2030	PV	36,500 tonne/year	1.98-4.00 $/kg (no distribution of H_2)
Vartiainen et al. (2022)	Various	2020	PV	Not specified (100 MW electrolyser)	1.0-2.7 €/kg (no storage & no distribution of H_2)
Vartiainen et al. (2022)	Various	2030	PV	Not specified (100 MW electrolyser)	0.7-1.8 €/kg (no storage & no distribution of H_2)
Vartiainen et al. (2022)	Various	2050	PV	Not specified (100 MW electrolyser)	0.3-0.9 €/kg (no storage & no distribution of H_2)
Raab et al. (2022)	Various	Not specified	Wind, PV, and Grid	225,482 tonne/year	4-6 €/kg (down to 2.5 €/kg with perspective cost data) (no distribution of H_2)
Scolaro & Kittner (2022)	Northern Germany	2025	Wind	10,040 tonne/year	4.9-7.25 €/kg (no distribution of H_2)
Olateju et al. (2016)	Alberta, Canada	Not specified	Wind	21,900 tonne/year	3.37-9.00 $/kg (no storage & no distribution of H_2, batteries)
Armijo & Philibert (2020)	Chile and Argentina	2020	Wind & PV	Not specified (60.2 MW electrolyser)	1.94-2.33 $/kg (no storage & no distribution of H_2)
Rezaei et al. (2021)	Lutak, Iran	Not Specified	Wind	4.09-5.49 tonne/year	1.375-1.59 $/kg (no storage & no distribution of H_2)
Jørgensen & Ropenus (2008)	Denmark	Not Specified	Grid with high variable renewable generation	Not specified	4.89-5.37 €/kg (no storage & no distribution of H_2)
Singlitico et al. (2021)	Northern sea, Denmark	20230	Offshore wind	Not specified (up to 12 GW electrolyser)	min value 2.4 €/kg (depending on the supply chain configuration)(no storage of H_2)
Glenk & Reichelstein (2019)	Texas & Germany	2020 & 2030	Wind	Not specified (0.01-0.29 kW electrolyser)	3.23-3.53 €/kg (2030: 2.5 €/kg) (no storage & no distribution of H_2)
Moran et al. (2023)	Ireland	2030	Wind, curtailed & grid	400-21000 tonne/year (2.5 – 138 MW electrolyser)	2.75-3.95 €/kg
Gallardo et al. (2021)	Chile	2018 & 2030	Solar PV and CSP with TES	16 ktonne/year (105.8-400.2 MW electrolyser)	2018: 2.2 2025: 1.67$/kgH2 €/kg
Gunawan et al. (2020)	Ireland	2020 & 2030	Wind and grid	2020: 13-39 ktonne/year, 2030: 16-49 ktonne/year (national production)	2020: 9-25 €/kgH_2, 2030: 6-15€/kgH_2

3 Systems side impact literature

A model that considers the effect on a wider energy system of a particular supply chain and/or the integration of different supply chains and locations within a particular energy system can be considered a systems side impact model. Normally, these models try to minimize the costs of the whole system from the perspective of the system operator. Some of the main objectives of energy systems modelling is to predict tendencies in prices, demands and supply availability, and propose policies.

With the decarbonization of energy systems, many modelling challenges need to be addressed. Pfenninger et al. (2014) describes four major challenges in the development of accurate energy systems models; issues with spatial and temporal resolution, uncertainty and transparency balancing, increase in complexity of the energy system, and assessing social risk and opportunities with human behaviour. According to Lai et al. (2021), current long-term electrical power system models do not properly address high renewable generation penetration and energy storage systems. They claim that current long-term electrical power system models, due to computational complexity and cost, cannot integrate the short-term temporal changes of energy storage and renewable generation. To accurately predict how energy systems are going to behave with high penetration of renewable generation, energy systems modelling research has developed quickly in the last years.

To address the challenges of high penetration of renewable generation such as intermittency and variability of supply, different approaches have been taken.

Despite the relatively recent interest in the impact of hydrogen on energy systems, some studies have been published with different focuses on the subject. According to the hydrogen system modelling taxonomy proposed by Blanco et al. (2022), there are many different approaches to studying the effects of hydrogen on energy systems. Starting with power system models, i.e. which consider the electric system of a region or nation, followed by energy system models which include the previous one, and integrated assessment model which comprises all previous-mentioned types of models, making it the most complete of those. There are other types of models mentioned with more specific purposes like the city or sectoral analysis such as transport focused models, but since those represent smaller or fractions of systems were not considered in this study. Since integrated assessment models are energy systems models with extra analysis on the carbon footprint of the systems or other environmental/social impact assessment, only power and energy systems models were considered as categories. It is interesting to mention that hydrogen supply chain models, according to Blanco et al. (2022), have not been integrated into the energy systems or integrated assessment models so far in any study.

In this section, power and energy systems models are described and analysed with examples of studies presented in literature, which are presented also in Table 6.

3.1 Power systems models

3.1.1 What defines a power system model

A power systems model is a type of model that only considers the electric sector, which includes the generation, transmission, demand, and sometimes distribution. Depending on the aim of the study the approaches and assumptions in each model can vary, but in all cases, a major emphasis on the power system is taken. Even though there are some exceptions, usually, power system models focus on searching for the least-cost solution while respecting constraints including delivering power to the demand centres, and limitations in generation. This is reached by varying the operation schedules of each unit included in the model and in most cases also by changing the capacity of the equipment involved. The usual parameters utilized by these types of models are the equipment specification, fixed and variable operating costs of each unit, the electric demand, and renewable power generation. It is also common for these types of models to compare different scenarios where demand response, a base load of certain units, different weather conditions and years, and flexible operation of units are considered to formulate the scenarios (see Table 5).

3.1.2 Different approaches and objectives of power system models

Different studies have made use of power system models to answer different research questions. Among them are the impact of including hydrogen systems within a power system Mirzaei et al. (2018); Ruggles et al. (2021); Nojavan et al. (2017); Zhang et al. (2020) and the sizing of hydrogen storage for improving energy resilience in a particular power system Ali et al. (2018); Marocco et al. (2023); Guerra et al. (2023). The impact of hydrogen systems in power systems was evaluated by adding a hydrogen demand Zhang et al. (2020), hydrogen production from excess electricity Ruggles et al. (2021), or using hydrogen to produce electricity Mirzaei et al. (2018); Nojavan et al. (2017); Marocco et al. (2023); Guerra et al. (2023). Besides, the sizes of the systems also varied, from relatively small systems in the MW scale Mirzaei et al. (2018); Nojavan et al. (2017); Marocco et al. (2023), up to whole countries energy systems Ruggles et al. (2021); Zhang et al. (2020); Ali et al. (2018); Guerra et al. (2023). Moreover, there are studies that considered investment as a central part of their analysis Ruggles et al. (2021); Marocco et al. (2023) and in other cases, only the impact on the operational level is evaluated (percentage of curtailment, operational costs, etc) Mirzaei et al. (2018); Nojavan et al. (2017); Zhang et al. (2020); Ali et al. (2018). Further, not every study considered the elements of the supply chain as part of the variables (size of equipment/units). Those that did consider the hydrogen supply chain elements as variables were able to evaluate the effect of different sizes of equipment in the performance of the power systems in environmental terms Zhang et al. (2020) or in fostering the investment in new renewable generation units Ruggles et al. (2021), as well as assessing the effect on the size of storage of different demand profile scenarios Ali et al. (2018). The different demand profiles are also recurrent in these types of models and the effect of including hydrogen systems and demand response programs on a power model has been substantially assessed Ali et al. (2018); Mirzaei et al. (2018); Nojavan et al. (2017); Ruggles et al. (2021).

3.1.3 Hydrogen in power system models

As mentioned previously, hydrogen systems can play an important role in power systems due to their flexible operation and capacity to store energy, but different challenges need to be addressed like the constraints in the transmission lines, gas storage, and profitability. One issue addressed in power system studies was the effect of including hydrogen on existing power systems. In general, the reported effects of hydrogen in power systems include: decrease in wind curtailment and daily operating costs Mirzaei et al. (2018), an increase in renewable generation investment Ruggles et al. (2021); Zhang et al. (2020), and retailers revenues increase Nojavan et al. (2017). However, if hydrogen storage is added to the system to produce electricity it could decrease the requirements for oversizing renewables capacity to fulfil the demand Marocco et al. (2023). In addition, hydrogen combined cycle gas turbines add inertia to the system, a feature that in a highly renewable penetration power system will be more scarce Guerra et al. (2023). Another topic evaluated by a couple of studies was the flexible operation of electrolysers, which could decrease curtailment of renewable power Ruggles et al. (2021), carbon emissions and systems costs Zhang et al. (2020). Besides, Ruggles et al. (2021) highlights how the flexible load generated by electrolysers is not tied to a certain daytime, which is a desirable feature for the operator.

3.1.4 Limitations of power systems models

Despite the variety of focuses in the power systems models presented above, none of the mentioned have considered other types of energy sectors, which is not realistic if hydrogen is produced due to its trans-sectoral nature. Besides, in some cases, hydrogen was considered for selling as a commodity (outside the energy system boundaries), and in others used as backup for electricity production. Both approaches could be considered at the same time and produce a more robust model at national scale. Furthermore, since renewable hydrogen is tied to the power sector, their interaction could include ancillary services revenues as part of a more complete analysis of the power market.

3.2 Energy systems models

3.2.1 Definition, parameters, and variables involved

An energy system model includes a power systems model as well as other energy carriers at large, meaning national or regional or transnational, scale. These other energy carriers include gas networks or other fuel supply chain system. Those supply chain normally interact with each other, e.g. gas networks interact with the power system when electricity is produced from gas turbines. As a general rule, these types of models are oriented to find the least cost solution of the whole system, simulating a central operator point of view. The total system cost includes operating costs and in some cases investment optimization. The usual variables of these systems are the operation of each of the units and, as mentioned, new investment if investment optimization is considered. Further, the parameters considered by these models are renewable generation profile, equipment specification, specific costs of investment, base installed capacity and transmission infrastructure. Morover, several different scenarios are usually evaluated in energy system models, e.g. different years, production of synthetic fuels from hydrogen, adding renewable targets or quotas of hydrogen, among others (see Table 5).

3.2.2 Effects of hydrogen in energy systems: operation flexibility

The presence of hydrogen increases the flexibility of energy systems. This is mostly due to the multi-sectoral nature and buffer effect that hydrogen storage can offer. In an optimization model, this can be expressed as an increase in the solution space or the degrees of freedom of the problem, produced by the addition of a new variable. By adding hydrogen systems into an energy system the operating space of the system increases and the optimal operating solution can have more slack without compromising fulfilling the energy demand or the cost of energy Chicco et al. (2020). Besides, hydrogen and power-to-gas technologies can decrease carbon and SOx emissions as well as the operational costs W. Liu et al. (2021) and total costs of the system (with investment included) He, Mallapragada, Bose, Heuberger-Austin, & Gençer (2021). Besides, if hydrogen systems are deployed within an energy system it increases the total variable renewable generation He, Mallapragada, Bose, Heuberger-Austin, & Gençer (2021). The increase in investment due to the new renewable capacity installed could lead to an increase in electricity prices (in an Irish context, around 1-2%) Longoria et al. (2021).

3.2.3 Effects on the investment

The investment in hydrogen production depends strongly on the new renewable capacity installed and on the renewable targets imposed. For instance, if high carbon taxes are imposed, the hydrogen industry development will be quicker and will reach big importance by 2040 and a moderate development by 2030 O'Dwyer et al. (2022). The technology that will be deployed for hydrogen production also depends on the policies applied, where Steam Methane reforming (SMR)-based hydrogen could dominate the industry if no carbon emission restrictions are applied Navas-Anguita et al. (2020); He, Mallapragada, Bose, Heuberger-Austin, & Gençer (2021), but if more strict restrictions are considered, renewable hydrogen comming from biomass gasification and water electrolysis will be the principal production technologies Navas-Anguita et al. (2020). As mentioned previously, the increase in investment in the energy sector will negatively affect the prices of electricity for the consumers, but the producers of renewable energy and PtG owners will be the big economically benefited entities due to the subsidies and other tributary benefits that will receive during the energy transition period Schlund & Schönfisch (2021). This points to the fact that implementing hydrogen nowadays is not a cost-optimal solution and enabling its deployment will require governmental fostering mechanisms such as subsidies or tax abatement.

Interestingly, the level of detail of the models affects the level of investment predicted. If a less detailed model is considered, variable renewable generation is over-invested and lower investment occurs for conventional CCGT plants. This is because of neglecting the importance of reserve requirements, which brings in curtailment and renewable integration costs underestimation leading to higher investment in a renewable generation but not necessarily with higher electrolyser investment O'Dwyer et al. (2022). Furthermore, hydrogen infrastructure could have an effect on the electric transmission infrastructure. If electrolysers are placed in strategic points, their deployment could lead to substituting the investment on grid reinforcement Longoria et al. (2021), but this depends on the scale of the projects and if are going to be centralized or scattered productions.

3.2.4 Power system, Gas network and hydrogen interaction

The capacity of hydrogen and synthetic methane to blend with natural gas in different proportions has led some researchers to study the effects of injecting hydrogen or synthetic methane into the gas network. As was mentioned before, adding hydrogen production as the new link between the power sector and the gas network results in more flexibility and less curtailment W. Liu et al. (2021). Fewer carbon emissions from the gas network are produced J. Liu et al. (2020); W. Liu et al. (2021), and lower operational costs of the overall system are reached J. Liu et al. (2020). Nevertheless, due to an increase in investment and electric demand, the electricity prices increase too Schlund & Schönfisch (2021). When hydrogen injection versus synthetic methane injection to the grid is compared, hydrogen deployment abates more carbon emissions in total and has lower operational costs, but absorbs less curtailment and power from wind farms due to constraints of allowed gas blending J. Liu et al. (2020). Another interaction point between gas networks and hydrogen systems is SMR-based hydrogen production which uses natural gas as the main feedstock. He, Mallapragada, Bose, Heuberger-Austin, & Gençer (2021) revealed that SMR-based hydrogen with carbon capture and storage will be only competitive if no or low (less than $50/tonne) carbon taxes are applied.

3.2.5 Greenhouse gas emissions consideration

Greenhouse gas emissions abatement is part of the analysis in many energy systems models, but different approaches are taken when considering this element. In the majority of cases, the emissions abatement is ignored, but when considered, they can be part of the objective function Longoria et al. (2021); He, Mallapragada, Bose, Heuberger-Austin, & Gençer (2021), a constraint Navas-Anguita et al. (2020), or an explicitly specific separated objective function W. Liu et al. (2021). In some cases, the greenhouse gas emissions are ignored in the optimization problem and take part in the final assessment and discussion J. Liu et al. (2020); Schlund & Schönfisch (2021). Common results obtained by the former are carbon abatement costs and total emissions of the system during the analysed period. In contrast, other studies that include the carbon emissions accounting as an element of the objective function that minimizes the system cost put a price on the carbon emissions and according to the value the weight of the emissions on the total cost changes Longoria et al. (2021); He, Mallapragada, Bose, Heuberger-Austin, & Gençer (2021). By adding caps, taxes, or other types of restrictions in the objective function different scenarios of emissions can be set, this allows to evaluate the effect of different policies on the total cost of the system or other model outputs Navas-Anguita et al. (2020). It is also possible to perform a multi-objective optimization with one of the objective functions being the carbon emissions minimization and the other the system cost W. Liu et al. (2021). This allows the system to evaluate the relationship between those two variables as a function of the other on a Pareto front. An important conclusion of the majority of the studies that involve carbon emissions optimization is that carbon emissions decrease in systems that include hydrogen is only possible if new renewable capacity is added into the system. Without new renewable capacity built the electricity consumption increases and with this the operational time of thermal units that rely on fossil fuels, hence, increasing the total emissions of the system Longoria et al. (2021).

3.2.6 Gaps in energy system models

In previous sections, it was shown how different supply chain configurations have been proposed and tested. Among the energy system model shown in this section, for the ones that included detailed supply chains, no one assessed other types of supply chain configuration, or many different hydrogen demand centres, and no marginal effect of choosing one type over another was evaluated. Further, a detailed operational model within energy systems models can have a significant effect on the final results, as shown by O'Dwyer et al. (2022) that have evaluated the effect of not having a detailed operational model in comparison with a more detailed one (i.e. including or excluding reserve requirements and inertia floor from the model). The study showed that with a less detailed model variable renewable generation is over-invested and lower investment occurs for conventional CCGT plants.

It is important to consider the effect of different types of supply chains, the addition of different demand centres, and the level of detail in the assessments due to the final effect on costs, investment and carbon emissions. This is especially relevant if the energy system level studies are intending to influence policy-makers to design energy markets that will target low-carbon technologies implementation at big-scale.

Table 5.

Type of model	Typical parameters	Typical Variables	Typical scenarios
Power systems models	Equipment specification, fixed and variable operating unit costs, power demand, renewable generation.	Operation of each unit, units capacities	Consideration of demand response, year, base loads, flexible operation of certain units, inclusion of hydrogen and renewables, weather conditions.
Energy systems models	Equipment specification, fixed and variable operating unit costs, base installed capacity and transmission infrastructure, demand (electricity, hydrogen, gas, etc) renewable generation profile.	Operation of each unit, units capacities.	Years, synthetic fuels production, adding quotas or targets, carbon emissions caps, other storage technologies.

Table 6.

Reference	Approach	Systems description	Novelty	Investment	Objective function	Supply chain level of detail	Variables & Scenarios	Parameters
Mirzaei et al. (2018)	Power system model.	Wind farm: 140 MW. Hydrogen storage: 180 MWh. 6-bus system.	Security constrained unit commitment model with the integration of hydrogen storage system, shifting demand response in a highly renewable system (wind).	No investment considered, only cost of storage and operation cost.	Minimize operation cost function.	Storage limits, fixed efficiency.	Variables: operation of each unit. Scenarios: cases with or without demand response and/or hydrogen storage.	Parameters: operation costs of units and storage, size of the units, wind generation, power demand.
Ruggles et al. (2021)	Power system model.	Whole USA electric market (CONUS).	By adding Flexible load to electric systems they evaluated the effect on electricity price, hydrogen cost, and if additional capacity is required to be installed.	Yes.	Minimize system cost.	Fixed efficiency value, hydrogen loss per hour in storage, storage limits.	Variables: Installed capacity and hourly operation of each unit. Scenarios: Dispatch generation, Dispatch+renewable+storage generation, Renewable+storage generation.	Parameters: fixed and variable costs, the hourly capacity factor for renewable generation, the variable cost for demand response, hourly demand, and annual flexible load constraint.
Nojavan et al. (2017)	Power system model.	A power system with a maximum load of 3500 kW, that includes a wind farm, PV generation and thermal units. Evaluation is done for 24 hours.	Real-time electricity price calculation in a power system with a hydrogen storage system and demand response. Considers uncertainty and a comparison done with time-of-use pricing in a smart grid.	No, only operation cost (energy purchase) and revenues are considered.	Maximize the expected retailer's profit (revenue minus cost).	Fixed efficiency, storage limit, and on-off system with variable input of power.	Variables: hourly operation of each unit. Scenarios: demand response implementation, real-time or time-of-use pricing scheme.	Parameters: renewables generation, unit specifications and constraints, power demand, electricity pool prices.
Zhang et al. (2020)	Power system model.	Western US power system with fuel cell vehicles hydrogen consumption.	Simulation of fuel cell vehicles time-varying refuelling demand met using electrolysers distributed along the power system. Increasing the flexibility of the electrolysers (oversizing of equipment).	No.	Minimize the operational cost of the system by meeting day-ahead load.	Fixed efficiency, storage limit, and on-off system with variable input of power.	Variables: operation of each unit, electrolyser size. Scenarios: business as usual, inflexible or flexible electrolyser operation).	Parameters: hydrogen en electricity demand, fossil fuel prices, units transmission lines available and specifications, wind and solar generation.
Ali et al. (2018)	Power system model.	Finland power system. 87 TWh renewable generation (70% wind 30% solar). 82 TWh demand. Between 46 and 74 TWh of hydrogen storage capacity is required.	Sizing hydrogen energy storage in consideration of demand response based on households heating in highly renewable generation power systems.	No, only sizing of storage capacity.	Minimizes hydrogen energy storage capacity to mitigate the daily variability of renewable generation.	Fixed efficiency, storage limit, and on-off system with variable input of power.	Variables: operation of the units. Scenarios: coordination of hydrogen storage and demand response, presence of a base-load generation, days of hydrogen storage requirements.	Parameters: renewables generation (sensitivity analysis done by changing the generation profile), baseload generation, heating systems technical details, power demand.
Marocco et al. (2023)	Power system model.	Power system of the island of Pantelleria, Italy. 27.3 GWh annual demand. Electrolyser: up to 10 MW, Wind farm: up to 70 MW.	Optimizes and compares batteries, hydrogen, and hybrid scenarios to fulfil a certain electric demand and evaluates the effect on the renewables investment requirements.	Yes.	Minimise the net present cost of the energy system.	Fixed efficiencies, storage limit, and on-off system with variable input of power.	Variables: annual installed capacity of technologies and storages in each year, operation of the technologies and storage. Scenarios: only batteries, only hydrogen and hybrid, and different years.	Parameters: Units CAPEX and OPEX, electricity demand, increase of demand per year, renewables capacity factors.

Guerra et al. (2023)	Power system model.	Spanish power system with high penetration of renewables.	Includes different flexible energy storage options and different climate conditions without compromising inertia.	No.	Rule-based model with a priority order for deployment of new technologies.	Volume loss rate in a salt cavern and compression losses, storage state, fixed equipment efficiency	Variables: Storage required, operation of units, fraction of conventional units replaceable. Scenarios: Weather conditions (Dry, wet, and normal year), year.	Parameters: Historical demand, power output of renewables, historical power exchanged by interconnectors, economic, emissions and technical parameters of each technology, capacity available of batteries, conventional renewable and non renewable generation.
Chicco et al. (2020)	Energy system model.	Adaptable system. In the case examples small scales (less than 1 MW).	Flexibility of distributed multi-energy systems general mathematical and graphical modelling framework is formulated to describe the operational characteristics of individual MES and aggregate DMES, including the role of multi-energy networks in enabling or constraining flexibility.	No.	Framework to evaluate the flexibility of a system. No fixed operation point was considered, hence no optimization was done in this study.	Fixed efficiency.	Variables: Operation of the units. Scenarios: different example cases.	Parameters: Size and specification of the units, demands, and operation costs.
J. Liu et al. (2020)	Energy system model.	39-bus power system and Belgian 20-node gas system.	Hydrogen and synthetic methane production in an energy system that includes gas network and power system is optimized to minimize costs.	No.	Minimize the total operational cost.	Fixed efficiency, storage limit, and on-off system with variable input of power, heating value calculation of Natural gas blended with hydrogen, and detailed pipeline operation constraints.	Variables: gas flow on the units. Scenarios: the presence of hydrogen or methane production, and coal power generation.	Parameters: wind generation, equipment specification, equipment size, operation cost, demand (gas and power)
Schlund & Schönfisch (2021)	Energy system model.	European gas and electric systems.	Assessment and quantification of the distributional effects of a hydrogen quota on the power and gas markets in the EU. Integration based on iterations of gas and electric markets in Europe with the addition of hydrogen production.	Yes.	Minimize the difference between the outputs and inputs of the gas and power models, which are investment models.	Fixed efficiency, the limit of hydrogen injection into the natural gas network, and hourly correlation of hydrogen production with renewable generation.	Variables: installed capacity, energy and storage flow. Scenarios: year (quota imposed).	Parameters: inelastic natural gas and electricity demand, emission trading system imposed, actual gas and power transmission capacity, approved future expansion of the network, injection limits of hydrogen into the gas grid, power generation from different sources, units specification.
Navas-Anguita et al. (2020)	Energy system model.	Spanish energy system and expected hydrogen vehicles fleet.	Techno-economic and environmental optimisation of the production of hydrogen in Spain, by implementing an energy system model with a life cycle assessment.	Yes.	Minimize cost of hydrogen production prioritizing the least cost option and the carbon footprint.	Different types of hydrogen production processes,	Variables: Investment in each production technology. Scenarios: year, hydrogen demand, carbon emissions cap.	Parameters: hydrogen demand per year, carbon footprint restrictions, investment and operation cost of each hydrogen production unit, and power produced each evaluated year from different sources.

O'Dwyer et al. (2022)	Energy system model.	Irish energy system in 2030 and 2040. Gas, power and hydrogen markets considered.	A case study exploring optimal investments in H2 generation and underground storage alongside other conventional generation and storage technologies in an energy system with a very high share of renewable generation.	Yes.	Minimize a cost function that includes investment costs, O&M costs, start-up costs, fuel costs, taxes and penalties associated with the slack variables of the demand balance and reserve constraints.	Start-ups, electrolyser efficiency that varies with electric input, different time resolution.	Variables: Unit and storage investment. Scenarios: case studies (global ambition, high fuel price, hydrogen network, technology breakthrough, variable renewable rnergy, restricted compressed air energy storage), operational level of detail.	Parameters: units and storage cost, base model installed capacity, demands, wind and solar generation.
W. Liu et al. (2021)	Energy system model.	39-bus power system and Belgian 20-node gas system.	Assessment of the integration of power-to-gas technology on an integrated power-natural gas-heating system and the effect over the flexibility, environmental impact, and cost of the system.	No.	Multi-objective minimization of operational cost and pollutant emissions,	Only synthetic methane production, fixed efficiency, gas storage limits.	Variables: operation of the units. Scenarios with and without power-to-gas.	Parameters: power and natural gas system characteristics (units, efficiencies, operational cost, etc), power-to-gas facilities and storage specifications demand of gas, heating and power, and wind generation.
Longoria et al. (2021)	Energy system model.	Irish power and heating markets.	Investment model implemented for the production and consumption of hydrogen for heating purposes from grid electricity. Evaluates the effect on infrastructure expansion, curtailment, electricity prices, zonal prices and emissions. Includes reactive power constraints.	Yes, including expansion of generation capacity and transmission system.	Minimize the total cost of the system, which includes: the NPV of the investment, variable costs, reliability, emissions, and operation and maintenance costs.	Fixed efficiency, reactive power consumption, storage limits, hydrogen leakage considered.	Variables: investment of each technology in each node, operation of each unit. Scenarios: business as usual, renewable target, electrolysers implementation, and renewable target+electrolyser implementation.	Parameters: Costs and specification of each unit, technology, and transmission system, heat demand profile in each node, carbon price, and power demand.
He, Mallapragada, Bose, Heuberger-Austin, & Gençer (2021)	Energy system model.	U.S. Northeast region power system with hydrogen demand for different sectors.	Energy system model that includes hydrogen and electricity demand. It considers interaction with the power system at different points of the hydrogen supply chain. Carbon emissions penalty included, and a range of different technologies for generation and storage.	Yes.	Minimize cost of hydrogen and electricity system mixed function.	Compression costs, storage balancing, shutting down and turning up electrolysers dynamics considered, storage recharging rate, pipelines constraints, transport time by trucks.	Variables: Storage and units investment, operation of units. Scenarios: range of CO2 prices, H2 demand and technology cost scenarios.	Parameters: Units and transmissions systems specific costs, emissions, efficiencies and other specifications, electricity and hydrogen demand in each zone, renewable generation.

4 Main challenges in the integration of production-side and system side models

In previous sections, it was shown that no existing hydrogen system model truly integrates a production-side supply chain model within a system-side impact one, and this is corroborated by Blanco et al. (2020). It is crucial for hydrogen deployment in energy systems to have accurate available models. Those models will eventually inform policymakers and should consider the technical constraints, but also the economic and social externalities that hydrogen will have on the energy system. Several issues were shown in previous sections and those are related to the nature of the variable utilized in the model (exogenous or endogenous), the optimization approach (cost minimization or profit maximization), and modelling techniques.

4.1 Exogenous/endogenous variables

The different types of models described in this review were classified according to their scope and objectives. The variables and parameters involved in each model are responsible for limiting a model to a certain category. In the case of PSSC models, as every single supply chain reported in literature considers a marginal effect over the system, their inputs are parameters that are essentially exogenized variables. Among those variables are electricity prices, electricity, heat and hydrogen demand, grid electricity carbon intensity, transmission constraints, and ancillary services requirements. The resolution of each exogenized variable varied from study to study, being constant in the simplest cases and an hourly variable in the more complex models. This issue has been reported before but for large-scale power-to-x plants, which produce chemicals, fuels, or other goods from electricity. Campion et al. (2023) mentioned that usually, models assume fixed electricity prices and steady-state operation, and those methodological biases have a great influence on the final cost results. Despite this, even that study (as all of them) assumed to have a marginal effect on the system, and the assumption is likely to be true in the cases in which the scale of the system is small. On the other hand, on the megawatt scale or gigawatt scale systems, the effect on the system cannot be neglected, and the exogenized variables will start to be dependent on the behaviour of the hydrogen production site. Besides, even in small-scale systems, if hydrogen production is already considered deployed at a system scale, the exogenized variables will be already affected by the presence of many other hydrogen production facilities. The optimal size and operation of a hydrogen plant cannot be obtained without taking into account the impact of hydrogen on variables like demands and prices.

Conversely, SSI models tend to consider only one configuration of the supply chain for hydrogen production. This means that they exogenize the optimization of site-specific hydrogen facilities, and the technical level of detail required to obtain an accurate optimal solution. Among those variables are the geographical location which comprises geological storage availability, transmission lines and exporting facilities, storage size, electrolyzer size, alternative energy storage technologies, for example, batteries, operation mode which includes curtailment only, hydrogen first, and electricity first, technologies available like PEM, Alkaline or SOEC electrolysers, hydrogen liquefaction, and compression. In the cases that a more detailed supply chain is proposed at a systems level, it also is very homogeneous, which means that every facility considered in the model has the same configuration. This last point is very unlikely to represent the future of hydrogen production, where each site will deliver, at least, slightly different supply chain arrangements that fulfil the geographical, meteorological, and local demand requirements. The minimum cost system with hydrogen participation cannot be determined without considering each specific site's characteristics, neither a minimum level of detail of the operation.

This issue was partially addressed by He, Mallapragada, Bose, Heuberger-Austin, & Gençer (2021), and shows that if compared with isolated single PSSC optimization models results, the integration of different sites within an SSI decreases the energy system decarbonization costs. However, their supply chain was also limited to certain configurations and the demand centre for hydrogen was limited to the transport and power sectors only.

We propose that a new modelling framework should consider as endogenous variables the different types of demands, prices of variable goods, supply chain configurations and technological options available, geographical locations, system services requirements, and carbon emissions of the system. This will allow an accurate integration between PSSC and SSI models.

4.2 Profit maximization vs cost minimization

The modelling approach is also very important to obtain an accurate model of hydrogen production when different players are considered within the model. Each model prioritizes different elements during the optimization, and each approach is more likely to generate results that are more alike to what one or other player would do according to their own interests.

The system cost minimization approach is aligned with what a systems operator would look for in a model. By minimizing the total cost of investment and operation, the model obtains results that could be feasible in a perfectly competitive scenario. Nevertheless, this approach does not consider the commercial reality of projects or investments, and the optimal results could make little sense in the real competitive market.

The profit maximization approach is more aligned with the investor's view and obtains results that generate the maximal benefit for the project. This also is disconnected from reality in terms of project externalities. By not considering the social welfare or environmental impact the feasibility of the optimized solution might not be aligned with the systems operator or governmental regulator's view.

To avoid this issue, both models should be applied to a big-scale energy system investment model, where both approaches could be applied at different levels of the model, or where both approaches applied separately interact with each other in an iterative way to obtain a final optimal solution.

4.3 Modelling techniques

As mentioned before, cost minimization models are usually used in systems which could have a central planner entity. Hence, the single linear or mixed-integer linear problem has a single minimization objective function. The set of constraints that follow the objective function can be equality or inequality conditions, and obey the Karush–Kuhn–Tucker conditions, which are the optimality conditions resulting from the first derivative tests of the optimization problem. These values include stationary condition, complementary slackness, primal feasibility, and dual feasibility. These conditions need to be fulfilled when an optimum value is found.

By having only one objective function, which is linear, the mathematical complexity and computational requirements to solve the problem are not as high as they would be if a non-linear problem or multiple objective functions were added to the system. This is the case with equilibrium models, which generate an equilibrium between demand and offer of different players, hence comprising different objective functions for each player that wants to maximize its profit. These models are subjected to the Nash-Cournot competition which establishes that according to the strategy that each player takes the rest of the players are going to react to obtain a new equilibrium in the system. This means that the demand and offer are affected by the players. This type of system is more likely to represent real liberalized energy systems more accurately than cost-minimization systems. Without this non-cooperative interaction between entities, the equilibrium model can be optimized as a cost-minimization problem. The computational requirements to model an equilibrium model with Nash-Caurnot competition are greater than a cost minimization optimization problem. To avoid long solving times, and high computational requirements, a big energy system model could be simplified by compromising the accuracy of the model. By applying equilibrium models in sub-models of the main energy system model the problem can be simplified, the computational times decreased and the accuracy maintained within a reasonable margin. The sub-models should be selected with the criteria of the modeller. Those should consider the nature of the sub-model, the number and influence of the players, the size of the sub-system itself, and the influence that it will have on the main optimization problem. (I would like to know if what I said here makes sense to you).

5 Conclusion

This review analysed the status of hydrogen production systems models and their integration with energy system models. Although detailed and exhaustive work has been published about hydrogen supply chain models, the relationship with their respective power markets or gas networks was normally neglected. This was due to small-scale hydrogen production with marginal effects over the system. Nevertheless, several studies of supply chains of hundreds or thousands of MW of power were reported without a reciprocal interaction with the energy system, unveiling a gap in the hydrogen supply chain literature. On the energy systems side, fewer studies have been reported but the interaction of the hydrogen systems and the effect produced on the energy system and market were reported in detail. Nevertheless, the level of detail of the studies on the supply chain level was lower and if the supply chain was modelled properly, it did not consider the marginal effect of changing the configuration as part of the sensitivity analysis. Besides, some topics were not identified among the studies reviewed, which included a lack of life-cycle assessments within energy systems, and case studies that evaluate the effect on the system of a big-scale hydrogen plant configuration and operation.

After analysing the difficulties of integrating both types of models to obtain a more robust modelling scheme for future development of policies about hydrogen production, three main challenges in models integration were identified:

A) Exogenized variables that are endogenous variables in the counterpart model. These variables in the PSSC model are normally related to the energy system that is almost completely ignored, such as electricity price, hydrogen or electricity demand, and transmission constraints. The SSI models normally exogenize hydrogen supply chain configurations (e.g. different technologies available), geographical location variables, and operation modes.

B) Different optimization approaches in SSI and PSSC. Usually, PSSC model minimizes the cost of production or maximizes the revenues of the project from the point of view of investors or project developers. On the counterpart, SSI models consider a least-cost optimization, which is the approach that a central system operator will take. Both types of models have advantages but to represent accurately the reality of hydrogen production on a system level, both should be integrated.

C) Modelling techniques and computational constraints. SSI models usually have more variables and the optimization problems are larger than the PSSC. Computational constraints of applying an equilibrium profit maximization optimization on an SSI model could lead to very long computational solving times. Hence, a different scheme of integrating profit maximization and least-cost optimization should be developed for integrating hydrogen PSSC models within SSI models.

The deployment of hydrogen at a big scale will add a new demand for electricity and a new offer of renewable fuel that could potentially help to decarbonize the energy, transport, and manufacturing sectors.

Producing a complete integrated model will enable the assessment of different types of policies' effects on the energy system and to take accurate decisions for the future of decarbonization.

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