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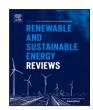
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#### Review article

# The role of hydrogen in integrated assessment models: A review of recent developments

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#### ABSTRACT

Hydrogen is emerging as a crucial energy source in the global effort to reduce dependence on fossil fuels and meet climate goals. Integrating hydrogen into Integrated Assessment Models (IAMs) is essential for understanding its potential and guiding policy decisions. These models simulate various energy scenarios, assess hydrogen's impact on emissions, and evaluate its economic viability. However, uncertainties surrounding hydrogen technologies must be effectively addressed in their modeling. This review examines how different IAMs incorporate hydrogen technologies and their implications for decarbonization strategies and policy development, considering underlying uncertainties. We begin by analyzing the configuration of the hydrogen supply chain, focusing on production, logistics, distribution, and utilization. The modeling characteristics of hydrogen integration in 12 IAM families are explored, emphasizing hydrogen's growing significance in stringent climate mitigation scenarios. Results from the literature and the AR6 database reveal gaps in the modeling of the hydrogen supply chain, particularly in storage, transportation, and distribution. Model characteristics are critical in determining hydrogen's share within the energy portfolio. Additionally, this study underscores the importance of addressing both parametric and structural uncertainties in IAMs, which are often underestimated, leading to varied outcomes regarding hydrogen's role in decarbonization strategies.

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Abbreviation	Full Form
AIM	Asia-Pacific Integrated Model
ALK	Alkaline Electrolyzer
AR6	Sixth Assessment Report
CCS	Carbon Capture and Storage
CHP	Combined Heat and Power
COP21	21st Conference of the Parties
DRI-EAF	Direct Reduced Iron - Electric Arc
	Furnace
ETS	Electrolyzer
GCAM	Global Change Analysis Model
GEM-E3	General Equilibrium Model for
	Energy-Economy-Environment
GHG	Greenhouse Gases
GRACE	Global Responses to Anthropogenic
	Change in the Environment
HYD	Hydro
IAMC	Integrated Assessment Modeling
	Consortium
IAMs	Integrated Assessment Models
IPCC	Intergovernmental Panel on Climate
	Change
IO	Intertemporal Optimization
LH <sub>2</sub>	Liquefied Hydrogen
LOHC	Liquid Organic Hydrogen Carrier
LP	Linear Programming
MARKAL	MARKet ALlocation
MCFC	Molten-Carbonate Fuel Cell
MERGE-ETL	Model for Evaluating the Regional and
	Global Effects of GHG Reduction Policies
MESSAGE	Model for Energy Supply Strategy
	Alternatives and their General
	Environmental Impact
Mt	Million tonnes
NLP	Non-Linear Programming
O&M	Operational and Maintenance
PEM	Proton Exchange Membrane
POLES	Prospective Outlook on Long-term Energy
TOLLO	Systems
PROMETHEUS	Energy-Environment-Economy Model
REMIND	REgional Model of INvestments and
1,2	Development
RES	Reference Energy System
RCP	Representative Concentration Pathways
RO	Robust Optimization
SMR	Steam Methane Reforming
SOFC	Solid Oxide Fuel Cell
SSP	Shared Socioeconomic Pathways
TIAM	TIMES Integrated Assessment Model
TIMES	The Integrated MARKAL-EFOM System
VRE	Variable Renewable Energy
WITCH	World Induced Technical Change Hybrid
WGIII	IPCC's Working Group III

#### 1. Introduction

There is a global consensus that anthropogenic greenhouse gas (GHG) emissions are responsible for global warming [1,2]. The Paris Agreement reached at the Conference of the Parties (COP-21), is devoted to keeping the increase in surface average temperature to less than 2 °C (SAT) [3]. In spite of this agreement, human-induced GHG emissions continue, resulting in an increase in global surface temperature of 1.1 °C above the pre-industrial levels (from 1850-1900) during the past decade (from 2011-2020) [2]. Several studies have provided a pathway to a net-zero and further net-negative emission regime and support the fulfillment of the Intergovernmental Panel on Climate Change (IPCC) targets [4-8]. Addressing these challenges requires a well-structured and sophisticated modeling approach using decision models, due to the complex interplay between the energy sector, society, economy, and climate systems [9]. Among these, integrated assessment models (IAMs) aim to link different disciplines by combining economic, social, and environmental data into a mathematical framework to evaluate the consequences of climate change and provide feedback on socioeconomic systems.

For example, since the publication of the second IPCC assessment report [10,11], IAMs have played a key role in the IPCC's Working Group III (WGIII) on mitigation. Consequently, WGIII research is largely dependent on IAM ensembles to provide a comprehensive framework to assess the complexities of climate change [12–14]. IAMs have been central in quantifying the technological and macroeconomic impacts of various decarbonization pathways, providing policy-relevant insights that are crucial for effective climate change mitigation.

To explore different future scenarios and their implications, Shared Socioeconomic Pathways (SSPs) have been developed [15]. SSPs outline various socioeconomic futures and, when combined with Representative Concentration Pathways (RCPs) [16], provide a comprehensive framework to examine the impacts of different climate policies and actions. These scenarios were fundamental to the IPCC Special Report on Global Warming of 1.5 °C (SR1.5) [13] and the Sixth Assessment Report (AR6) [14], enhancing our understanding of the relationship between potential temperature outcomes and climate models. In these reports, various scenarios are divided into eight temperature-based categories (C1-C8) based on projected temperatures and associated risks, assessing global warming by evaluating simulated peak temperatures in the 21st century [17]. C1 to C3 categories are considered the lowest temperature outcomes: C1 includes limiting warming to 1.5 °C (with the probability higher than 50%) with no or limited overshoot; C2 includes returning warming to 1.5  $^{\circ}\text{C}$  (with the probability higher than 50%) after a high overshoot; and C3 limits warming to 2 °C (with the probability higher than 67%). Higher emission scenarios are also categorized, projecting temperature rises of 2°°C (with the probability higher than 50%) (C4), 2-2.5 °C (C5), 2.5-3 °C (C6), 3-4 °C (C7), and over 4 °C (C8) by 2100 [18].

One of the challenges of these modeling efforts is to correctly integrate the fast technological advances in the description of the global energy transition. This is the case of hydrogen, for example, which displays a rising significance as a central vector for achieving decarbonization [19]. Hydrogen demand reached 94 million tonnes (Mt) in 2021, going beyond its pre-pandemic levels and contributing to about 2.5% of global final energy consumption, a growth supported in part by a solid interest in new applications [20]. This upward trend continued into 2022, with demand further increasing to 95 Mt [20]. However, the production, distribution, and consumption infrastructure

remains a bottleneck; therefore, ongoing research and strategic planning are essential to overcome these challenges and pave the way for a sustainable hydrogen future [21,22].

The potential expanding role of hydrogen in the global energy landscape is underscored by governmental interest. Since September 2021, new national strategies have been adopted, taking the total number of countries with hydrogen strategies to 26 countries in 2021 [23], and 41 countries in 2022 [20]. Concrete policies are being shaped in regions like the EU, US, and Germany to support commercial-scale projects for low-emission hydrogen production and infrastructure [20]. However, a significant gap between these aspirations and reality remains due to the lack of policy momentum in fostering hydrogen demand [24]. As a result, the role of hydrogen as a potential energy vector in the context of diversifying and decarbonizing the global energy portfolio has been actively pursued at national and international levels [25–27]. To support these efforts, it is essential to properly categorize the orientation of the various models that are currently accessible, as there is a variation in the focus of models, which might range from examining macroeconomic effects to assessing technological viability.

To answer this question, we categorized here the studied literature based on their hydrogen supply chain configurations, integrating hydrogen system processes into IAMs and examining decarbonization policies. This study aims to address the following key research question: How do different IAMs incorporate hydrogen technologies, and what are the implications for decarbonization strategies and policy development, considering the underlying uncertainties? Each section of the article delves into specific aspects: the types of IAMs used, sectoral coverage of hydrogen technologies, technological characteristics, and the varying assumptions and uncertainties that influence the results. By systematically reviewing these elements, we aim to provide a comprehensive understanding of the current state of hydrogen modeling and identify areas for future research.

#### 2. Hydrogen supply chain configuration

Although hydrogen is the most common element in the universe, it is rarely found in its pure form on Earth. Instead, it needs to be extracted and separated from compounds containing carbon and oxygen using feedstocks such as biomass, fossil fuels and water, and energy sources ranging from fossil to nuclear and renewable energies [28]. Various methods, such as thermochemical, electrochemical, and biochemical processes, are used to produce hydrogen [29, 30] (Fig. 1). Despite thermochemical methods being the predominant and established techniques for producing hydrogen, recent years have seen considerable progress in biochemical and electrochemical processes [31]. Conventional thermochemical processes like steam reforming and gasification have been the mainstay, utilizing heat to chemically transform carbon-based fuels into hydrogen [32]. These processes, while effective, often depend on non-renewable resources such as fossil fuels, which are carbon-intensive and raise sustainability concerns although these carbon-emitting hydrogen production methods can be retrofitted with carbon capture technologies to reduce the amount of GHG emissions [33].

In response to the concerns of GHG emissions from thermochemical production methods, there has been a notable shift towards zero-emission hydrogen production methods [29]. Hydrogen production methods based on renewable sources are becoming more economically viable [34]. Using renewable and nuclear sources such as solar, wind, hydro, geothermal, and ocean thermal, electrochemical hydrogen production is gaining traction [35]. These sources not only minimize GHG emissions but also improve the adaptability of hydrogen production, particularly in isolated or off-grid locations. A promising approach for eco-friendly hydrogen production is the use of water as a feedstock in various sophisticated electrolyzers [36]. Currently, the three primary technologies for electrolysis are Raney-Nickel electrodes (Alkaline), Polymer Electrolyte Membrane (PEM) either anion

exchange or proton exchange, and Solid Oxide Electrolyzer Cell (SOEC), each varying in electrolyte material, efficiency, and operating conditions [37–39]. Moreover, biochemical methods for producing hydrogen are showing great promise. Processes such as fermentation and photobiological generation utilize microorganisms and sunlight to produce hydrogen in a renewable and eco-friendly manner [40]. These emerging biochemical-based technologies, while still in their new stages, could signify a progressive step toward a sustainable hydrogen economy, leveraging renewable resources and advanced technologies to reduce reliance on fossil fuels and minimize the carbon footprint of hydrogen production [41].

Hydrogen-based synthetic hydrocarbons represent another innovative application of hydrogen in the energy transition. Hydrogen can be combined with carbon dioxide captured and oxygen through processes such as methanation and Fischer–Tropsch synthesis to produce synthetic hydrocarbons [42]. Their potential for carbon neutrality further enhances the sustainability of these synthetic hydrocarbons, as they can function within a closed carbon cycle by utilizing carbon captured from industrial processes or directly from the atmosphere [24]. These energy carriers are generally easier to store and transport than hydrogen due to their higher energy density, stable form at standard conditions, compatibility with existing infrastructure, and reduced leakage risk [43,44].

The logistics and distribution phase is vital in the hydrogen supply chain, encompassing a range of subprocesses. Due to its low volumetric energy density, these include liquefaction and compression of hydrogen, various storage strategies, and its subsequent distribution. However, there is an associated energy and cost penalty with compression and in particular with liquefaction. This stage is essential for ensuring hydrogen's availability and accessibility as a fuel source. Liquefaction of hydrogen is the process of converting hydrogen gas into liquid hydrogen (LH2) by cooling it to extremely low temperatures. Hydrogen becomes a liquid at a temperature of -252.87 °C at atmospheric pressure. This process significantly increases the hydrogen energy density by volume, making it more efficient for storage and transport, particularly over long distances, where pipelines may not be feasible or cost-effective. Hydrogen can also serve as an energy storage solution, storing surplus energy from intermittent renewable sources, thereby improving the stability and reliability of energy systems [45-47]. Alternatively, synthetic hydrocarbons provide a more convenient solution for storage and transportation than hydrogen, as they can be stored at ambient temperatures and pressures [43]. Stored hydrogen can be used directly by end users or converted into different forms of energy carriers. It can also be transmitted for various applications, including use in fuel cells, combustion engines, or as a feedstock for chemical processes.

Hydrogen can be distributed using pipelines, via rail and road, through shipping, or delivered through refueling stations [48]. Its transmission can take several forms, including liquid, compressed gas, or carriers like ammonia, and involves decisions between long-distance transmission and local distribution [49]. Although hydrogen has traditionally been produced and utilized close to its point of use due to its low volumetric energy density, which complicates and increases the cost of long-distance transport, there are significant ongoing developments and economic analyses dedicated to enhancing the efficiency and feasibility of long-distance hydrogen transport [50]. These include retrofitting existing natural gas pipelines and exploring international shipping, indicating a shift towards a more globally integrated hydrogen market [51].

In general, therefore, hydrogen could be a versatile energy carrier with broad end-use applications, showcasing its potential as a clean fuel alternative in various sectors [52]. Hydrogen-based energy carriers can be utilized as a fuel in the transportation sector for vehicles such as cars, buses, airplanes, and shipping, capitalizing on its high energy efficiency and low emissions [53,54]. In industrial processes, hydrogen acts as both a feedstock and fuel, instrumental in the production of

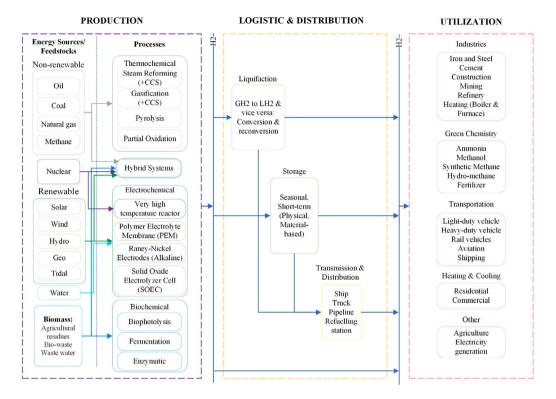


Fig. 1. Hydrogen supply chain.

chemicals, steel, and powering industrial machinery [55–57]. Also, since hydrogen-based synthetic hydrocarbons can mimic the chemical structure of conventional fossil fuels allowing them to be used in existing engines, vehicles, and fuel distribution systems, offering a practical decarbonization solution in hard-to-abate sectors [58]. They can be used in power generation, either directly or through fuel cells, to produce electricity and heat, showcasing their utility in both domestic and industrial contexts [59]. These applications illustrate hydrogen's transformative potential in driving the energy transition toward a decarbonized future, with its adoption in various sectors contributing to the increased resilience and sustainability of energy systems.

#### 3. IAMs considering hydrogen

IAMs are comprehensive frameworks that incorporate insights across diverse sectors such as energy, land use, and the broader economy, along with their associated GHG emissions. They are also linked with climate systems to facilitate an exploration of the intricate interplay between climate and socioeconomic and technological advancements [60]. In this study, our attention is particularly directed toward IAMs that have explored the integration of hydrogen within the broader context of energy systems and climate change mitigation strategies. Furthermore, among the models reviewed in the AR6 [14] and those retained by the Integrated Assessment Modeling Consortium (IAMC) [61], we have focused specifically on models that contain internal climate modules or incorporate linkages to external climate models. Subsequently, the general characteristics of IAMs that incorporate hydrogen technologies into their frameworks will be outlined, followed by an evaluation of methods to address uncertainty in the various research studies examined.

IAMs are also designed to capture the intricate feedback loops and trade-offs between energy, economic, and environmental systems. These models incorporate interactions across sectors such as energy production, distribution, transportation, and utilization, including industrial processes, though the level of detail and accuracy varies depending on the model's structure and scope, as exemplified by the

IMAGE model [62]. Feedback within the system can influence energy markets, such as fossil fuel markets, by reducing demand, which may alter global energy prices and emissions trajectories. Additionally, IAMs consider trade-offs between sectors, such as the allocation of limited renewable energy resources between electricity generation and hydrogen production, or balancing emissions reductions between transportation and industrial processes. The ability to capture these dynamics varies depending on the model's structure, with bottom-up (B–U) models offering detailed sector-specific insights, while top-down (T–D) or hybrid models are better at representing macroeconomic feedback and global interactions [63].

IAMs also facilitate policy design, analysis, and implementation by modeling intricate interconnections across various domains [64]. For instance, they contribute to achieving the Paris Agreement's goals [65-67], energy transition strategies towards low-carbon, efficient, and renewable energy systems [68-70], managing natural resources and addressing policies in agriculture, water, land use, and air quality [71, 72], assessing adaptation measures for reducing vulnerability to climate change effects [73] and exploring geoengineering options as countermeasures for deliberate interventions in the Earth's systems to counteract or mitigate the impacts of climate change [74,75]. Considering this context, our analysis encompasses 12 distinct families of models from 50 studies, representing all articles related to hydrogen integration in IAMs identified through comprehensive searches in Web of Science (WOS) and Google Scholar, as listed in Appendix A: AIM/Hub [76, 77], GCAM [78], GEM-E3 [79], GRACE [80], IMAGE [62], MERGE-ETL [81,82], MESSAGE [83], POLES [84], PROMETHEUS [85,86], REMIND [87], TIAM [88], and WITCH [89]. Each IAM offers diverse approaches for exploring "the solution space" in climate change research [90].

#### 3.1. Modeling paradigms and characteristics

In our analysis, IAMs vary significantly in their details and complexity in capturing feedback, interactions, and linkages they include. Some models represent the entire Earth system using an aggregated

structure [e.g.,91,92], while others represent more detailed structures from multi-discipline sciences [e.g.,87,93]. This variability underscores the challenge of applying a "one-size-fits-all" approach to model classification within our study. One classification separates models into two categories: those that offer specific, sectoral information on complex processes, namely detailed process-based models, and those that estimate developmental scenarios and future pathways, named costbenefit models [94]. Our focus extends to how these IAMs can be distinguished based on their model structure degree of spatial detail, geographical coverage, solution method, time horizon, representation of feedback, and solution concept [90,95]. This classification extends further with the study of impacts and adaptation [96], carbon dioxide removal [97] geoengineering technologies [98], macro-economy features, technological detail, treatment and sensitivity analysis of uncertainty [99].

From other perspectives, the studied IAMs can be divided based on their modeling approaches, considering their economic approaches, mathematical structure, framework, modeling perspective, and spectrum. Table 1 illustrates the typology of the studied IAMs. Models differ in their economic perspective, using either General Equilibrium (GE) or Partial Equilibrium (PE) approaches [100]. GE models aim to capture the interactions between different sectors of the economy. Computable General Equilibrium models (CGEs) are an important example of GE models with a more detailed representation of the behavior of households, firms, and the government [101]. PE models, for their part, are less comprehensive and focus on a specific market or sector of the economy. In addition, the methodology adopted by different IAMs can range from optimization to econometrics, game theory, and agent-based modeling. They have various mathematical structures and problems, from linear and nonlinear programming to simulation problems. IAMs differentiate by their solution approaches: recursive dynamic models with myopic foresight, where agents respond based on immediate outcomes without full future insight, and intertemporal optimization models, where decisions are made with either perfect or limited foresight.

IAMs can be further classified into two types based on their study of the climate system: those with internal climate modules and those linked to external climate models [102]. Models with internal modules (such as WITCH, MERGE-ETL, etc.) offer simplified climate system representations, allowing quick climate impact assessment for policy analysis, but with less detailed simulations. IAMs—such as MES-SAGEix, REMIND, IMAGE, GCAM, etc.—that are coupled to external models—MAGICC [103] and Hector [104]—deliver more accurate climate projections by adding advanced climate model capabilities, but at a higher computing cost. This classification reflects the balance between efficient scenario exploration and detailed climate process analysis, influencing the insights derived for climate policy and research.

The studied IAMs cover a diverse range of time horizons, time steps, technological change, levels of technological detail, and geographical coverage (see Table 2). The objective, structure, level of detail, and process capture capacities of distinct IAMs vary significantly. Therefore, based on their strengths and weaknesses, each IAM may be more effective in answering specific issues and less suitable for others. Yet, a study of the ensemble of IAMs provides a more robust analytical framework to investigate many elements of the complex interplay between the economy, society, and the environment, and to further assess the interactions between alternative strategies to address certain climate change or energy policy issues.

There are a variety of characteristics across IAMs in terms of their modeling paradigm and economic coverage approaches. IAMs can also be distinguished based on their representation of the energy and economic systems, with B–U, T–D, and hybrid models being the main categories. In the B–U modeling approach, the reference energy system (RES) component represents the energy system's structure. It includes various processes or technologies, commodities, and the flows that

link commodities to processes of the same type. Fig. 2 illustrates this setup with a network diagram, a representation derived from the examination of articles and reports focused on hydrogen modeling. The boxes represent various processes and technologies within the hydrogen supply chain. The RES includes production, logistics and distribution, and utilization phases. The commodities, such as various forms of hydrogen, electricity, and heat, or the useful demand, are depicted as vertical lines. Arrows illustrate commodity flows, linking the boxes denoting processes to the lines representing commodities. This RES is a comprehensive representation of the hydrogen supply chain, including the majority of available technologies. Depending on the research objectives, modeling methodology, data availability, and technologies relevant to the specific geographic region, the scope of included technologies may be expanded or narrowed. For instance, in the MERGE-ETL model, the production sector is described with greater detail, whereas the hydrogen demand within the utilization sector is treated as an aggregated final demand [105].

In B-U partial equilibrium models, integrating the hydrogen energy system into the model requires embedding the configuration of the hydrogen energy supply chain into the model, defining commodity details of the processes from production to end-use application, and eventually, incorporating the projection assumptions and technoenviro-economic characteristics of production, delivery and utilization technologies. This paradigm follows a disaggregated view; a more detailed description of the technical-economic characteristics is used (e.g., availability factor of technology) to find the ideal pathways of hydrogen production. The B-U approach integrates hydrogen into energy systems using key mathematical formulations that focus on cost optimization, energy balance, and constraints related to production, storage, transportation, and utilization. Detailed equations are provided in Section 1.1 of the Supplementary Material. Many current IAMs are hybrids, combining energy systems with macroeconomic or multisector models, and explicitly incorporating key sector technologies to study energy-economy interactions [90]. Therefore, hybrid models can also employ a bottom-up RES to represent detailed technological pathways and energy flows.

The approach of modeling can vary significantly in T-D models, influenced by the characteristics of the model and the research questions being addressed. Typically, the production module in these models illustrates the conversion of various inputs, like different energy sources, into economic production. An example of this production structure is depicted in Fig. 3. In CGE models, production functions such as Cobb-Douglas, Leontief, and Constant Elasticity of Substitution (CES) are commonly employed. The choice of production function is guided by the modeling approach and the relationship between inputs. Each sector's output level is set to maintain market equilibrium. A common approach to integrating hydrogen into T-D models is through a CES production function, which accounts for costs, technological changes, and policy incentives, with detailed formulas in Section 1.2 of the Supplementary Material. Fig. 3 illustrates the hydrogen production process, which employs multiple layers of nested CES functions. The top layer of the nested structure includes the combined primary inputs of labor, capital, and energy, along with intermediate inputs. In this modeling approach, labor and capital are typically considered to have a quasi-complementary relationship, whereas the elasticity of substitution between capital/labor and energy is higher. In the factor market, it is assumed that capital and labor can substitute for one another as their relative prices shift [106]. The energy inputs reveal the interplay between various sources of hydrogen production, categorized into ELEC, which includes electricity-based methods, and NELEC, which encompasses non-electricity-based methods such as biomass or fossil fuel processes. In this structure, capital also includes the distribution, transmission, production, and storage of hydrogen.

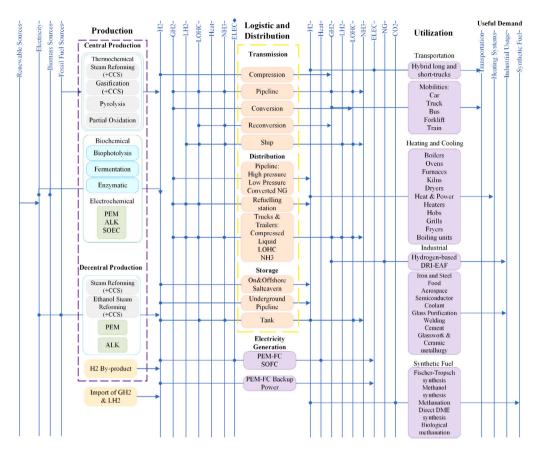


Fig. 2. RES of the hydrogen supply chain in a typical B-U approach.

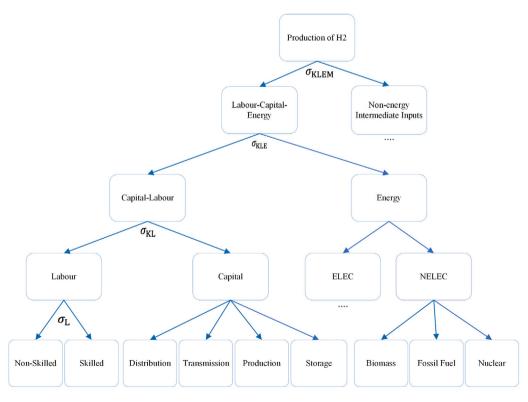


Fig. 3. Production structure of the hydrogen supply chain in a typical T–D approach ( $\sigma$  represents the CES parameter).

Table 1
Typology of studied IAMs.

IAMs	Economic <sup>a</sup> approach	Mathematical <sup>b</sup> structure	Modeling spectrum	Model perspective	Climate modeling
AIM/Hub	GE	RD/S	Myopic	Top-down	External Models
GCAM	PE	RD/NLP	Myopic	Hybrid	External Models
GEM-E3	GE	RD/NLP	Myopic	Top-down	External Models
GRACE	GE	RD/S	Myopic	Top-down	External Models
IMAGE	PE	RD/S	Myopic	Top-down	External Models
MERGE-ETL	GE	IO/NLP	Perfect foresight	Hybrid	Internal Modules
MESSAGE	GE	IO/LP	Perfect/limited foresight	Hybrid	External Models
POLES	PE	RD/S	Myopic	Top-down	External Models
PROMETHEUS	PE	IO/LP	Perfect foresight	Bottom-up	External Models
REMIND	GE	IO/NLP	Perfect foresight	Hybrid	External Models
TIAM	PE	IO/LP	Perfect foresight	Bottom-up	Internal Modules
WITCH	GE	IO/NLP	Perfect foresight	Hybrid	Internal Modules or External Models

The data presented in our table primarily derives from the Integrated Assessment Modeling Consortium [61] database and model documentations.

Table 2
IAMs temporal, technological, and regional characteristics.

IAMs	Time Horizon	Timestep <sup>a</sup>	Technological Change	Technological <sup>b</sup> detail	Geographical <sup>o</sup> Coverage
AIM/Hub	2005 to 2050-2100	1 year	Exogenous	Mid	Mid
GCAM	2015-2100	5 timesteps	Exogenous	High	High
GEM-E3	2014 to 2100	5 years	Endogenous	Low	High
GRACE	2014-2100	1 year	Exogenous	Low	High
IMAGE	2005 to 2050-2100	15 years	Endogenous	High	High
MERGE-ETL	2000 to 2150	10 years	Endogenous	Mid	Low
MESSAGE	2010 to 2100	5 years	Exogenous	High	Low
POLES	2015-2100	1 year	Endogenous	High	Mid
PROMETHEUS	2000-2100	1 year	Endogenous	Mid	Low
REMIND	2005 to 2100-2150	5-10 years	Endogenous	High	Low
TIAM	2005 to 2100	5-10 years	Exogenous	High	Mid
WITCH	2005 to 2100-2150	5 years	Endogenous	Low	Mid
		•			

For clarity and simplicity, we have reported on only one representative model from each IAM family based on the IAMC database [61] (e.g. TIAM-UCL from the TIAM family).

#### 3.2. Sectoral coverage of hydrogen systems

The studied IAMs highlight the potential role of hydrogen technologies for achieving significant reductions in carbon emissions by 2050 and 2100 while underlining the challenges of properly representing the full complexity of the hydrogen system. This study evaluates approximately 40 hydrogen-related technologies. Fig. 4 illustrates the analysis frequency for the 40 hydrogen-related technologies studied in 50 reviewed articles. For instance, utilization technologies are discussed in 40 articles, whereas storage technologies are examined in 10 articles. These IAMs vary in their hydrogen technology modeling approach; some focus on a particular sector, [107,108], or multi sectors analysis [109]. Some studies take a more comprehensive approach, assessing both the supply and demand side and exploring the full range of processes from hydrogen generation to its end use [70,110].

Assessment of the most common components within the hydrogen supply chain across IAMs reveals that the majority of research focuses on the production and utilization phases, despite the equal importance of other areas such as distribution and storage. Fig. 4 shows that production methods, particularly electrochemical processes, are examined in more than half of the studies, followed by fossil and biomass-based production methods. Technologies used by end users receive as much attention in studies as those used in production. Focusing primarily on

a single end user, such as the transportation or industrial sectors, to access the role of hydrogen technologies in decarbonization pathways is a common approach [111,112]. For instance, various studies on transportation illustrate the importance of hydrogen as a fuel not only for light-duty vehicles but more importantly for heavy-duty vehicles, shipping, and aviation [113,114]. In the industrial sector, the role of hydrogen is becoming increasingly significant. It is directly applied in high-energy-demand sectors such as steel and iron and serves a vital role in the chemical industry [25]. Synthetic fuels produced from hydrogen can be employed in various industrial processes, such as chemical manufacturing, steel production, and refining, where they can replace conventional fossil fuels [26]. This involves using hydrogen in chemical reactions to produce alternative fuels, a process that is gaining attention as a sustainable energy solution. This dual application of hydrogen, both as a direct energy source and a vital component in synthesizing eco-friendly fuels, highlights its growing importance in IAMs which evaluated industrial processes [67].

The generation of electricity from hydrogen is part of strategies aimed at decarbonizing energy systems, particularly highlighted in recent research [109]. In our classification, we treat the production of electricity using hydrogen as a distinct category due to its significance, although it could technically be regarded as a subset within utilization. The potential of hydrogen to act as a long-term storage option

<sup>&</sup>lt;sup>a</sup> GE and PE stand for General Equilibrium and Partial Equilibrium respectively.

<sup>&</sup>lt;sup>b</sup> The mathematical structure of models was mainly Intertemporal Optimization (IO) or Recursive Dynamics (RD) with (Non)Linear Programming ((N)LP) formulation or Simulation (S).

<sup>&</sup>lt;sup>a</sup> TIAM-UCL and REMIND contain 5-year timesteps up to 2070 and 2060 and 10-year timesteps afterward.

<sup>&</sup>lt;sup>b</sup> A qualitative assessment considering into Low (less than 40), Mid (between 40 to 60), and High levels (more than 60), based on [61]. Following a similar approach to [90], the assessment evaluates the level of detail in energy and land-use sectors.

<sup>&</sup>lt;sup>c</sup> The number of regions covered in the models is considered either Low (less than 14) Mid (greater than 15 or less than 26) or High (greater than 27).

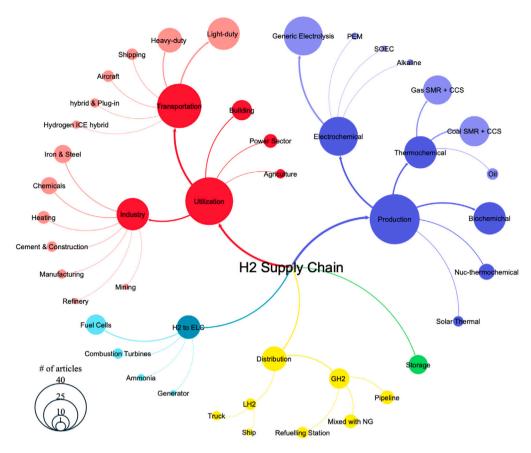


Fig. 4. Frequency of hydrogen supply chain technologies in 50 reviewed articles. The size of the bubbles corresponds to the number of articles analyzed for each technology.

complements the intermittent nature of variable renewable energy (VRE) sources such as wind and solar, thereby ensuring an electricity supply better aligned with demand [115–117]. Finally, examining the distribution aspect of the hydrogen supply chain reveals that, for nearterm emission-reduction strategies, blending hydrogen with natural gas as a means of reducing hydrogen distribution costs emerges as a feasible option. To meet long-term objectives, an increase in trade is anticipated, where potentially the transportation of liquefied hydrogen via ships becomes a prevalent method for international trade [26]. In addition to models that focus on transmission, those that address both light and heavy-duty vehicles follow how hydrogen is supplied at refueling stations as a distribution option [118].

Fig. 5 shows the number of hydrogen supply chain technologies (processes) evaluated in each IAM. Looking closely at the link between different technologies and their inclusion in various IAMs, it appears that REMIND [87,119] and TIAM [120,121] have explored additional applications in the utilization sector. In addition to these, some other models like WITCH and MESSAGE-GLOBIOM [117] have also assessed nearly the entire spectrum of the hydrogen supply chain mentioned in Fig. 4. Approximately seven production technologies have been scrutinized in research using the MESSAGE-GLOBIOM [122] and GCAM models. Models incorporating T–D and some hybrid approaches, treat the utilization sector as an aggregated final demand [105,123]. They concentrate on various production methods within their framework. This is in contrast to the research conducted with the T–D IMAGE model, which focuses on hard-to-abate sectors, viewing them as end users [25].

#### 3.3. Parameters, inputs, and assumptions

To embed hydrogen systems into IAMs, parameters, inputs, and assumptions serve distinct roles. Parameters as internal data within the

models undertake to define the structure and behavior of the model and need to be calibrated. However, inputs and assumptions are external data fed into the model to represent various aspects of the system being studied, such as economic or environmental data.

Through the disaggregated modeling approach in B-U models, there is a wide range of parameter values in the hydrogen system [124] both within a model (varying by the different representations of each technology and by region) and across those (varying by the projection assumptions). Techno-enviro-economic characteristics of hydrogen production technologies contribute to evaluating the technological feasibility, environmental impact, and economic viability of different technologies used to produce hydrogen. In models with multiple representations of technology types, the technology mix is explicitly examined through a trade-off between various types (with different efficiency and cost-effectiveness), while in other models, this transition is implicitly applied based on one type getting more efficient and cost-effective over time [125]. Based on the reviewed literature, some models represent multiple technologies within a single hydrogen production pathway. For instance, MESSAGE-ix includes various types of biomass gasification, both with and without CCS. On the other hand, some models include only a single representative technology for each pathway; for example, the WITCH model considers only one type of biomass for hydrogen production [126]. The structural representation of technology refers to the technical and operating characteristics of data on capital cost, O&M cost, energy efficiency, and lifetime.

Capital cost of hydrogen technology. The investment or capital cost of hydrogen technologies considered in IAMs is also called overnight construction cost. The anticipated amount of this element of cost is also determined based on the discount rate and availability factor assumptions, and hydrogen plants' lifetime [127]. In this study by Bolat and Tiel, the contribution rates of capital cost in total cost for SMR and electrolyzer technologies are approximately the same and are lower

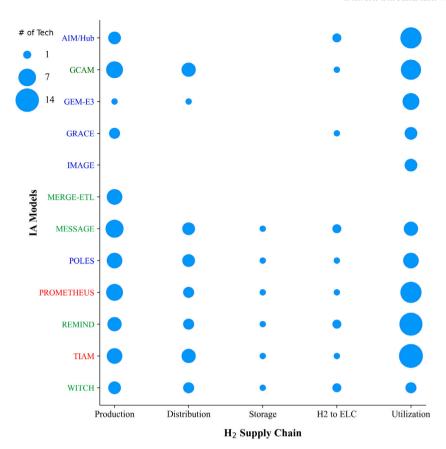


Fig. 5. Number of hydrogen supply chain processes evaluated in each IAM. Colored IAMs represent their modeling paradigm: T-D (Blue), Hybrid (Green), and B-U (Red).

than those of coal and biomass gasification technologies [127]. The available numerical data on the capital cost of hydrogen production for some global IAMs is provided in Table 3:

 $\begin{tabular}{ll} \textbf{Table 3} \\ \textbf{Capital cost of hydrogen production technologies in the studied IAMs (in US$2010/kW)}. \\ \end{tabular}$ 

Model	Conversion Technology							Reference
	CG	CG+	BG	BG+	SMR	SMR+	ETS	
AIM/V2.0	2981	3103	2604	3451	1016	1518	1455	[128]
TIAM-Grantham	1050	2822	3135	8779	313	1160	1057	[33]
MERGE-ETL	1200	1400	1600	1800	800	1000	N/A	[82]

CG: Coal Gasification, CG+: Coal Gasification+ CCS, BG: Biomass Gasification, BG+: Biomass Gasification+ CCS, SMR: Steam Methane Reforming, SMR+: Steam Methane Reforming+ CCS, ETS: Electrolyzer.

IAMs make dynamic or static assumptions about the capital cost and conversion efficiency of technologies. In MESSAGEix-GLOBIOM\_1.0, as a member of the MESSAGE family, and IMAGE 3.0, capital costs vary across regions and over time. Similarly, WITCH-GLOBIOM 4.4, part of the WITCH family, assumes that capital costs for power plants vary regionally and change dynamically over time.

O&M cost of hydrogen technology. Fixed O&M costs are typically a fixed percentage of the capital cost of hydrogen production, and this ratio is assumed to remain constant over time. For most IAMs, this percentage is the same across all regions, but across models, the percentage could be different. For reference, IEA [129] gives a percentage of 3%–6% of capital cost (on average) for the fixed O&M cost of all technologies, however, a wide range of 1%–7% can be found among IAMs [127]. While most IAMs assume that the ratio of O&M costs to capital costs is not spatial, WITCH-GLOBIOM 4.4 ratio is region-dependent and is subject to the IEA's assessment [127]. Based on the reported data, variable and fixed O&M costs of hydrogen production account for 1% and 4% of annual capital expenditure, respectively [130]. The variable

O&M can also be considered with the exogenous assumption of fuel cost or endogenously changing based on the extraction cost of the fuels. The available numerical data on the O&M cost of hydrogen production for some global IAMs are provided in Table 4:

Table 4
Fixed O&M cost of hydrogen production technologies in IAMs (in US\$2010/kW).

•	Model	Conversion Technology							Reference
		CG	CG+	BG	BG+	SMR	SMR+	ETS	
	AIM/V2.0	232.63	346.82	1114.4	943.37	83.24	120.28	346.92	[128]
	TIAM-Grantham	47.03	54.55	33.86	47.03	17.55	35.11	29.78	[33]

CG: Coal Gasification, CG+: Coal Gasification+ CCS, BG: Biomass Gasification, BG+: Biomass Gasification+ CCS, SMR: Steam Methane Reforming, SMR+: Steam Methane Reforming+ CCS, ETS: Electrolyzer.

Conversion efficiency. The conversion efficiency reported by IAMs is the so-called net efficiency after subtracting internal losses such as fuel conditioning and pumping. It is worth noting that the efficiency is reported based on an average through all types of operations, not only for hydrogen. IAMs generally consider the conversion efficiency of the technology to be an exogenous input to the model, constant or evolving over time to match the expected technological learning. Table 5 represents data on conversion technologies in some available IAMs:

Conversion efficiency of hydrogen production technologies in IAMs.

Model	Conv		Reference					
	CG	CG+	BG	BG+	SMR	SMR+	ETS	
AIM/V2.0	60	58	60	55	76	69	69	[128]
TIAM-Grantham	63	38	63	37	81	44	80	[33]
MERGE-ETL	60	55	55	52	75	70	70	[82]

CG: Coal Gasification, CG+: Coal Gasification+ CCS, BG: Biomass Gasification, BG+: Biomass Gasification+ CCS, SMR: Steam Methane Reforming, SMR+: Steam Methane Reforming+ CCS, ETS: Electrolyzer.

*Lifetime.* IAMs usually assume that the lifetime of a given technology does not change over time. The only exception is MESSAGEix\_GLOBIOM\_1.0 which assumes the lifetime of the technology of biomass with CCS varies over time [83,131,132].

The changes over time in the techno-economic characteristics of the hydrogen supply chain are projected in terms of the associated assumptions. The projection approaches consider either static or dynamic assumptions on these characteristics. It is worth noting that the IAM team may use just one of the strategies to predict characteristics for all technologies in the model or employ various strategies for different technologies. However, details regarding hydrogen technologies have not been published for the majority of the models. The assumptions on characteristics projections in some IAMs considering hydrogen systems can be found in Table 6.

Table 6
Assumptions on energy system characteristics in IAMs [124].

Model	Efficiency Improvement	Capital Cost
MESSAGE	Static	Both
TIAM	Static	Both
WITCH	Dynamic	Both
AIM-Hub	Static	Both
GCAM	Static	Static
IMAGE	Static	Both
PROMETHEUS	Dynamic	Both

Generally, T–D models require relatively aggregated data on the levelized cost of hydrogen production, as the cost for producers in these models does not account for the detailed characteristics of energy production technologies [70]. However, some hybrid IAMs also incorporate the levelized cost of hydrogen production. For example, MERGE-ETL uses the levelized cost of hydrogen production as an endogenous (dynamic) characteristic, as described in section 1.3 of the Supplementary Material. These levelized costs of hydrogen are shown in Table 7, reflecting a range of values for different hydrogen production methods and highlighting ETS as the most cost-effective option.

Table 7
Initial (2010) and floor levelized cost of Hydrogen production by conversion technologies in the MERGE-ETL model (Unit: US\$/GJ/year).

Model	Conver		Reference					
	CG	CG+	BG	BG+	SMR	SMR+	ETS	
Initial Cost	11.14	11.90	13.14	13.87	9.42	10.02	6.70	[82]
Floor Cost	10.50	11.30	12.80	13.40	8.90	9.60	6.20	

CG: Coal Gasification, CG+: Coal Gasification+ CCS, BG: Biomass Gasification, BG+: Biomass Gasification+ CCS, SMR: Steam Methane Reforming, SMR+: Steam Methane Reforming+ CCS, ETS: Electrolyzer.

In models with T-D approach, it is primarily required to define the substitution parameters of energy carriers by model calibration for embedding hydrogen energy systems [133]. The amount of hydrogen contributed to the total supply of non-electric energy carriers is then determined based on the associated elasticity of substitution and their relative price or cost of the producer (levelized cost of hydrogen production). As another approach for hydrogen modeling, Wei and Glomsrod developed a T-D CGE model in which at the top level, the elasticity of substitution across different hydrogen technologies is considered a value of 2. At the middle level, fuels used by each technology and value-added are aggregated through a Leontief function at the middle level with an elasticity of 0, which indicates a fixed proportion in transforming other energy to hydrogen in terms of energy values. Using an alternative modeling approach at the last level, the value added for each technology is combined with labor and capital using a CES function with an elasticity of 0.3, the same as for other production sectors in the model [70].

Cost-effectiveness is an important metric that is generally used in the study of hydrogen pathways. However, an inefficient pathway that requires a relatively large amount of energy is not desirable because a larger amount of fossil fuels or hydrogen needs to be used to satisfy the demand. Therefore, hydrogen supply chains are assessed primarily based on energy, economic, and environmental effect metrics [134]. It should be noted that the primary purpose of using hydrogen is decarbonization, and its contribution to reducing  ${\rm CO}_2$  emissions can be seen as a performance criterion.

Reviewing the literature shows that including environmental externalities such as human health, ecosystem quality, and resource depletion in the total cost of hydrogen systems (TCH) provides a "real" total cost of production [135,136], and delivery [134]. Results showed that environmental externalities can account for a large portion of the total hydrogen cost (ranging from 14% to 88%), highlighting the importance of involving external environmental impacts in the assessment. Among the technologies reviewed in this study, SMRs with CCS are deemed the most cost-effective due to the lowest levelized cost of production and lower direct CO2 emissions. While biomass and coal can be considered relatively cheap feedstocks, in practice, the "real" costs of their gasification are significantly higher due to the large externalities [135]. Among green hydrogen technologies, Solar PV electrolysis is more expensive than wind and nuclear, and its externalities from manufacturing crystalline silicon panels are also greater and lead to the weakest overall economic performance. The results of the TCH analysis for hydrogen technologies are summarized

$$TCH_{CG} > TCH_{BG} > TCH_{SolarPV} > TCH_{BG+} > TCH_{CG+} > TCH_{Wind} > TCH_{Nuclear} > TCH_{SMR} > TCH_{SMR+}$$

On the logistic side, a regional delivery-oriented study [134] shows that compressed hydrogen, as a promising option for hydrogen delivery, has a landed cost of 2.4 USD/kg and for transportation and power industry use is approximately 6.8 USD/kg¹. In addition, liquid NH₃, as another potential option, has cost ranging from 2.9 to 3.4 USD/kg. Pipeline transmission of 70 bar hydrogen has the lowest "energy loss" for distances less than 4500 km and is followed by liquid hydrogen and liquid organic hydrogen carriers (LOHC). Hydrogen storage is also an important cost driver at around 32% of TCH. For SMR and Autothermal Reforming (ATR), hydrogen storage costs accounted for the largest share of total capital costs of delivery, approximately 48% and 34%, respectively.

#### 3.4. Dealing with uncertainty

Quantifying and dealing with uncertainty could be a significant challenge, highlighted by the systems' complex and interconnected nature of IAMs. The challenge of modeling processes and commodities, mapping technological progress, and future climate conditions bring inherent uncertainties to the integration of hydrogen systems into IAMs. In assessing and exploring the impact of hydrogen-related policies, through IAMs, there could be two primary sources of uncertainty including structural (related to the choices of the model structure), and parametric associated with inputs and parameters of the hydrogen system [137].

Parametric uncertainties emerge from incomplete knowledge about the empirical values of model parameters, while structural uncertainties are related to the assumptions within the model equations defining its structure [138]. A common observation across different scales is that the majority of analyzed cases focus on parametric uncertainty, while a smaller portion addresses structural uncertainty [99,139]. To manage uncertainties, particularly parametric uncertainties, IAMs employ a variety of advanced methods, including Monte Carlo simulations, Bayesian inference, sensitivity analysis, scenario analysis, robust optimization, and stochastic programming. Additionally, machine learning approaches such as ensemble learning, Gaussian Processes, and deep

 $<sup>^{1}\,</sup>$  Landed cost indicating distribution cost is calculated under the assumption that distances are not longer than 2000 km.

learning models with uncertainty quantification could be applied to further enhance decision-making reliability [140]. Common approaches for addressing parametric uncertainty in IAMs that model hydrogen pathways include scenario analysis, stochastic programming, robust optimization, and simulation [137,141]. The selection of a specific technique for managing uncertainty should take into account factors such as the availability of data, the range of uncertainties to be addressed, and the nature of the policy questions being investigated. Each of these methods has a unique way of dealing with the uncertainty of input parameters and characteristics of the hydrogen system with a common goal of measuring how changes in parameters affect the output of the model and its related policy insights.

In the reviewed articles, only four models used uncertainty methods beyond basic scenario planning and sensitivity analysis. [120,142] used Monte Carlo simulation within the TIAM model to address uncertainties associated with parameters such as technology costs, resource potentials, and climate sensitivity. They examined how these uncertainties affect energy transition pathways, the effectiveness of climate policies, and the risks associated with clean energy technologies such as hydrogen. [123] relied on a similar approach to examine the efficiency and consequences of global warming reduction policies by incorporating the uncertainty of several parameters, such as the cost of hydrogen production from different sources. The majority of the reviewed studies on hydrogen rely on scenario analysis. It starts with establishing a base case scenario and then explores the effects of uncertain policy measures or external factors through alternative scenarios, incorporating various constraints and assumptions. However, this approach has its critics due to several shortcomings. Usher and Strachan criticized the deterministic approach as inadequate for complex issues riddled with uncertainties [143]. Morgan and Keith argued that scenarios with detailed narratives might narrow the perceived range of possible outcomes, leading to cognitive biases [144].

Examples of dealing with structural uncertainties include those taking a multi-model approach. In the reviewed articles, less than 20% of the studies use a multi-model approach to address structural uncertainty and achieve more reliable results. For example, models such as GEM-E3 and GCAM, despite not always being the subject of single model studies [68,145], are frequently incorporated into extensive multi-model investigations [69] and are crucial for constructing scenarios within the SSP frameworks [146]. This approach considers the results of different model applications using the same model inputs as can be seen based on AR6 data.

The data derived from multiple models, which account for structural uncertainty, provide a foundational database for numerous research studies and policies, particularly those featured in the AR6 databases [147]. An important effort to do a multi-model analysis is the study done by IPCC WGIII for ARs and special reports. In these reports, SSP scenarios have been studied to provide a range of possible results by different models. Within categories C1 to C3 (Fig. 6), which consider scenarios that limit warming to 2 °C or lower (with a probability higher than 67%), the production levels are compared using these models. In this analysis, out of the 541 vetted scenarios related to categories C1-C3, 67 belong to C1, 101 to C2, and 225 to C3, all derived from 12 primarily studied IAMs, report hydrogen as a secondary energy source. The variability in results reported across different models in each category is mostly due to structural uncertainty, which is one of the main contributing factors. Statistical analysis indicates that B-U models, particularly those with a high level of technological detail, demonstrate increased levels of hydrogen production. In general, "technological detail" and "technological change" have statistically significant effects on H2 production, while "model perspective" has a lesser but still notable impact, and the "economic approach" shows no significant influence B. The REMIND and MESSAGE-GLOBIOM models, with their high technological detail and B-U approach to modeling energy systems, stand out by projecting higher production levels in

their respective scenarios [109], around 100 EJ per year, compared to other IAMs, such as WITCH and GCAM [148,149].

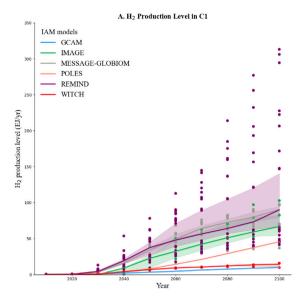
IPCC AR6 indicates that to keep global warming under 1.5 °C, it may be necessary for low-carbon energy sources to make up more than 70% of the world's primary energy supply by the year 2050 [18]. Delving into the details of hydrogen production as depicted in Fig. 7, it becomes apparent that its production levels vary significantly across different C categories. Specifically, the average production level in the C1 category is nearly five times greater than in the C8 category. A notable observation is that tighter restrictions on warming levels correlate with an increase in hydrogen production. Climaterelated policies, which restrict GHG emissions, underscore the growing significance of alternative energy sources like hydrogen in meeting overall energy demand by 2100 [150]. The shaded areas around the lines represent the uncertainty and variability in hydrogen production estimates across different C categories over time. This highlights the importance of addressing uncertainty in decision-making to achieve more robust outcomes and effective policymaking.

#### 4. Hydrogen and decarbonization policies

Policy analysis that builds on IAMs employs a methodology in which a baseline scenario is enhanced through the implementation of a specific policy intervention [18]. Research indicates that hydrogen as an energy source becomes economically viable mainly under strict climate mitigation strategies, efficiency norms, or introducing market-driven incentives such as fossil fuel taxes [113,120,151]. Findings suggest that while cost reductions in low-carbon hydrogen can significantly boost its consumption, in terms of its overall market share, this leads to a slight reduction in fossil fuel dependency and associated carbon emissions. Reducing the costs of low-carbon hydrogen is beneficial, but without sufficient policy measures, it is considered insufficient to achieve significant climate benefits [70]. Effective policy actions are crucial to direct investment to achieve interim climate goals efficiently [66]. There exists a positive relationship between carbon pricing and hydrogen's role in the energy sector [114]. The emergence and success of a hydrogen-based economy will also greatly depend on technological progress and focused initiatives to avoid investment in non-sustainable hydrogen production methods [120].

Hydrogen production tends to be significantly higher in scenarios with stringent policy frameworks [152,153] or specific scenarios aimed at promoting hydrogen or hydrogen-based energy carriers use [154, 155]. This trend indicates a positive correlation between policy-driven scenarios and the anticipated levels of hydrogen production by the end of the century. As hydrogen becomes a more prominent component of the energy mix, the reliance on electricity will require substantial increases in generation capacity (Fig. 8). In these scenarios, the pivotal role of electricity in electrolysis, the primary method for producing green hydrogen, becomes particularly pronounced. Consequently, the integration of hydrogen into future energy systems not only depend on robust policy support but also on strategic investments in expanding and decarbonizing the electricity grid.

Hydrogen presents a feasible solution for hard-to-abate sectors, such as heavy transport, aviation, and high-heat industrial processes [25,69]. In industries like cement and chemicals, where direct electrification is challenging, the shift towards carbon-neutral alternatives like biomass or hydrogen, or indirectly through hydrogen-based synthetic fuels, is viable [26,67,114]. Policies and mechanisms that promote the use of hydrogen in industry, including technology R&D, carbon pricing, subsidies, and regulatory frameworks that encourage or require low-carbon hydrogen adoption have been studied [69,156–158]. They can drive the early adoption of hydrogen technologies, by creating an opportunity for investment and technological advancements. This can lead to reducing the costs of hydrogen technologies and facilitate the development of industrial hubs for large-scale hydrogen production and utilization. However, the effectiveness of these policies depends on



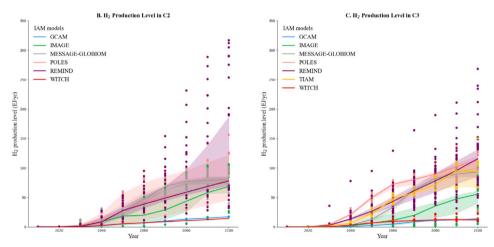


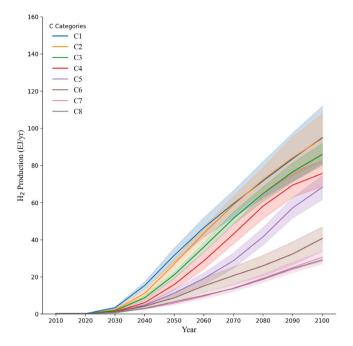
Fig. 6. In panel A–C, the 2020–2100 annual time series of hydrogen production level is plotted at 5-year intervals for reviewed models within the C1 to C3 temperature category. The graphs show median pathways (dark lines), the interquartile range (IQR, shaded regions between the 25th and 75th percentiles), and outliers for each model (individual points). The interactive format of these graphs is available at the following link: InteractiveGraphs.

their coordination across different governance levels and their ability to address economic and technical challenges [56].

Scenarios with hydrogen adoption in the transportation sector are primarily driven by robust policies and measures such as rebates, stricter emissions regulations, and the establishment of extensive refueling infrastructure [155,159,160]. The effectiveness of these policies is crucial, as the transportation sector often needs more direct incentives than carbon taxation alone to drive change [68]. Within the transport sector, for light duty vehicles complementary policies, such as feebates on internal combustion engines and rebates for fuel cell electric vehicles (FCEV), can further accelerate the transition to hydrogen [155]. Furthermore, early investments in FCEV research and development, coupled with infrastructure and fuel subsidies, can significantly support the adoption of these vehicles [161]. Hydrogen also shows great promise in long-haul freight transport due to its advantages over battery technologies, although energy consumption for compression and liquefaction remains a challenge [160]. Beyond freight, the potential of hydrogen-powered buses is also gaining attraction [160]. However, studies suggest that the long-term economic viability of these technologies depends on several factors: reducing the costs of hydrogen and synthetic fuel production [43], enhancing

refueling infrastructure [107,159], and securing regulatory support alongside advancements in vehicle technology [43,119]. On the other hand, in scenarios where political resistance is high, conventional internal combustion engines and hybrid vehicles maintain their dominance, with only modest adoption of hydrogen and synthetic fuels. These contrasting pathways highlight the decisive role of policy in shaping the future landscape of hydrogen production and vehicle adoption.

Fig. 8 illustrates the uncertainty in hydrogen production and consumption values, which highlight the spread and variability of the data across different years and energy sources. The presence of outliers and the distance between the median and mean values further emphasize the variability and potential uncertainty in production and consumption estimates in different sources and sectors. Another notable point in the graph is the discrepancy between the total amount of hydrogen production and consumption, particularly evident in the year 2100. This difference can stem from several factors. For instance, many models, especially T–D models, report only production data and do not account for consumption. The number of reported scenarios for production is almost double compared to those for consumption. A second factor contributing to this gap is energy losses or the use of hydrogen in unreported sectors. This non-transparent data leads to a high level



**Fig. 7.** Hydrogen production levels among C categories (2020–2100): The lines represent production trends for each category, with shaded areas indicating the 95% confidence intervals, reflecting the uncertainty and variability in the estimates.

of uncertainty, exacerbating the discrepancy between production and consumption estimates.

As illustrated in Fig. 8, it is projected that by 2100, around 50 EJ per year of hydrogen will be produced, primarily from electricity, which could contribute significantly to the demand sector. It is projected that total production will reach almost 70 EJ/yr. The hydrogen demand in "other sectors" represents a significant portion of the total hydrogen consumption. However, this specific segment is not explicitly described in the IIASA database. It may encompass hydrogen that could potentially be employed in electricity generation, as suggested by insights from the literature. Following this, the industrial and transportation sectors are expected to become the primary consumers of hydrogen, leveraging it as a key energy source to drive their operations and significantly reduce their carbon footprints. There is increasing confidence that hydrogen can play a significant role in specific sectors, particularly in the transport and industrial sectors. However, there is less consensus on the timing and volumes of hydrogen use, and there are varied perspectives on the effectiveness of different hydrogen production methods [150].

#### 5. Discussion and conclusion

This paper presents an extensive review of the literature on IAMs, studying the technological characteristics of hydrogen technologies in decarbonization pathways across different sectors to meet ambitious global climate goals, considering the underlying uncertainties. We classified the literature studied according to their respective hydrogen supply chain configuration, including how hydrogen systems are integrated into IAMs and their decarbonization policies. This analysis outlines 12 families of IAMs, each with differing complexities, scopes, and technological details, while also highlighting the increasing focus on hydrogen in stringent climate mitigation scenarios, along with the varying assumptions and uncertainties that significantly influence the outcomes of these models.

Two keys to scaling up hydrogen's role are supportive policies and economic incentives, both amidst a backdrop of diverse assumptions on its techno-economic aspects that shape decarbonization paths. Many studies identified hydrogen as a cornerstone element in the decarbonization of specific sectors. While some aspects of hydrogen's supply chain and applications have been studied in depth by the reviewed IAMs, we noticed that other sectors, such as the utilization of hydrogen in electricity generation or as seasonal storage, received less attention. Mostly, hydrogen's utilization in transportation, particularly through fuel cells in heavy-duty vehicles, and in hard-to-abate sectors, such as iron and steel production have been explored by various IAMs. For example, based on the C3 scenario implemented by IAMs, the share of hydrogen in final energy could reach 17% by 2100 and it is expected that the transportation and industrial sectors will be the main hydrogen users [150]. This emphasizes the vital importance of hydrogen in these sectors, highlighting the need for a holistic and thorough examination of its use in all possible applications.

Navigating uncertainties within IAMs related to technology representation, inputted policies, and model structure is essential, as these factors influence hydrogen's potential for emission reduction. IAMs incorporate different approaches to address parametric uncertainty, like technology cost projections. These models explore multiple pathways by varying assumptions about learning rates, capital costs, and operational efficiencies for hydrogen technologies. However, these traditional approaches have limitations, as they rely on a narrow set of outcomes and overlook the variability of real-world systems, including dynamic interactions between policies, markets, and technological adoption. Structural uncertainty is often examined through multi-scenario analyses that consider diverse policy frameworks, such as carbon pricing, subsidies for green hydrogen, and renewable energy mandates. IAMs use SSPs and RCPs to account for variations in economic growth, population dynamics, and climate mitigation ambitions, offering a range of potential outcomes for future hydrogen demand.

Our review indicates that the integration of hydrogen into decarbonization strategies is sensitive to various assumptions like technological progress and policy support. The reported variations in hydrogen production levels by the IPCC AR6 also illustrate this issue, arising from diverse assumptions, widely spread inputs, different sectoral coverage, and modeling approaches across IAMs. Both parametric and structural uncertainties play a crucial role in shaping the outcomes of IAMs, particularly when considering hydrogen-based technologies as cutting-edge solutions. This highlights the need for rigorous modeling approaches to capture these uncertainties effectively.

#### 5.1. Gaps and future research

Designing effective climate policies and producing reliable scientific results become significantly more difficult due to varying outcomes from different climate models and IAMs, all stemming from underlying uncertainties. Our review highlights a gap in IAM studies addressing hydrogen technologies and uncertainty. Utilizing effective uncertainty analysis approaches helps deal with parametric and structural uncertainties for a more accurate representation. Future studies could address the significant gap in understanding the structural uncertainty of hydrogen systems within IAMs by exploring how variations in model design, assumptions, and methodologies influence results. Investigating these uncertainties would enhance the robustness of projections and provide more reliable insights into hydrogen's role in decarbonization pathways.

Studied models often rely on deterministic or simplified probabilistic methods, which may not adequately capture the complexities and uncertainties inherent in hydrogen production, distribution, and utilization systems. Common parametric uncertainty approaches such as stochastic programming, robust optimization, and simulation can be employed to address variability in hydrogen parameters and system behaviors. Complementing these traditional methods, predictive approaches like Bayesian methods and machine learning techniques offer advanced capabilities for uncertainty quantification, bridging the

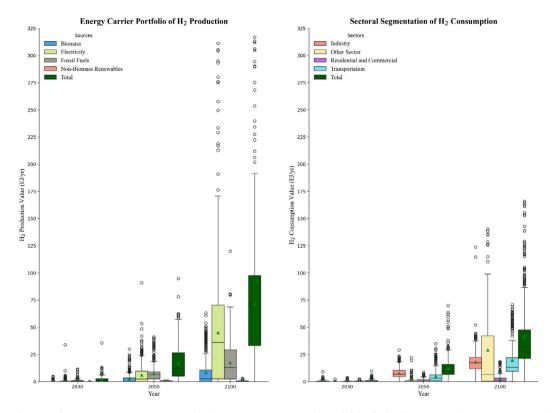


Fig. 8. Hydrogen production and consumption mean in scenarios that limit warming to 2 °C (with a probability higher than 67%) or lower (IPCC C1–C3). The interactive format of these graphs is available at the following link: InteractiveGraphs.

gap between predictive techniques and optimization, and enhancing decision-making under uncertainty. Techniques such as neural networks, decision trees, and ensemble learning can be utilized to refine parameter estimates, optimize scenario pathways, and identify key drivers of uncertainty.

Despite the value of feedback loops and trade-offs in IAMs, challenges persist in capturing the complexities of real-world systems. For instance, many IAMs oversimplify the impacts of large-scale hydrogen production on industrial processes or the interplay between hydrogen-based infrastructure and transportation costs. Addressing these short-comings requires future IAM research to prioritize higher temporal and spatial resolution, dynamic policy feedback, and multi-sectoral optimization frameworks. Such advancements would better account for the intricate feedback loops and trade-offs that hydrogen introduces across different sectors. Ultimately, this enhanced modeling would offer deeper insights into hydrogen's long-term effects and synergies in the broader energy, economic, and environmental landscape.

There has been significant progress in improving the accessibility of model outputs in the evolution of IAM transparency in models' documentation and, particularly evident in the AR6 database [147]. However, the transparency of inputs and underlying assumptions remains a critical area for improvement, as highlighted by previous studies [162]. While the focus on outputs has undoubtedly improved, the clarity of the foundational assumptions and input data in AR6 and our review of 50 papers could be further enhanced to foster a deeper understanding and trust in these models. In this context, our findings reveal a significant gap between the robust data on the techno-environmental-economic characteristics and the projection assumptions of hydrogen systems, a gap that has also been identified in earlier research [99]. Considering this issue would not only aid in the reproducibility of research, but also in creating more informed and effective climate policies, building upon the significant achievements of AR6 and the ongoing work within the climate modeling community. Regarding the data used in modeling, while IAMs typically operate on longer time scales, real-time data can be integrated to capture

short-term dynamics and system behaviors, thereby providing more robust representations of storage capacities, transportation logistics, and infrastructure utilization within the hydrogen supply chain.

Additionally, there is a significant lack of data on the associated costs of these processes in IAMs, which hinders an accurate evaluation of the economic viability and scalability of hydrogen systems. It remains unclear whether hydrogen-related technologies and their costs are included in end-use calculations or treated as part of the production stage. These costs may be incorporated into the total cost, influencing overall estimates, or omitted entirely, leading to increased uncertainty. They are not explicitly detailed in the AR6 database or the reviewed literature, with the results indicating that these processes have been studied in only a limited number of cases. Future research should aim to clarify this issue and reduce uncertainties surrounding hydrogen integration into energy system models.

Among hydrogen infrastructures, production and consumption have received considerable attention, as these areas are critical for understanding the potential and challenges of integrating hydrogen into energy systems. It is important to recognize that the differences between hydrogen production and consumption levels observed in the results underscore the influence of uncertainties, and future studies should explore this in more detail. However, while much emphasis has been placed on reducing hydrogen production costs, greater focus is needed on developing an efficient, robust infrastructure to support storage, transportation, and distribution.

Hydrogen storage can be a pivotal element for enabling the large-scale deployment of VRE [117,163], and progress in hydrogen storage technologies can further promote and extend the field of hydrogen applications. Moreover, the literature reveals a significant gap concerning solutions for large-scale transmission and distribution. As the demand for clean hydrogen, particularly in industries such as steel production, continues to rise, it becomes increasingly efficient to connect supply and demand centers and utilize decentralized production methods. However, the development of cost-efficient hydrogen transmission methods remains a challenge. High transmission and distribution costs

Table A.8
Full list of reviewed references categorized based on models.

Model	Reviewed References				
AIM	[110]				
GCAM	[78,113,164,165]				
GEM-E3	[114]				
GRACE	[70]				
IMAGE	[25]				
MERGE	[82,105,123]				
MESSAGE	[115,117,122,166,167]				
POLES	[84,116]				
PROMETHEUS	[168,169]				
REMIND	[67,87,108,109,111,119,155,170–172]				
TIAM	[26,112,118,120,121,142,170,173–175]				
WITCH	[107,126]				
Multi-models	[66,68,69,145,146,153,176,177]				

can dramatically escalate the overall expenses associated with hydrogen, thereby impacting its commercial viability and economic competitiveness. IAMs could help meet this challenge by guiding strategic planning.

#### CRediT authorship contribution statement

Sara Ghaboulian Zare: Conceptualization, Data curation, Formal analysis, Methodology, Software, Visualization, Writing – original draft. Kamyar Amirmoeini: Conceptualization, Data curation, Formal analysis, Methodology, Writing – original draft. Olivier Bahn: Project administration, Supervision, Validation, Methodology, Investigation, Writing – review & editing. Ryan C. Baker: Funding acquisition, Validation. Normand Mousseau: Supervision, Validation, Investigation, Writing – review & editing. Najmeh Neshat: Writing, Conceptualization, Data curation. Martin Trépanier: Supervision, Validation, Investigation, Writing – review & editing. Qianpu Wang: Funding acquisition, Validation.

#### Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Olivier Bahn reports financial support was provided by National Research Council Canada. If there are other authors, they 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. Reviewed articles

Table A.8 presents an extensive list of reviewed articles, organized into 12 IAM categories and one multi-model category, encompassing studies involving more than one model.

Table B.9
Results of multi-way ANOVA.

Model characteristic	sum_sq	df	F	PR(>F)
Technological Detail	209 709.440716	1.0	217.184876	1.184469e-34
Model Perspective	12753.995869	1.0	13.208633	3.469297e-04
Economic Approach	549.945230	1.0	0.569549	4.512453e-01
Technological Change	17 394.446682	1.0	18.014500	3.232708e-05

#### Appendix B. Statistical analysis

To better assess the contribution of modeling characteristics to hydrogen adoption levels from a statistical perspective, an analysis was carried out on 225 scenarios from the AR6 database within the C3 category, as this category contains a larger number of scenarios compared to the others. We focused our analysis on the C3 category within the AR6 database, as it encompasses scenarios with less stringent climate targets and moderate levels of mitigation. Moreover, the C3 category includes a wider variety of integrated assessment models, such as IMAGE, GCAM, MESSAGE, POLES, REMIND, TIAM, and WITCH, thereby providing a greater number of scenarios for robust inter-model comparison and analysis. In order to statistically compare the variability within IAMs to the variability between them, ANOVA (Analysis of Variance) was used to determine whether the means of different models with varied characteristics are significantly different from each other in hydrogen production level. The influences of several factors including technological detail (198 scenarios as High and 27 scenarios as Low), model perspective (48 scenarios as T-D and 177 scenarios as B-U), economic approach (156 scenarios as GE and 69 scenarios as PE), and technological change (148 scenarios as Endogenous and 77 scenarios as Exogenous) were assessed and the results provided insights into the significance of these factors in determining hydrogen production levels as follows. Based on Table B.9, "Model perspective" contributes meaningfully to explaining the variance in hydrogen production levels. The "Economic approach"s contribution to explaining the variance in hydrogen production level is minimal. The practical impact of "technological detail" on hydrogen production might be relatively major compared to other factors or the overall model, and "technological change" explains a substantial amount of variance in hydrogen production level because of a very low p-value. While it should be noted that sum sq represents the variability explained by each factor (Model Characteristic); df (Degrees of Freedom) represents the number of independent pieces of information for each factor, while F(F-statistic) is the ratio of the variance explained by the factor to the unexplained variance (error term), and in the last column, PR(>F) is the p-value, indicating the significance of the factor's effect. A small p-value (e.g., less than 0.05) suggests that the factor has a significant impact.

#### Appendix C. Supplementary data

A description of the mathematical formulations related to the B–U and T–D modeling approaches, as well as the incorporation of learning curves, can be found in the Supplementary Material file.

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.rser.2025.115544.

#### Data availability

Data will be made available on request.

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