A taxonomy of models for investigating hydrogen energy systems

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ABSTRACT

Hydrogen can serve multiple purposes within the energy system, from flexibility provider, to decarbonizing hard-to-abate sectors, to chemical feedstock. A range of model paradigms have been developed to assess the potential for hydrogen energy systems while accounting for the unique characteristics of hydrogen. This study proposes a taxonomy to classify models of hydrogen energy systems. The taxonomy is based on a review of 29 studies that proposed a taxonomy for energy models in general. This review identified 124 categories that are commonly used to map models, which were grouped into six major categories. This general taxonomy was then adapted to hydrogen, leaving only 32 categories in four major categories. Nine hydrogen archetypes that cover the entire spectrum of studies of hydrogen energy systems were identified. Each of these archetypes was mapped against the categories defined which allowed identifying common gaps across archetypes and degree of interrelationship between them. The environmental and high spatial resolution aspects are only covered by one archetype. The correlation between archetypes assessed in this study can be used to identify opportunities for soft-linking. All the archetypes provide partial answers and using a modeling suite composed of various models could address shortcomings of individual archetypes. All models have a strong focus on technology and costs, with other aspects such as the innovation cycle, market design and policy levers to promote deployment receiving little focus. Capturing these dynamics in the hydrogen archetypes would enable a more holistic analysis and would also facilitate subsequent action.

Highlights

- A taxonomy to classify hydrogen models is proposed based on a review of 29 studies
- Nine hydrogen archetypes covering the entire range of studies are defined
- Each archetype is characterized using the hydrogen taxonomy
- Challenges for each archetype are discussed together with potential solutions

Keywords: Hydrogen; Model; Taxonomy; Classification; Archetypes; Challenges.

Abbreviations:

AIM-Enduse Japan	Asia-Pacific Integrated Model applied to Japan
AIM-Hub	Asia-Pacific Integrated Model (Includes Japan, Vietnam and India)
BET	An IAM: a multi-regional, inter-temporal general equilibrium model
BLUES	Brazilian Land Use and Energy System
CCS	Carbon Capture and Storage
China TIMES	Application of TIMES to China

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CHP	Combined Heat and Power
COFFEE-TEA	COmputable Framework For Energy and the Environment-TEA
DoE	Department of Energy
DNE21+	a Global model for Energy and Climate Change Assessment, Japan
EFOM	Energy Flow and Optimization Model
ESM	Energy System Model
ESOM	Energy System Optimization Model
ETSAP	Energy Technology Systems Analysis Program
FCEV	Fuel Cell Electric Vehicle
GEM-E3	General Equilibrium Model for Economy-Energy-Environment, Greece
GHG	Greenhouse Gas
GLOBIOM	Global Biosphere Management Model
HSC	Hydrogen Supply Chain
HOMER	Hybrid Optimization Model for Electric Renewables
IAM	Integrated Assessment Model
IEA	International Energy Agency
IFs	International Futures, USA
IMACLIM	a hybrid dynamic general equilibrium model of the world economy that covers the period 2001–2100, France
IMACLIM-NLU	is intended to study the interactions between energy systems and the economy, to assess the feasibility of low carbon development strategies and the transition pathway towards low carbon future.
IMAGE	Integrated Model to Assess the Global Environment
IPCC	Intergovernmental Panel on Climate Change
iPETS	Integrated Population Environment Technology Science model
LCA	Life Cycle Assessment
LEAP	Low Emissions Analysis Platform
MARKAL	Market Allocation
MESSAGE	Model for Energy Supply Systems Alternatives and their General Environmental Impact
MESSAGE-GLOBIOM	MESSAGE (as above) with GLOBIOM (as above)
OSeMOSYS	Open Source Energy Modelling System
POLES	Prospective Outlook on Long-term Energy Systems
PyPSA	Python for Power System Analysis
RE	Renewable Energy
REMIND	REgional Model of Investment and Development
SD	System Dynamics
SHIPMod	Spatial Hydrogen Infrastructure Planning Model
TEA	a Computable General Economic (CGE) model, Brazil
TIAM	TIMES Integrated Assessment Model
TIAM-UCL	as above adapted by UCL (as below)
TIMES	The Integrated MARKAL-EFOM System
UCL	University College London
UniSyD	Unitec System Dynamics model
VRE	Variable Renewable Energy
VWM	Value Web Model
WITCH	World Induced Technical Change Hybrid

1 Introduction

There is a pressing need to reduce greenhouse gas (GHG) emissions and limit global temperature rise [1]. The global energy sector including electricity, industry, transport, and buildings represent almost three-quarters of the global GHG emissions [2]. Emissions have not yet peaked, making it necessary to use all available means to transform energy systems [3]. Hydrogen can complement other decarbonization strategies such as electrification and renewable electricity. The net result can lead towards optimal net-zero emission energy systems [4]. Although most hydrogen is still produced from fossil fuels, with high CO_2 intensity, electrolytic hydrogen from renewables has gained significantly more momentum in recent years.

Hydrogen is a versatile energy carrier: it can be produced from multiple energy sources and transported and stored in numerous ways. This flexibility is advantageous for mitigation efforts. Yet hydrogen deployment to date is predominantly confined to the industrial sector, with infrastructure limited to about 4500 km of hydrogen pipelines [5] and six operational underground storage facilities worldwide [6]. This versatility means that assessing the role of hydrogen in the energy system is a multi-dimensional field involving complex interactions between a large array of techno-economic, social and environmental factors. A single energy model will only capture some relevant aspects of the impacts of hydrogen, giving a partial picture of the solution. Hence several models are necessary to obtain holistic insights.

Previous literature (see Section 2.1) proposes a taxonomy to classify energy models in general, but none of them takes into account the unique characteristics of hydrogen (see Section 3.1). This creates the need to understand the scope and the questions that each model is best suited to address when evaluating the role of hydrogen in the energy system. This study presents a tailored taxonomy for hydrogen model archetypes and uses it to identify potential gaps and synergies between archetypes. This structured approach allows the systematic characterization of archetypes of various types of models representing distinct aspects of the energy system. It can help the community to identify the best combination of models to use depending on the problem definition.

Previous studies have identified some modeling challenges in energy systems models in general [7-10]. Energy models including hydrogen should consider additional complexity and uncertainty from innovation processes (i.e. learning and cost curves), technology penetration, business models, and market/political/geographical opportunities and constraints. The proposed taxonomy in this work accounts for these specific items enabling a clearer identification of the challenges and potential solutions.

The structured approached is reflected in the following Sections. In Section 2, the taxonomy of existing energy models is analyzed and six main categories are identified. In Section 3, a new taxonomy is presented for hydrogen energy system modeling. In Section 4, 12 archetypes of hydrogen models are identified and nine are discussed in detail. In Section 5, the challenges of modeling hydrogen in the nine archetypes are discussed along with solution strategies. The paper concludes in Section 6 with comments on the new hydrogen-focused modeling taxonomy and the nine model archetypes.

2 Model taxonomy for energy models

This section examines some common categories used to classify energy models based on previous reviews explaining the typical split within each category. This is done based on a review of previous model taxonomies (for energy models in general), which is adapted later on (Section 3) to hydrogen.

Energy models are computational tools that aim to determine the technology mix to satisfy a foreseen energy demand satisfying multiple constraints (e.g. cost, environmental impact, resilience). These models arose during the oil price shocks of the 1970s when oil-importing economies sought alternative ways to meet energy demand [11]. At that time, governments were responsible for energy planning and centrally assessed alternative energy, new capacities to satisfy the increasing demand.

Today, the same paradigms from half a century ago no longer apply. Dispatchable electricity generation is becoming displaced by variable renewable generation technologies such as wind and solar. Further, in the past electricity demand was seen as fixed, but today electricity demand is becoming increasingly flexible through smart grids and demand response markets [12]. Digitalization of control of both supply and demand is creating more interconnected systems [13]. Both sides of the market can now continuously change in real-time. In addition, the use of renewable generation technologies, especially roof-top solar-PV, is leading to decentralization [14]. This new feature again deviates from the previous models of centralized generation. Thus, the tools from the past need to be modified to account for these emerging trends.

Multiple energy models have arisen over the years. Differentiators include a) the part of the energy system that is covered, b) geographical boundaries, and c) spatial and temporal resolution. Several reviews have identified multiple categories to identify models that are suitable for specific questions. In this section, a meta-analysis of energy system reviews by others is presented which provides a blueprint for a hydrogen taxonomy (Section 3).

2.1 Mapping of categories for the taxonomy

To identify the categories for classifying energy models 49 reviews were surveyed and 29 of these were used as input to the taxonomy. A table with the specific categories surveyed by each review is available in the General Archetypes Excel sheet of the Supplementary Information of this article. The steps followed for this review were:

1. Identify energy model reviews with a high citation score.
2. Expand selection based on references known by the authors.
3. Select recent energy systems reviews that cited those from Steps 1 and 2.
4. Identify remaining energy systems reviews not covered in Step 3.

The criteria used to include reviews in the list of 29 were that they:

- had an extensive classification system and involved a cross-comparison of specific models.
- did not include an extensive survey of models but proposed a model taxonomy that was complex enough to compare with other reviews [15-19].
- reviewed a large number of models despite using limited categories [20, 21].
- were a meta-analysis of reviews [22-25].

The criteria to exclude reviews were:

- Only had a few, non-exhaustive categories to classify models or did not apply it to specific models [26-40].
- focused exclusively on challenges and gaps [7, 41].
- focused on a narrow aspect of the energy system or the energy transition without having an extensive review of the classification [42-48].
- focused on a scenario or output comparison rather than model comparison [49-52].

A total of 124 categories to classify energy models were identified (see the General Archetypes Excel sheet in the Supplementary Information). These were aggregated into 27 major categories colored green in Figure 1 with the darker green indicating more reviews. These categories were then further clustered into six broader ones colored blue in Figure 1. The more broadly covered categories were the methodology and mathematical approach, which almost every review covered. Most reviews covered multiple sub-categories for these, except for [21, 53], which only surveyed two. These were closely followed by the temporal resolution and spatial coverage which 20 and 19 reviews respectively surveyed. On the other extreme, aspects like transparency, irrationality, market representation, and policy were covered by only a handful of reviews.

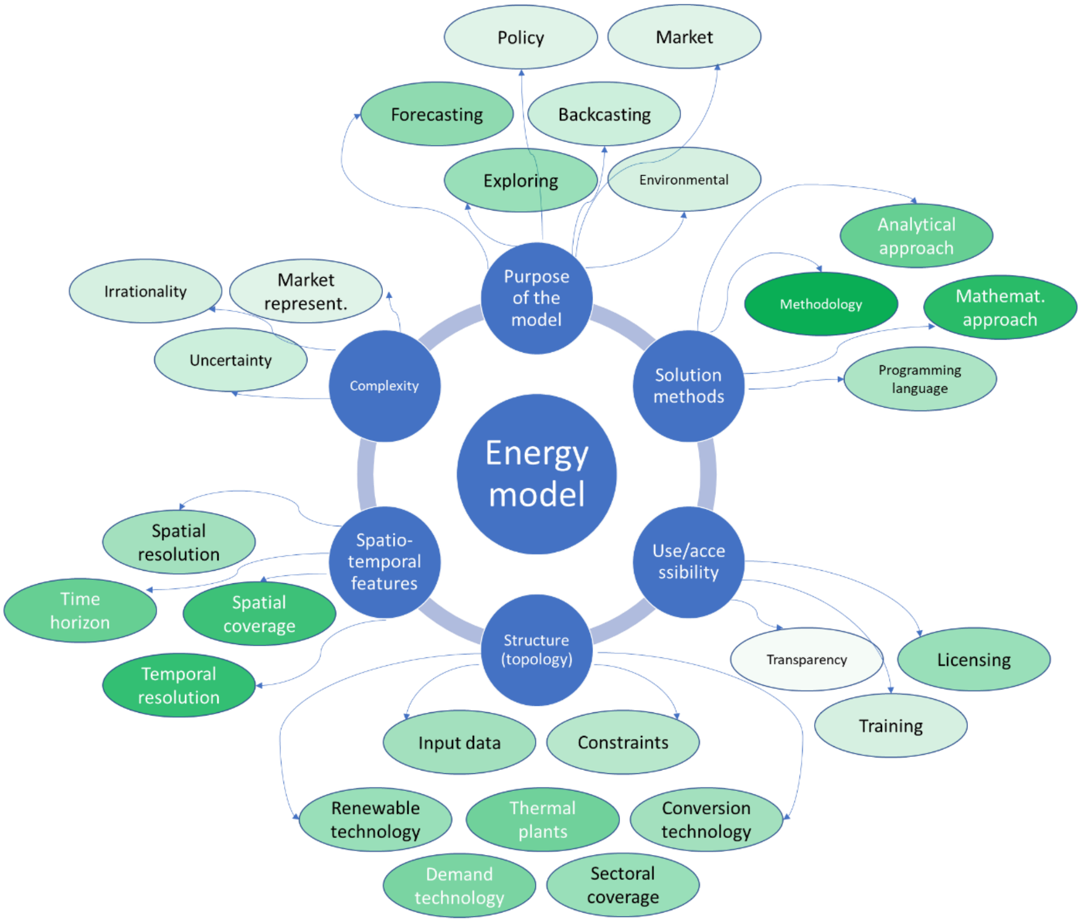


Figure 1. Model taxonomy to classify energy system models. Categories with relatively greater numbers of reviews are colored with darker shades of green.

Two reviews focused on hydrogen energy systems. Li et al. [54] focused on a specific subset of hydrogen models, namely optimal hydrogen supply chains. This type of model usually has a high spatial resolution. This resolution is for capturing transmission and distribution infrastructure distances. In turn, this provides for connecting supply and demand centers and covering hydrogen value chains excluding or greatly simplifying the rest of the energy system (see geospatial archetypes in Section 4.8). This study maps optimization parameters, parts of the hydrogen value chain, spatial scale, and whether the mathematical description is available across 32 publications. This study also reviews decisions over different time horizons, performance metrics (cost, environmental, safety), uncertainty, model constraints, and solution methods.

Gondal et al. [55] argued that energy models are needed to assess the potential of a hydrogen economy developing in specific energy systems. This study introduced 12 criteria to select a suitable model for hydrogen in the economy. It briefly describes 17 models. Some of the shortcomings identified in the review of these models are already outdated. It does not explain the criteria used to select models and only briefly describes each model (one or two paragraphs). Finally, it does not include hydrogen in all cases, does not use the criteria introduced, and does not make a cross-comparison between models.

3 Model taxonomy for hydrogen models

The taxonomy introduced in Section 2 covers the entire range of features that a model can have. In turn, it enables the classification of almost any model. At the same time, hydrogen has unique characteristics that require specific modeling features. This section introduces these characteristics (Section 3.1) and then adapts the taxonomy from Section 2 to hydrogen (Section 3.2).

3.1 Hydrogen characteristics important for modeling

1. **System-wide scope**. Hydrogen can be produced from multiple sources and be used across multiple applications, it couples different sectors, and it can be transformed to other molecules such as ammonia, methanol, and synthetic fuels. This means its uptake is defined by the competition with multiple technologies and its evaluation should cover all sectors. Including all the pathways in production, transformation, and end-use applications becomes crucial to rigorous modeling.

2. **Flexibility provision to the power sector**. Electrolyzers can provide additional flexibility to the grid [56]. They have a fast response, and their load can adjust to follow renewable generation. Other technologies such as batteries, grid extension, interconnection capacity, demand response, and flexible generation can also provide this flexibility [57]. Robust modeling needs to include all these options at different time horizons to avoid overestimating the role that electrolyzers can have.

3. **High temporal resolution**. Modeling the flexibility of electrolyzers requires an adequate time resolution. For example, a low temporal resolution is inadequate for assessing the potential for integrating renewable electricity production in an energy system containing electrolyzers.

4. **Life cycle assessment**. Hydrogen does not emit any CO_2 upon use or any pollutant when used in fuel cells. All the emissions are in the production, transport, and conversion processes. Thus, a model would need to include the life cycle to make sure the role of hydrogen is not overestimated by not considering the environmental penalties upstream. The use of life cycle assessment (LCA) would prevent economic and environmental impacts shifting across categories.

5. **Systemic drivers**. The role of hydrogen will be determined by competing pathways that are considered (e.g. bioenergy, nuclear, CCS) and by system drivers such as level of ambition for GHG mitigation or level of carbon tax.

6. **High spatial resolution**. This is needed because renewable generation is very location specific. At the same time, hydrogen infrastructure planning should consider multiple spatial constraints (e.g. water availability, existing natural gas pipelines, ports). Accordingly, a high spatial resolution is needed for capacity expansion decisions to be able to determine the progressive steps required to connect sites with high-quality renewable resources with demand centers [58].

7. **Consumer behavior**. Many models use a cost optimization approach, but some hydrogen applications might arise in the context of a broader range of criteria. For example, for residential heating, heat pumps [59] are the most efficient method and are expected to represent the bulk of the energy demand in most countries, but other factors such as level of insulation, space availability, or limited electricity grid capacity might make hydrogen more attractive for niche conditions.

8. **Development uncertainty.** Assumptions about future abundant green power and affordable CCS technologies are driving the current policy momentum [60]. In addition, future scenarios frequently assume a decline in investment costs of electrolyzers and fuel cells, as seen with solar PV, wind, and batteries [61]. A model should be able to determine the most influential parameters and assess the impact of different future developments.

9. **Climate variability.** Wind and solar generation are dependent on weather and climate. Modelers can use a broad range of weather profiles from a range of years to ensure a robust and resilient power system. Such range coverage can cause an excess of capacity to cover extreme climate years.

3.2 Adapting the general model taxonomy to hydrogen

The specific characteristics of hydrogen that are identified in Section 3.1 highlight the need to adapt the general taxonomy (Figure 1) to capture better the specificities of hydrogen. This is done in Figure 2, which selects the four major categories that are most relevant to hydrogen and expands them into more specific categories that are applicable to hydrogen. This is effectively adapting the general taxonomy for hydrogen. The rationale for the specific choices is explained below.

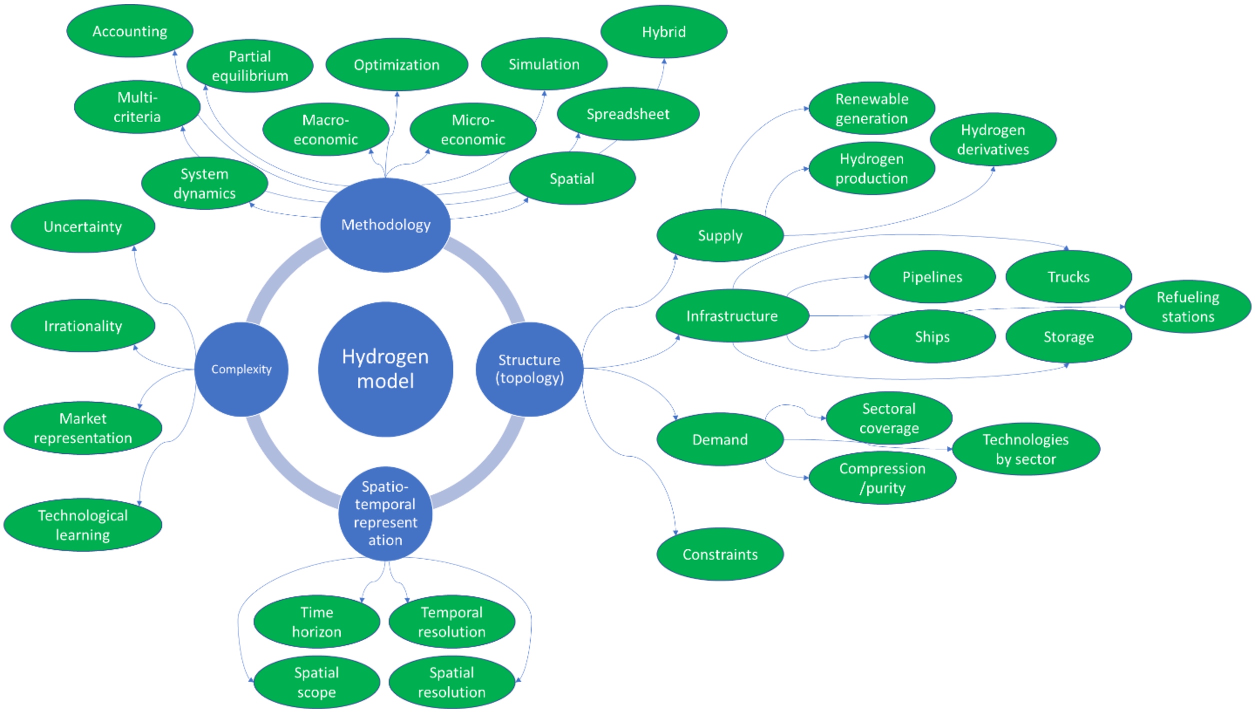


Figure 2. Model taxonomy to classify energy system models based on features required for hydrogen.

The role electrolyzers can have as flexibility providers and the need for higher spatial and temporal resolution (see Section 3.1) justify the need to have the spatiotemporal representation as one major category for hydrogen. Answers from a model with a broad geographical scope that only considers transmission capacity between regions will be different from a model with the representation of each user and supplier with specific routes for the infrastructure and focused on each transmission/distribution pipeline. Similarly, a model from the latter category can capture the contribution to grid services of electrolyzers. And only models covering multiple decades can give insights into the capacity needed to satisfy long-term demand.

The second major category in Figure 2 is model topology, which is justified by the need to use a model that includes multiple applications and transformation pathways (including derivatives) in all the sectors. For instance, a model that does not include ammonia as a possible carrier to satisfy (international) shipping demand is limiting ex-ante the potential that hydrogen can have in such a sector.

The third major category for the hydrogen taxonomy is complexity since hydrogen transgresses from technology to behavioral aspects, markets, and policy (see characteristic 7 from Section 3.1). This justifies the need to use models that consider a broader range of criteria (beyond cost) for decision making. Attributes that have a substantial impact on the transformation and configuration of the energy system include 1) path dependence, 2) non-linearity, 3) non-ergodicity (this means that past data or behavior cannot be relied upon to explain what might happen in the future), 4) lock-in, 5) irreversibility, 6) the role of institutions, and social context [39]. For example, a model that only looks at the transport sector and assesses the fuel cell electric vehicles (FCEV) penetration considering safety, sustainability, comfort, perception, performance, and reliability will result in a different hydrogen role from one system-wide cost optimization model.

Many of the hydrogen technologies are still in early stages, which makes crucial the exploration of uncertainties (see characteristic 8 from Section 3.1) and the impact input values could have on the role of hydrogen in a model. These can result in tipping points. When reaching such a point, a radical change in technology mix takes place. Models that can systematically assess the effect of different hydrogen technology performances can address uncertainty. Models that can handle a stochastic approach would also provide statistical insights into hydrogen deployment options.

Hydrogen can be coupled with variable renewable energy. This raises the need for a high temporal resolution and flexible time-slicing methods that can adapt to the profiles from a specific year (instead of the sampling intervals remaining constant regardless of the profile).

The specific combination of features for a model inherently affects the hydrogen representation in the model and the capacity and activity for those hydrogen technologies. For example, an analysis might estimate the energy efficiency measures and technologies for the residential sector. The answer will be different when comparing a macro-economic model aiming to determine the impact of this sector on a future gross domestic product than from a bottom-up model that represents all relevant building types and has an explicit spatial representation (e.g. district heating might be more attractive than individual hydrogen boilers).

4 Model archetypes for hydrogen

This section identifies the model archetypes for hydrogen and uses the categories from the taxonomy from Section 3.2 to discuss each one. Examples of application from literature are given to provide a sample of the typical use but the focus is on the characterization of each archetype and the review of examples is not exhaustive.

Based on a literature review, hydrogen models are classified into 12 archetypes. Nine of these 12 (see Figure 3) are discussed using the taxonomy introduced in Section 3. Table S1 of the supplementary information contains a table with the strengths and weaknesses for each archetype.
The nine archetypes are:

1. Integrated Assessment Models
2. Energy System Models
3. Power models
4. Integration models for variable renewable energy
5. models focused on Cities
6. Islands/Off-grid
7. Sectoral analysis
8. Geo-spatial analysis and Networks
9. Integrated Life Cycle Assessment (LCA) and hydrogen ESM

For the remaining three of the 12 model archetypes, the categories from the taxonomy were mapped but they were excluded from the detailed analysis for various reasons. First, technology-centered studies go through the fundamental principles of design and operation, possible improvements, and areas for further research but miss the system-wide perspective. Second, economic studies investigate the cost prospects and comparison with other competing technologies on a pure cost basis without considering the interaction with the rest of the system. Third, supply chain studies extend the scope of the evaluation to cover the path from an energy source to end-use but disregard competition with other pathways and the rest of the energy system.

The relationships between the different archetypes are presented in Figure 3. The green lines denote the boundaries of the scope for each archetype, the blue (dashed) arrows show relationships between different archetypes and the blue boxes refer to the elements that are part of each archetype. Some of the archetypes (e.g. IAM) include several elements, while archetypes with a narrower scope (e.g. islands) include a single blue box. At the same time, some archetypes are a subset of others (e.g. power is a subset of an ESM or IAM) and some partially overlap (e.g. an ESM and geospatial analysis).

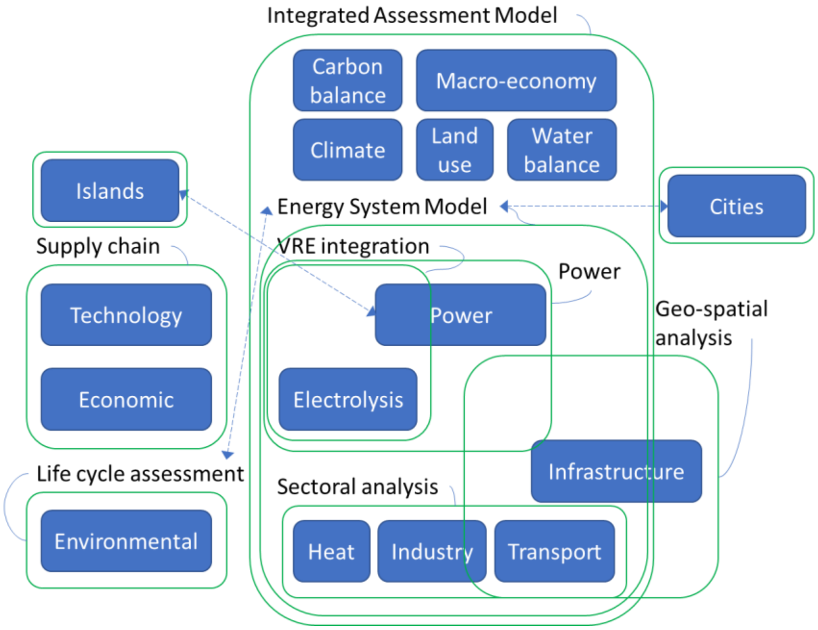


Figure 3. Boundaries and relationships between hydrogen model archetypes.

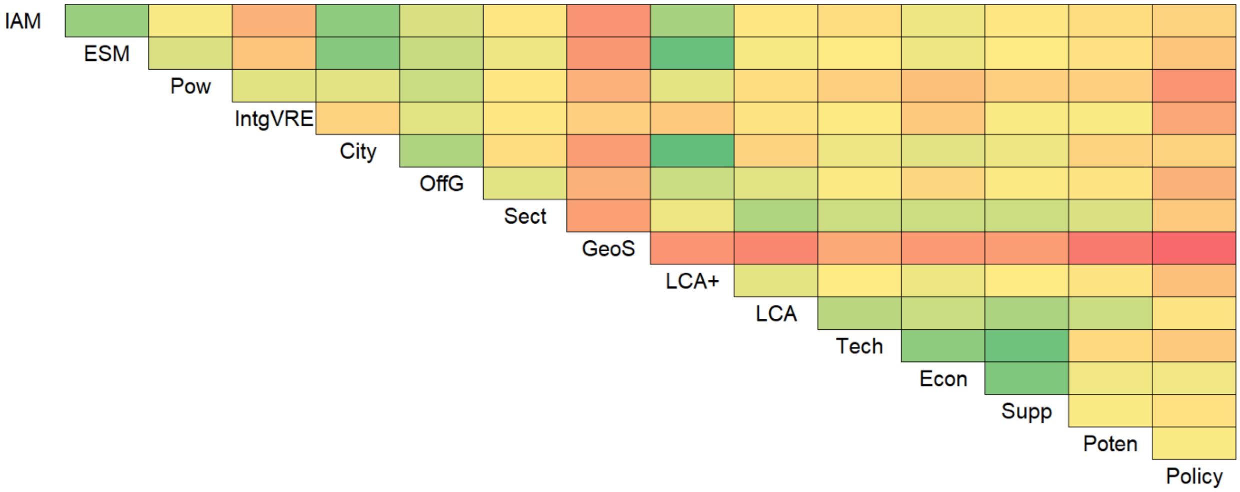
Infrastructure is partially outside the energy model envelope because geospatial analyses usually include more detail of the infrastructure. Examples include trucks or specific storage sites as distinct from generic storage components in ESM. Technology assessments, economic, and supply chain studies lie outside the boundaries of what energy models are meant to cover.

The nine archetypes related to energy models are not all mutually exclusive. For example, an ESM, by definition, covers the entire energy system. But in doing so, it needs to have a simplified representation of the different parts of the system to remain tractable. This need is crucial when covering a large geographical area. It thus includes the power, buildings, industry, and transport sectors. It also overlaps with a power model or models focused on specific sectors. Also, ESMs and cities archetypes are not fundamentally different. Both these are models with the possibility of covering all the end-use sectors. The difference lies in the spatial boundaries, with the cities archetype focusing on urban systems and energy models for regional analyses and larger areas. Modelers can also identify soft-linking possibilities to extend a modeling framework using the representation in Figure 3.

This hydrogen archetype classification is complementary to two examples from the literature that attempt to classify hydrogen models. The first example is from McDowell et al. [62]. They introduced three model archetypes for hydrogen. 1) bottom-up energy system models, 2) system dynamics and agent-based simulation models, and 3) infrastructure optimization models. The present study overcomes three disadvantages of this classification. First, only these three categories are covered – it does not cover the entire spectrum of studies. Secondly, the hierarchy does not systematically identify the difference between types of models. And thirdly, this proposal does not establish a relationship with other types of models.

The second example is from the U.S. DoE [63]. They use a six levels hierarchy to cluster models. 1) Policy scenario and integration, 2) Financial and employment, 3) Market assessment, 4) Environmental and lifecycle, 5) Vehicle penetration, components, and infrastructure, 6) Vehicle assessment. The advantage of this hierarchy is that it goes from overarching categories (Policy) to specific aspects (Vehicle assessment). A disadvantage is the focus to date on hydrogen FCEVs as an option to diversify from oil rather than a systems perspective. The hierarchy does not yet cover potential hydrogen applications beyond cars or hydrogen derivatives. Further, the criteria to use a specific module over another and information flow between modules are not clear.

The taxonomy categories were mapped for each hydrogen archetype (see the Hydrogen Archetypes Excel sheet in the Supplementary Information). Then the correlation between pairs of archetypes was quantified by using the number of categories each pair had in common as proxy (see “Hydrogen archetypes” tab of the Excel file in the Supplementary Information and Figure **4**). This comparison includes all types of hydrogen studies (LCA+, potential and policy) to be able to benchmark the archetypes and understand not only how archetypes relate to each other but also how they relate to other common types of hydrogen studies.



Green squares denote high correlation between archetypes and red squares denote low correlation. IAM = Integrated Assessment Models; ESM = Energy system models; Power = Power models; IntgVRE = Integration models for variable renewable energy; City = Use for cities; OffG = Islands and off-grid applications; Sect = Sectoral applications; GeoS = Spatial analysis and networks; LCA+ = Studies integrating LCA and ESM; LCA = Studies performing only the life cycle assessment; Tech = Technology; Econ = Economic; Supp = Supply chain; Poten = Studies looking at hydrogen potential; Policy = Most effective instruments for hydrogen uptake.

Figure 4. Correlation between hydrogen model archetypes based on similarities across dimensions of the hydrogen taxonomy.

Some of the archetypes have very similar dimensions. This similarity leads to a high correlation between some archetypes. For example, *LCA+* is highly correlated to *ESM* since *LCA+* refers to the combined use of LCA and ESM for prospective analysis of the background data for the LCA and other impact categories beyond climate change that affect the cost optimization solution (see Section 4.9). Similarly, *City* and *ESM* are highly interrelated. Both are energy models that differ only in the system size to which they are applied. On the other end, a spatial analysis considering the infrastructure and specific routes has limited overlap with an LCA study that uses energy and material flows to assess the environmental impact of hydrogen technologies or value chains.

4.1 Integrated Assessment Models (IAMs)

Integrated assessment models (IAMs) are widely used to understand the options for and consequences of reducing greenhouse gas (GHG) emissions and have featured prominently in all five IPCC reports. They are valuable because they represent the development of interacting human and earth systems (e.g. energy, economy, climate, land use) [64]. There are considerable variations in the design and application of IAMs. These result in varying levels of detail and approaches to modeling the energy sector.

Some models have a complex energy model at their core and perform the soft linking with other models. For example, the MESSAGE ESM is soft-linked to the GLOBIOM land-use model. TIAM-UCL is an energy system model with an integrated climate component but without a land-use component. IMAGE is an integrated system dynamics model of energy systems, other human activities, and natural systems. Other models have a basic or no representation of the energy system, which is a consequence of the broader scope of IAMs.

As an example, Table 1 shows hydrogen production technology representation for 18 IAMs. Models that consider the energy system in detail tend to represent hydrogen production from electrolysis, natural gas, biomass, and coal, both with and without carbon capture and storage (CCS). Two models also consider thermochemical routes.

Table 1. Representation of hydrogen production technologies in a range of IAMs [65].

	AIM-Enduse Japan	AIM-Hub	BET	BLUES	COFFEE-TEA	China TIMES	DNE21+	GEM-E3	IFs	IMACLIM	IMACLIM-NLU	IMAGE	IPETS	MESSAGE-GLOBIOM	POLES	REMIND	TIAM-UCL	WITCH
Coal w/o CCS					X	X						X		X	X	X	X	
Coal w/ CCS			X		X	X						X		X	X	X	X	
Natural gas w/o CCS				X	X	X						X		X	X	X	X	
Natural gas w/ CCS				X	X	X						X		X	X	X	X	
Oil w/o CCS				X	X							X			X		X	
Oil w/ CCS				X	X							X					X	
Biomass w/o CCS				X	X							X		X	X	X	X	
Biomass w/ CCS				X	X							X		X	X	X	X	
Nuclear															X			
Solar												X			X			
Electrolysis	X		X	X	X	X						X		X	X	X	X	

Using the taxonomy introduced in the present study, most IAMs have a low spatio-temporal resolution since they aim to cover aspects beyond energy and need to reduce model complexity in other areas. Regarding model topology, IAMs do not exploit the full range of pathways hydrogen can have and some of them still focus on road transport [65] since the interest on hydrogen started there and the review cycles for IAMs are usually slow. Hydrogen derivatives are hardly used and the use of ammonia for shipping or synthetic fuels for aviation is lacking. Regarding complexity, some of the models include endogenous learning and there have been some attempts to include behavioral aspects for passenger vehicles [65].

4.2 Energy system models

ESMs are economic models used to explore the potential evolution of energy systems in future decades [46]. ESMs provide an understanding of decarbonization pathways for economies, by counting GHG emissions from all sources and constraining total future GHG emissions. To produce credible scenarios, ESMs must represent a wide range of low-carbon energy technologies and commodities, including hydrogen technologies.

Regarding the spatio-temporal category of the taxonomy, modelers have built ESMs for local, national, and global scales. At larger scales, ESMs often represent collections of energy systems in various geographical regions that interact by trading commodities. Very few models have sufficient spatial resolution to adequately model the lower initial costs of developing hydrogen valleys or industrial clusters. For electricity specifically, production variations in regions with a high proportion of VRE creates a need for high temporal resolution. However, increasing the temporal resolution increases the model size and solution time. Hence most models make trade-offs between temporal resolution, solution objectives, and model paradigm. This limit results in a few representative time slices for most ESMs and the need for a separate model that focuses on renewable integration in the power system. ESMs are well suited for capacity expansion problems involving multiple decades as time horizons.

Regarding topology, ESMs represent energy demand and ways to balance demand and supply across whole economies. Hence modelers can use ESMs to identify trade-offs between sectors. The coverage of energy flows and emissions varies between models, with upstream energy technologies (e.g. oil extraction) and non-energy emissions often omitted from models. Infrastructure is typically simplified; for example, it is often represented as a fixed additional cost that disregards distance between assets.

The formulation of simulation models is forward-looking; they assess the future performance of a system based on an initial set of assumptions, which makes them faster to solve. As a result, they can use the higher temporal resolution and can represent non-linear relationships. Optimization models on the other hand, are normative searching for the system design that satisfies a set of constraints (commonly including future GHG emissions) [66] The choice between these paradigms depends on the purpose of the exercise. Combination of these paradigms is also possible [67] but no examples specific to hydrogen were found.

4.2.1 Simulation model paradigm

Some policymakers use simulation models to develop long-term scenarios, particularly in less developed countries. For example, several countries use LEAP (the Low Emissions Analysis Platform) [68]. EnergyPLAN [69] has been used multiple times to assess the role of hydrogen across sectors. The IEA's World Energy Model (used for the World Energy Outlook [70]) also uses a simulation approach [71].

The key advantage of simulation models compared to optimization models are that they are simpler to construct. Simulations are particularly well suited to balancing energy demand, for which cost optimization is often only one of many drivers. This feature makes them useful for hydrogen when behavioral aspects determine the technology mix. An example is FCEV penetration, for which cost is only one factor to consider.

4.2.2 Optimization model paradigm

Policymakers widely use energy system optimization models (ESOMs) to identify low-cost futures. For example, the IEA ETSAP technology collaboration program developed the TIMES model generator. Modelers have used this generator to create least-cost energy models across ranges of spatial scales in more than 40 countries [98]. A recent survey of ten global and national TIMES optimization models found that all included hydrogen energy systems to some extent [99]. Modelers are increasingly using the open-source OSeMOSYS model generator [100] to create models of energy systems of less developed countries. Optimization objective functions either or both minimize cost and maximize welfare. These models optimize systems across several decades. Hence the temporal resolution of optimization models is coarse (longer time steps) compared to simulation models.

Another class of least-cost models uses system dynamics (SD). For example, the SD model UniSyD has been used to explore energy system futures at the regional level in three countries, including Japan [72]. SD models can perform analyses at a significantly higher temporal resolution in a given processing time than models based on linear programming. In turn, SD models facilitate a robust representation of the role of electrolytic hydrogen and associated renewables in supporting the grid. They can also readily process non-linear algorithms such as those used to model consumer choice. Such choices are crucial when modeling hydrogen in the transport fleet. However, they have the disadvantage of requiring significantly more effort to define relationships between variables.

Economic data used in ESOMs include capital costs, fixed and variable operations, maintenance costs, and discount rates. Technology attributes include lifetime, availability/capacity factor, energy conversion efficiency. Technology component types number up to about 1000. For nascent hydrogen technologies, there is often much uncertainty about this economic and technical data. Models pass this uncertainty through to the model output. Hence, ideally, uncertainty analyses can be used to explore the implications of the data uncertainty, rather than relying on the modeler's judgment.

4.3 Power System Models

Power models are used to design and optimize generation capacity to fulfil carbon abatement targets and the resulting increase in electricity demand from conventional electricity consumers, electrification of new consumers (e.g. vehicles), and sectoral coupling applications (e.g. electrolyzers) [4, 73]. The trade-off for models of this archetype is that by reducing the sectoral scope compared to ESMs or IAMs, some information from other sectors is needed as exogenous input with the advantage of being able to model the power sector in more detail. For example, the extent of electrification rate for spatial heating, transport and industry are normally based on modelling outputs from IAM and energy models, and often are accompanied by an assumption of share of electrolysis connected to the grid (see Figure 5).

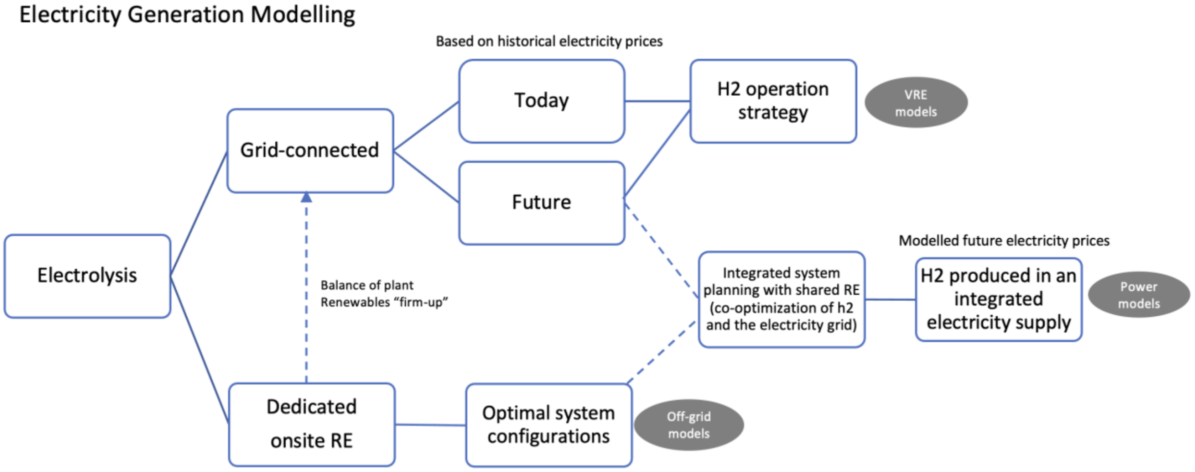


Figure 5. Roles for VRE models, power models, and off-grid models.

With the arise of hydrogen as an additional component of the power system, the optimization objective is often broadened to cover power and hydrogen costs while meeting temporal electricity and hydrogen demand subject to new constraints associated to hydrogen like electrolysis ramping constraints, minimum turndown for the electrolyzers, diurnal and long-term storage, among others.

Referring to the hydrogen taxonomy introduced in this paper, in terms of spatiotemporal resolution, power models usually use an hourly resolution. This is enough to capture variability of wind and solar and the flexibility needed to integrate these resources, yet low enough that an entire year can be represented. This temporal resolution still does not capture the full flexibility of electrolyzers which can respond within seconds.

The spatial resolution can range from a single node with a copper-plate assumption to a multi-node model with locational marginal prices. With more nodes, the role of electrolyzers could be different since it would take into account potential trade-offs with line congestion and transmission expansion. In terms of topology, this type of model is usually restricted to the power-hydrogen interface (i.e. the electrolyzer) and does not usually cover any hydrogen infrastructure (e.g. pipelines) or downstream use (e.g. refueling stations).

In terms of complexity, hydrogen technologies do not have endogenous learning curves and uncertainty is usually captured through a deterministic analysis changing individual input parameters. The market representation is limited to the power market rather than the hydrogen market and the consideration of hydrogen supply and demand. Power models have similar paradigms as energy models (see Section 4.2) and can also be simulation models.

This hydrogen archetype is of particular interest to potential exporting countries to understand the impact of large-scale hydrogen exports from grid electrolysis on the electricity system [74]. With the trend towards sector coupling and (indirect) electrification of all sectors [75], power models have been recently expanded to cover more than the power sector, thus, going one step closer to energy models and blurring the lines between one and another. An example is PyPSA in Europe [68, 76, 77] which can use hourly resolution and plant dispatch but also covers the transport and industry sectors.

4.4 Integration models for variable renewable energy

VRE models are a subset of power models (see Figure 3), which focus on the interface between electrolysis and the grid without considering the broader aspects of the power system (e.g. thermal generators). Models of this archetype can be differentiated by the electricity source of the electrolyzer. In one configuration, the electrolyzer can be connected to the grid and the focus is on operation strategies for the electrolyzer considering the increasing price volatility in the spot market [78, 79]. These VRE models typically use historical spot prices and assume flexible electrolysis could produce cost-competitive hydrogen by taking full advantage of price valleys while avoiding price peaks.

Another configuration of the VRE model [80, 81] is when the main source of electricity is dedicated renewables but with grid access for "firm-up" and "balance of plant" purposes. This is different than full off-grid models (Section 4.7) where even this supplementary electricity is supplied by dedicated renewables. The aim of these models is to design an onsite renewable generation system for hydrogen production while reducing the need for local energy storage and curtailment. Some models now include hydrogen derivatives, such as ammonia [82] and renewable methane [83].

Referring to the hydrogen taxonomy introduced in this study, the classification for models of this archetype is closely related to the power models. The main difference in the taxonomy compared to power models is the spatial boundaries. While the power system models cover the entire set of generators, electricity users, and in some cases, the grid, VRE models focus on the VRE generation and the electrolyzer. Historically, the focus has been even narrower restricted to wind generation since its stochastic behavior (as opposed to solar) makes a flexible load like electrolyzers more attractive to compensate for the variability.

4.5 Sectoral applications

Models of this archetype focus on specific sectors of the energy system. The most common type is power models (see Section 4.3), but there are also models that focus on the transport sector [84], and more specifically, passenger vehicles [85], models that focus on the heating sector [86] and others. The advantage of these models is that by narrowing down the scope, it allows for a more detailed representation of the technologies, the actors, and the evolution of the system. Dedicated sectoral models unlock new business cases for hydrogen that are not captured in system-wide models. For instance, a model focusing on the residential sector could have the type of building, vintage, and efficiency standards, allowing to identify specific buildings where hydrogen might be a better solution than heat pumps.

Referring to the hydrogen taxonomy, first, the temporal resolution needed is much lower than an hour in cases where the objective is determining the technology mix. The higher resolution is only needed when the sectoral models are coupled with the electricity system. Second, regarding topology, models of this archetype rely heavily on the end use usually disregarding hydrogen supply and infrastructure [87]. Fixed costs or fixed assumptions for the supply are usually considered since the focus is on technology competition for the downstream use. Third, this model archetype is better at representing complexity by capturing consumer behavior and part of the irrationality [88]. Technology learning and uncertainty can also be represented in this type of models, especially when system dynamics models are used [89].

The sectoral focus of this model archetype also means that the input data is different than other models. For instance, the behavior of the users of passenger vehicles usually comes from consumer choice models [90] that can be translated into disutility or intangible costs that can be used in transport models [91]. As with ESM, this model archetype is also moving in the direction of incorporating lifecycle data and expanding the boundaries from use to construction and materials [87]. Sectoral models for transport are also moving in the direction of ESM and IAM, while the representation of transport in these models is also improving, thus effectively closing the gap between these archetypes [92].

4.6 Energy models for cities

Hydrogen deployment plans go further than a national scope and have inspired growing interest at the regional and urban scale. An emerging challenge for many governments and firms is to expand hydrogen demand, which is still very limited today at the urban level. Considering that most of the global population lives in cities, the role of regional/metropolitan/urban governments is crucial in downscaling national hydrogen targets into specific and feasible goals.

This modeling archetype closely resembles ESMs. It can use a simulation or optimization approach in the methodology, and it covers from supply to infrastructure and end-use in the model topology. The main difference lies in the spatial scope. While ESMs tend to cover regions, countries, or continents, the cities archetype has smaller boundaries, constrained to a city. An example where this different scope can make a difference is when providing hydrogen to nodal areas where vehicles will refuel is an urban planning issue (allocating hydrogen refueling stations), geospatial optimization, and knowledge on transport demands [93]. And for heating and cooling services, hydrogen can displace natural gas. This change requires investment in hydrogen infrastructure in buildings and streets. Hence, hydrogen will have a substantial role in municipal decarbonization policies.

A recent example of the application of this model archetype is Uyar et al. [94]. They studied the need for hydrogen in 2030 for the city of Burdur, Turkey, considering three scenarios (a business-as-usual plus two alternatives). This work evaluates two different hydrogen penetrations in the transport sector of Burdur. For this, an optimal mix of infrastructure and balanced production and consumption is developed using a TIMES-Burdur model. Other examples of applications to cities include [95, 96].

Previous work points out the need to develop hydrogen modeling with a broader sectoral disaggregation while maintaining improved spatial resolution. To date, few detailed macro-level studies have this broad scope. These studies focused on hydrogen demand. There are no studies where modelers have evaluated infrastructure deployment or urban production using ESMs.

4.7 Islands and off-grid systems

Remote energy systems such as those located on some islands or on-shore off-grid systems, historically depend on imported fossil fuels. Renewable energy is increasingly displacing fossil fuels in these systems. The motivations for this displacement are fuel costs, energy security, and local pollution reduction. Like ESM, this model archetype can use an optimization or a simulation approach. They can cover power only or the entire system. According to [97], three different classes of bottom-up energy system models are normally applied at islands level. Most of the models used are static or short-term models.

The spatial scope of this model archetype is constrained to an island or a stand-alone off-grid system. Off-grid networks cannot fall back on intermittently importing electricity from adjacent regions. Hence their assessment is a reliability problem. Modelers use a wide range of model types, resulting in a range of temporal resolutions: from seconds to annual time-steps. The model complexity varies greatly, with some models including technology learning, as well as uncertainty regarding the variability of renewables.

Chade et al. [98] presented a feasibility study of a wind-hydrogen system using HOMER [99]. This study was of Grimsey Island (Iceland). This work resulted in recommending the implementation of a system consisting of wind, hydrogen, and diesel. The Arctic area has excellent wind potential with seasonal variations, combined with high energy prices. Ringkjøb et al. [100] analyzed the transition of the energy systems of an Arctic settlement to renewables using the TIMES modeling framework. One of the main findings from that work suggested that a stochastic modeling approach is critical in studies of remote Arctic energy systems and that modeling the variability of renewables is crucial for a remote settlement.

4.8 Geo-spatial and network models

This model archetype is also commonly called hydrogen supply chain (HSC) models [101]. These tend to focus only on the hydrogen system, being able to represent it at a much greater level of detail than other archetypes where modelers tend to include only a subset of hydrogen technologies. As there is little hydrogen delivery infrastructure in most countries, policymakers need to understand how to best develop infrastructure to meet increasing demand for hydrogen over time. By representing different types and costs of infrastructure spatially, and different sizes of production plants, HSC can produce infrastructure development plans [101-103].

Many supply chain models are optimization models [101]. Modelers use either of two mathematical approaches: 1) linear programming and 2) mixed-integer models. Most ESOM modelers use the linear paradigm, but this is not feasible for HSC if an assessment of a broad range of plant scales is required. Hence, supply chain models tend to be mixed-integer models that represent infrastructure using "lumpy" rather than continuous (linear) investments [102].

An example for the UK is the Spatial Hydrogen Infrastructure Planning Model (SHIPMod). For this model, cost-optimal scenarios have predicted distributed production facilities at the early stage of a transition followed by the gradual development of a national pipeline network as demand increases [104]. Another example is the Value Web Model (VWM), which adopts a high temporal resolution with the aim of more accurately assessing the role of hydrogen storage in a supply chain [105] and has been used to explore the potential impacts of carbon policies on hydrogen development [106].

4.9 Integration of LCA and ESM

Most hydrogen models developed to date do not involve a robust sustainability component. The combined use of ESOMs and Life Cycle Assessment (LCA) [107, 108] can overcome this limitation. In particular, LCA – as a standardized methodology to comprehensively assess the environmental performance of production systems [109] – could enrich hydrogen ESOMs by serving as a source of sustainability indicators to be integrated into the models [110]. In other words, as shown in Figure 3, there is a potential link between the environmental and modeling archetypes. There are two ways of implementing this synergy. Firstly, using outputs of ESMs for the background data in prospective LCA studies of hydrogen technologies such as the implementation of fuel cell electric vehicles [111]. Secondly, the endogenous integration of life-cycle sustainability indicators into energy systems models [107].

In terms of the hydrogen taxonomy, this hydrogen archetype is suggested to have almost the same classification across dimensions than the ESM when understanding the latter as the core component while LCA expands the scope in one dimension (environmental). This also opens up another possibility in the methodology dimension of performing multi-objective optimization: cost from ESOMs and LCA indicators [112]. In the complexity dimension, the combination with LCA adds one more layer of complexity because of the different boundaries. For example, an ESM is usually constrained to a country or region, while the LCA covers all the lifecycle stages which can include materials and construction outside the geographical scope of the ESM and outside the GHG target of the jurisdiction the ESM is meant to cover. The LCA is also dependent on technology performance that changes over time. LCA usually does not consider this aspect and this change in performance needs to be consistent with the change in the ESM [107, 108].

There are only a few examples in the literature of effective integration of life-cycle indicators into hydrogen ESOMs. One is Navas-Anguita et al. [112], who assessed the prospective integration of hydrogen from both techno-economic and environmental performance perspectives. They developed and applied a framework based on energy systems modeling enriched with carbon footprint indicators. This framework allowed the assessment of scenarios characterized by alternative carbon footprint restrictions that directly affected the solution of the optimization model. Additionally, an outcome of hydrogen energy systems models enriched with life-cycle indicators is the future trends of these indicators [113, 114].

5 Challenges of modeling hydrogen and potential solutions

This section discusses the challenges associated with including hydrogen in the model archetypes identified in Section 4. This allows identifying synergies and gaps between them and selecting the best combination of model archetypes to use depending on the targeted questions.

The main challenge resulting from the inclusion of hydrogen in energy system models is to accurately model economic, technological, social, political, and environmental effects with sufficiently high temporal and spatial resolution.

Table 2 gives a range of examples in each of the critical areas for hydrogen systems based on the authors experience.

Table 2. Emerging hydrogen modeling challenges for energy system models.

Learning/cost curves	**Business models**
• On-site hydrogen production at community, commercial, and industrial level. • Process and delivery methods for import/export of hydrogen. • Hydrogen fuel used in ships, aircraft, trains, and heavy vehicles. • Recovery of high purity hydrogen from geological storage in abandoned oil and gas reservoirs • Recycling and disposal of hydrogen technology components. • Fuel cells, electrolyzers, and batteries.	• Rates of return in commercial and industrial sectors on investment in hydrogen technologies and how these may vary as the technology matures. • Propagation of hydrogen refueling stations. • Internalization of externalities such as health and pollution costs at local, regional, and global levels.
Technology penetration	**Market/political/geographical**
• Solid storage in transportation and stationary applications.	• Consumer behavior in the purchase of new and second hand FCVs.

• Production of other H_2 based molecules from emerging technologies such as catalyst-based hydrogenation from renewable resources • Electrolyzers to maintain power quality. • Combined heat and power applications.	• Cross-sector market dynamics including competition for natural resources between the downstream hydrogen, electricity, and heating sectors. • Political and regulatory engagement with the adoption of hydrogen technologies. • Geographic constraints on hydrogen production and use.

Effective modeling requires a combination of access to appropriate data and the optimal use of one or more of the model archetypes outlined in Section 4. Model selections can be made using a hierarchy of decisions: Objective / Purpose, Use / Accessibility, Structure, and spatiotemporal representation. Further iterations can assist in refining model choice.

5.1 ESMs and IAMs

A survey of TIMES optimization models found that most represented hydrogen production by electrolysis. 60% considered one or more carbonaceous fuels with carbon capture and storage (CCS)[115]. Most models represented hydrogen-fueled road vehicles, but many did not consider hydrogen options in other sectors of the economy. Detailed representations of hydrogen delivery infrastructure were rare. Models did not generally account for hydrogen gas pressure and purity across system components. These findings are consistent with another review by Quarton et al. [116]. They also found limited consideration of hydrogen options outside of electrolysis and mobility, and these findings are likely to also apply to IAMs with detailed energy system representations. Hydrogen derivatives such as ammonia and synthetic aviation fuels have potentially crucial future roles, but most energy system models do not account for these products.

ESOMs have low spatial and temporal resolutions due to broad coverages of energy systems and long-time scales. Hence these models do not entirely resolve the costs and opportunities for integrating VRE generation into energy systems. This lack of integration makes them unsuitable for representing power-to-gas from excess VRE generation unless an approach can be parameterized using information from a separate higher-resolution model [117].

Another weakness of these models is the assumption of perfect foresight, which means that strategies to mitigate risks and uncertainties are not considered unless complex uncertainty studies are performed. For example, if the demand growth of hydrogen is considered perfectly predictable, the risks and uncertainties about the cost of hydrogen delivery infrastructure are low. Some studies have examined the consequences of having limited foresight [118], but not for hydrogen systems.

A limitation of system dynamics-based ESMs and IAMs is that they require a high level of specificity in the relationships between variables and a complex model structure. This specificity is needed to account for variable interdependencies. These models can also be sensitive to the outcomes of algorithms used to model behavioral factors such as consumer choice.

5.2 Power models

Future studies need to optimize the concurrent production of hydrogen and electricity. However, incorporating time-varying hydrogen value chains (i.e. hydrogen conversion, transportation, distribution, logistics and time-varying market demand) into the power system modelling within one planning framework is likely to be hindered by computational challenges such as the risk of numerical instability. Moreover, there is a need for a holistic modeling of multiscale energy storage technologies in the electric grid, both from the planning (e.g. siting and sizing of hydrogen systems for seasonal storage), and production cost perspectives (e.g. how hydrogen storage could support the grid via provision of operating reserves, replacing peak generation capacity, supplementing transmission, and improving the resiliency of the power grid).

It is also desirable for power models to account for 1) year-to-year weather variability and the impact of climate change on renewable resources and 2) hydrogen production across multi-decade periods, but this can be computationally challenging. Common simplifications include use of time-slices [119], rolling-horizon [120, 121], or a green-field approach that overlooks the existing infrastructures and the underlining transition [122-127]. In addition, most of these power models are deterministic and set up under a range of scenarios; stochastic modelling and robust optimization would be a future direction for these models to include uncertainty with the hope of augmented progression in computational techniques and facilities.

5.3 Integration models for variable renewable energy

One challenge for this model archetype lies in the narrow scope. By limiting to the VRE and electrolyzer interface [128], the optimal solution for this system might differ from the optimal solution for the entire system. For instance, using low-cost electricity for an electric vehicle might turn out better than using it for the electrolyzer. By omitting the rest of the power and energy system, only sub-optimal solutions are found. Similarly, when the scope is narrowed down from entire regions to single wind turbines and single equipment [129], attenuation effects of wind across a larger geographical area are missing, leading again to a different local solution that might deviate from the system-wide optimal operation.

Another challenge lies in the lack of consideration of the hydrogen users. The boundaries of this model archetype are usually up to hydrogen production. However, if the tolerance to fluctuations of different users is considered and hydrogen storage is introduced, a different production profile might be obtained. For instance, one user (e.g. industry) might require a stable supply profile which would make the use of storage necessary and would change the optimal size of the electrolyzer with respect to the renewable generation capacity.

These gaps are usually covered by combining this model archetype with broader power system models. The VRE archetype provides insights into the electrolyzer operation and flexibility at the local level, while the power system models provide insights into the interaction of the electrolyzer with the rest of the network.

5.4 Sectoral applications

The main challenge for this model archetype lies is rooted in the sectoral scope. Focusing on a single sector means that price dynamics for energy carriers used across sectors are not well captured. For instance, hydrogen prices depend on the range of technologies used to produce it and demand from all the sectors, but a transport model cannot represent the willingness to pay or demand from industry. This means that many of the price inputs are fixed which eliminates the feedback between sectoral demand and prices. Similarly, limited resources that are used across sectors, in particular bioenergy, are not allocated efficiently.

Sectoral models also do not work well with technologies that have different inlet and outlet streams that transgress across sectors. For instance, a district heating model that is supplied with combined heat and power (CHP) units would need a representation of the power sector as well to accurately determine the best operating mode for the CHP unit that is not only driven by the heating demand. Similarly, sectoral models cannot make trade-off with emissions from other sectors as the overall target is reduced.

As the energy system decarbonizes, the electricity share is expected to increase to at least half of the final energy demand (from about 20% today) [4]. This means that electricity will play a larger role in sectoral models and a low temporal resolution used so far might not be enough for decarbonized systems. Thus, a challenge for sectoral models is how to transition to high temporal resolution models, with a broader scope including parts of the power system to capture price signals for individual users, while still maintaining the details of the sectoral representation and remaining a tractable problem.

5.5 Energy models for cities

Hydrogen is an energy carrier in the sense of electricity and fuels. Hence ESMs can model hydrogen as an energy carrier. However, the application of ESM at the city level is not as widespread as it is at more geospatially broad levels. While the reasons for that might be several (e.g. data acquisition, traditions in energy planning, lack of background in municipal energy and climate policies), the upsurge of hydrogen means an opportunity to fill that gap.

As previously stated in Section 4.6, hydrogen will be required in transport to transform current vehicle fleets into zero-emission fleets. Accordingly, ESM will have to deal with the geo-spatial location of hydrogen refueling stations and assist in evaluating scenarios where hydrogen is produced on-site or is transported by truck or by pipeline, depending on the delivery costs and lifecycle emissions involved, all at once. And with more focus on residential or tertiary sectors, ESM will improve techno-economic efficiency and add detail on building performance (temporal resolution and seasonal storage). This focus will lead to a higher level of disaggregation and will enhance urban planning processes. Further, city-level energy system modeling can enable the efficient development of long-term energy and climate policies. In turn, including hydrogen allows for providing clean city-level energy-consuming services wherever electrification is less techno-economically efficient.

5.6 Islands and off-grid

Generally, isolated areas have specific characteristics that need to be considered individually for each case. One main challenge is to model the variability of renewables for energy systems at islands or other off-grid systems where a high proportion of the energy generation is variable renewables. This challenge is most significant when the security of supply is paramount. Hybrid energy systems comprising more than one energy source are crucial for reducing the system costs [100, 130] and exploiting the complementarity of diverse resources (e.g. solar and wind power). Additionally, some isolated areas have extreme climates and thereby higher requirements of the energy system operation.

Another challenge is to have an adequate time resolution for the system under consideration. An increase in temporal resolution allows for more constraints to be considered, including renewable resource availability, operation, and the dynamics of the electricity demand, thereby avoiding sub-optimal energy systems with reduced cost-effectiveness.

Although a general challenge with any energy system model, the computational burden also limits the resolution of this model archetype. There is a clear trade-off between having a high time-resolution, sector-coupling, techno-economic details, as well as including constraints regarding reliability and robustness of the power grid.

5.7 Geo-spatial and network models

Supply chain models require exogenous assumptions about the operation of the hydrogen system. Many models require the user to specify demands for hydrogen and how they change in each region over time. Hence these models cannot be used to compare hydrogen with other low-carbon options. Further, models with detailed spatial and temporal resolutions ideally need to consider interactions with other sectors (e.g. through power-to-gas). Low-resolution models do not fully resolve these interactions. To address this issue, some models (e.g. the VWM [105]) selectively represent alternatives to hydrogen (notably electrification) in several sectors, but at the cost of increasing the model complexity.

Given the high cost of infrastructure at the start of a transition to hydrogen, there is a focus on hydrogen valleys and industrial clusters as small geographical areas with high potential demands in the near term [131]. Although supply chain models tend to have higher spatial resolution than energy system models, modelers tend to choose this resolution to reflect geographical regions rather than potential hydrogen demand regions. Hence delivery costs are modeled across region boundaries rather than within them, and low-cost, short-haul delivery options are not considered. Work is needed for such models to resolve the benefits of developing hydrogen valleys in the early part of a transition.

5.8 Integration of LCA and hydrogen ESM

Key challenges for this model archetype are, first, lessons learned from prospective LCA studies [111, 132] should be implemented at the foreground and background life-cycle inventory level to enhance the suitability of the subsequent life-cycle indicators implemented in the model. In doing so, circular computational issues should be avoided, e.g. due to the link between electricity and hydrogen under demand/supply aspects. Second, the main scope challenges involve moving from single-region and single-sector models to multi-regional and multi-sectoral models. In this sense, current attempts are limited to a national scope and road transport [114]. This broadening requires accounting for both hydrogen production and use. It also implies using a higher time resolution (currently limited to one year). When expanding this scope, double-counting and trade-imbalance issues should be avoided [107].

Lastly, other issues concerning the scarce literature available in this specific field, namely the current limitation to carbon footprint as the only life-cycle indicator [112-114], should be understood as minor. This conclusion arises from noting that the availability of appropriate life-cycle inventories conditions the computation of life-cycle indicators. In turn, carbon footprint estimation and life-cycle indicators can use the same inventories. Hence robust carbon footprint estimation and quantitative life cycle assessments go together.

6 Conclusions

Hydrogen is a versatile energy carrier that can be used across all sectors, it can perform multiple functions from sector coupling to complement of electrification, and it requires special features for modeling. No single model can capture this complexity and the use of multiple modeling frameworks is needed to assess its role in a future low-carbon system. This study proposes nine modeling archetypes that cover the entire spectrum of applications. To systematically map the features of each archetype, this study has also proposed a modeling taxonomy that has been adapted to hydrogen. This taxonomy includes four major categories.

The nine modeling archetypes identified in this study are Integrated Assessment Models (IAM), Energy System Models (ESM), power models, integration models for variable renewable energy, and models for Cities, Islands/off-grid, Sectoral analysis, Spatial analysis and networks, and Environmental.

There are three main findings regarding the archetypes. The first finding is that some categories are well covered by multiple archetypes while there are some that are only covered by one. For example, if the question of an analysis is to understand the role that sector coupling can have in a low-carbon future, IAMs, energy models, power models, cities, integration models could all provide an answer to the question to a different extent. However, if the initial question relates to the environmental impact, it leaves the LCA archetype as the only suitable choice to answer the question. Thus, the choice of modeling archetypes is to be reduced both based on the types of questions to be answered and the modeling features of hydrogen that need to be more detailed. Second, the categories mapped allow assessing the interrelationship between archetypes. One use of these correlations is to identify archetypes that are complementary and that if used together through soft-linking, would cover a lot of the relevant aspects for hydrogen. Third, the mapping exercise allowed identifying gaps that are common for all archetypes. Given the common conception of models, there is a lot of focus on technology and costs across all archetypes. Other aspects such as environmental impact, the innovation cycle, market design and policy levers to promote deployment are much less covered. However, as these aspects are embedded into the modeling framework, it would enable not only a more holistic analysis, but it would also facilitate the translation of modeling output into concrete actions that policymakers can take to achieve the modeling outcomes.

While the study identifies specific challenges for each archetype, there are common challenges across them. First, that no single archetype covers all the features and applications. This makes necessary the use of soft-linking or modeling suites with various archetypes to be able to provide holistic answers where gaps of one model are covered by another one in the modeling suite. Second, that not all the archetypes make full use of the potential hydrogen has. This creates the need to revisit each archetype and ensure that is suitable for modeling low-carbon systems and adapted to fully take advantage of the features hydrogen provides. Third, is that hydrogen is relatively new for some of the modeling archetypes (e.g. IAM), while at the same time, it is a nascent set of technologies with limited experience across some applications. This means that there is lack of suitable and validated data that can be consistently used across archetypes to model hydrogen.

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