



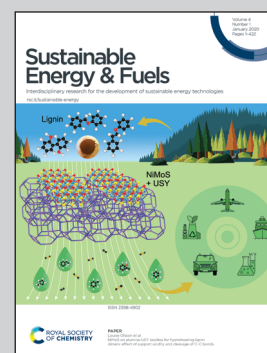
Showcasing research from the group of Dr Sheila Samsatli at University of Bath, UK.

The curious case of the conflicting roles of hydrogen in global energy scenarios

A collaboration between the IEA Hydrogen Implementing Agreement Task 38 and the group of Dr Samsatli, developing large, high-fidelity optimisation models, such as the Value Web Model, for integrated energy value chains that preserve the environment, biodiversity and ecosystems services.

Hydrogen is a crucial element in future low-carbon energy systems, where higher penetrations of renewables will require more responsive networks including load balancing, energy storage and sector coupling. However, it is puzzling that hydrogen does not play a more prominent role in global energy scenarios. This paper discusses the reasons for this and provides recommendations for energy scenario development so that hydrogen will be represented more consistently and to its full potential.

As featured in:



See Sheila Samsatli *et al.*, *Sustainable Energy Fuels*, 2020, 4, 80.

Cite this: *Sustainable Energy Fuels*,
2020, 4, 80

The curious case of the conflicting roles of hydrogen in global energy scenarios

Christopher J. Quarton,^a Olfa Tlili,^b Lara Welder,^{cd} Christine Mansilla,^b Herib Blanco,^e Heidi Heinrichs,^c Jonathan Leaver,^f Nouri J. Samsatli,^g Paul Lucchese,^h Martin Robinius^c and Sheila Samsatli^{id}*^a

As energy systems transition from fossil-based to low-carbon, they face many challenges, particularly concerning energy security and flexibility. Hydrogen may help to overcome these challenges, with potential as a transport fuel, for heating, energy storage, conversion to electricity, and in industry. Despite these opportunities, hydrogen has historically had a limited role in influential global energy scenarios. Whilst more recent studies are beginning to include hydrogen, the role it plays in different scenarios is extremely inconsistent. In this perspective paper, reasons for this inconsistency are explored, considering the modelling approach behind the scenario, scenario design, and data assumptions. We argue that energy systems are becoming increasingly complex, and it is within these complexities that new technologies such as hydrogen emerge. Developing a global energy scenario that represents these complexities is challenging, and in this paper we provide recommendations to help ensure that emerging technologies such as hydrogen are appropriately represented. These recommendations include: using the right modelling tools, whilst knowing the limits of the model; including the right sectors and technologies; having an appropriate level of ambition; and making realistic data assumptions. Above all, transparency is essential, and global scenarios must do more to make available the modelling methods and data assumptions used.

Received 21st September 2019
Accepted 8th October 2019

DOI: 10.1039/c9se00833k

rsc.li/sustainable-energy

1. Introduction

In order to combat climate change there is increasing interest in achieving net-zero greenhouse gas (GHG) emissions before the end of the century.¹ Energy systems decarbonisation is an essential part of this, as energy sectors contribute around three-quarters of global GHG emissions.²

Renewable energy technologies have progressed tremendously in recent decades, now offering economically credible alternatives to fossil fuels in many sectors.³ However, these technologies are fundamentally different to fossil fuels, so a like-for-like replacement is not possible. Renewable resources such as wind and solar are diffuse and intermittent, creating new challenges for matching energy supplies to

demands, in both time and space.^{4,5} Furthermore, fossil fuels have unrivalled storage capabilities. It is essential to find low-carbon energy storage options, for temporal balancing of supply and demand, and use in transport.⁶ We need to develop technologies that will enable increased energy systems flexibility and interconnectivity, while maintaining reliability and stability.^{7,8}

In this context, hydrogen has potential. Apart from small reserves of “natural” hydrogen,⁹ hydrogen is not a resource that can be extracted at scale in the same way as fossil fuels. However, it can be produced with minimal GHG emissions, for example through electrolysis powered by renewable electricity,¹⁰ or from bioenergy or fossil fuels with carbon capture and storage (CCS).¹¹ Hydrogen has many possible energy applications, including for heating, transport, industry, and electricity generation.^{12,13}

Energy scenarios can provide valuable insights into possible future trajectories of energy systems. Many different national, regional and global energy scenarios exist. Some scenarios, such as those produced by global institutions (e.g. ref. 14–16), can be very influential to political discourse.

However, energy scenarios are generated using various methods and, given the complexity of the systems being represented, it is unsurprising that the scenarios produce differing results. In particular, the prominence of hydrogen in different scenarios varies noticeably. Hanley *et al.*¹⁷ reviewed the role of

^aDepartment of Chemical Engineering, University of Bath, Claverton Down, Bath BA2 7AY, UK. E-mail: s.m.c.samsatli@bath.ac.uk

^bCEA, I-tésé, Université Paris-Saclay, Gif-sur-Yvette, France

^cForschungszentrum Jülich, Institute of Energy and Climate Research – Electrochemical Process Engineering (IEK-3), Wilhelm-Johnen-Straße, 52428 Jülich, Germany

^dChair for Fuel Cells, RWTH Aachen University, c/o Institute of Electrochemical Process Engineering (IEK-3), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

^eCenter for Energy and Environmental Sciences, IVEM, University of Groningen, Nijenborgh 6, 9747 AG Groningen, The Netherlands

^fSchool of Engineering, Unitec Institute of Technology, Auckland, New Zealand

^gProcess Systems Enterprise Ltd., London SW7 2AZ, UK

^hCEA, Université Paris-Saclay, Gif-sur-Yvette, France



hydrogen across different energy scenarios, finding a range of results regarding the uptake of hydrogen. Whilst many scenarios included some hydrogen in the transport sector, uptake of hydrogen in other sectors varied significantly depending on the emphasis in the scenario design. Furthermore, the review found a correlation between the level of ambition (e.g. decarbonisation or renewables integration targets) and the contribution of hydrogen in the scenario results.

Given hydrogen's potential to transform energy systems, the variation in its contribution in global energy scenarios is surprising. Whilst Hanley *et al.*¹⁷ identified some of the trends in hydrogen prevalence, they did not explore the reasons for differing results in detail.

In this perspective, we assess hydrogen's potential as a contributor to energy systems, and examine the methods used in global energy scenarios in order to understand the reasons for differing results regarding hydrogen. We focus on global energy scenarios produced by prominent institutions, as these are typically the most influential. The entire scenario development process is considered, including conceptualisation, model construction, and input data. Based on this analysis, we suggest some best practices for energy scenarios so that they can provide the best insight, and correctly quantify the potential of energy technologies such as hydrogen.

Section 2 provides an overview of hydrogen as an energy carrier. Section 3 provides details of hydrogen prevalence in scenarios from 12 global studies. In Section 4, the reasons for varying results between scenarios are discussed. Finally, some conclusions and suggestions for best practice in scenario development are provided in Section 5.

2. Opportunities for hydrogen in energy systems

There are many possible pathways for hydrogen in energy systems and in some cases they are already being realised in real projects. In this section, the main pathways are summarised; an overview is provided in Fig. 1, whilst Pivovar *et al.*¹⁸ describe them in more detail.

Currently, most hydrogen is produced from fossil fuels, such as reforming of natural gas or gasification of coal. Similar processes can be used to convert biomass feedstocks to hydrogen.¹⁹ Water electrolysis has been used to produce hydrogen in certain industrial applications for over a century, but in recent decades it has seen growing interest due to newly emerging technologies and availability of low-cost electricity.¹⁰ Many future projections for hydrogen are based on large contributions from electrolysis but there are other new technologies emerging, such as thermolysis and photolysis, that may offer a more efficient use of thermal or solar energy for hydrogen production.²⁰

Applications of hydrogen include conversion to electricity using a fuel cell,¹⁹ contributing to industrial processes,^{21,22} and combustion for heat and/or power generation.²³ Hydrogen can be stored in quantities from MW h to TW h, for example in pressurised cylinders or underground in salt caverns, depleted oil and gas reservoirs and saline aquifers.^{19,24} Pressurised hydrogen storage has a volumetric energy density greater than 500 kW h m⁻³, far exceeding low-carbon energy storage alternatives (up to 1.5 kW h m⁻³ for pumped hydro storage (PHS) and 12 kW h m⁻³ for compressed air energy storage (CAES)).²⁵

Hydrogen's high energy density makes it particularly interesting for system-wide energy balancing. Hydrogen could be

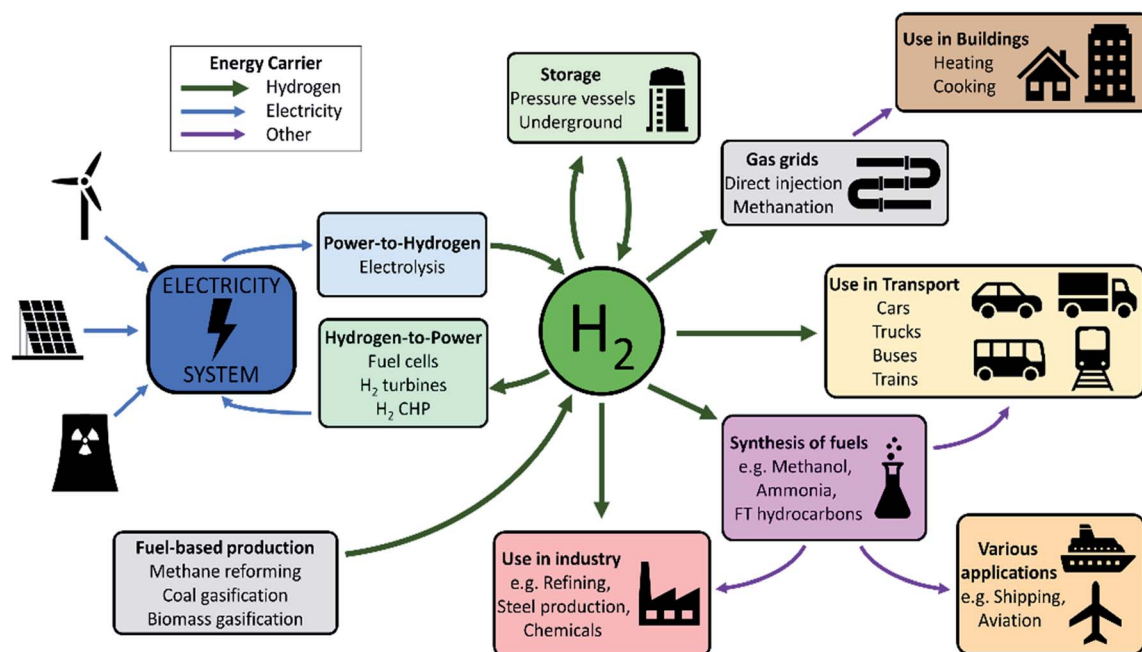


Fig. 1 Overview of key hydrogen production and usage pathways. With multiple production options and applications, hydrogen could be valuable in providing flexibility and sector-coupling to energy systems.



manufactured from electricity at times of excess supply, stored, and later converted back to electricity or used for other purposes at times of high demand.¹⁰ However, hydrogen storage round-trip efficiencies are around 20–36%, which is low compared to alternatives (PHS: 70–85%; CAES: 65–80%; battery: 86–95%).⁶ Therefore, the value of hydrogen energy storage depends on the trade-off between the benefits of time-shifting bulk energy, and the costs of the efficiency losses.

Whilst hydrogen for electricity storage has not yet been deployed at large scale, already several projects have deployed electrolyzers to absorb electricity from wind farms, to be stored and used at a later date in various applications (for example Energiepark Mainz²⁶ and Lam Takhong²⁷). For the 2020 Olympics, Tokyo plans to power the Olympic village with hydrogen from solar-powered electrolysis.²⁸

Hydrogen's suitability for storage also makes it appealing as a transport fuel. A hydrogen fuel tank and fuel cell can provide the electricity supply for an electric vehicle, or hydrogen can be burned in an internal combustion engine. Hydrogen is seen as a possible low-carbon fuel in transport sectors that require long ranges, such as road freight, rail and shipping.^{13,29} Hydrogen in passenger vehicles could also offer greater driving ranges, faster refuelling times and in some cases lower cost of ownership compared to battery electric vehicles.^{30,31}

The transport sector has seen the greatest interest in hydrogen so far and there is considerable interest globally in expanding the use of hydrogen as a transport fuel. There are over 350 hydrogen fuelling stations worldwide, across the Americas, Europe, Asia and Oceania.³² Hydrogen buses are in use in many cities around the world including in USA, Japan, China and several countries in Europe.^{33,34} Alstom have developed a hydrogen train, the first of which went into operation in Lower Saxony, Germany in 2018.³⁵

Hydrogen is already a key chemical component in many industrial markets: the main applications include ammonia synthesis (55% of hydrogen demand); hydrocracking and hydrodesulphurisation in refineries (25%); and methanol production (10%).³⁶

Nonetheless, the “hydrogen economy” is still in the early stages of development. In most applications, there has been limited deployment of hydrogen beyond demonstration projects.³⁷ Most of the hydrogen used today is produced on-site for specific applications. Consequently, there has been limited infrastructure development other than for transportation between chemical manufacturing sites. Today, there are around 16 000 km of hydrogen pipelines globally¹² compared to 2.91 million km for natural gas.³⁸ For expansion beyond the chemical sector, it will be necessary either to build new hydrogen infrastructure, or to utilise existing infrastructure (e.g. partial injection or conversion of existing gas networks).³⁷

Low-cost, low-carbon hydrogen production at scale is also still a challenge. Conventional production such as steam methane reforming (SMR) would require carbon capture and storage (CCS) to minimise GHG emissions, but this adds around 45% to the cost,¹¹ and CCS deployment remains limited. Low-carbon production of hydrogen using electrolysis requires both significant electrolysis capacity and sufficient low-carbon

electricity production. Although costs of renewable electricity are falling rapidly with increasing installed capacity,³ electrolysis installed capacity is low and reductions in capital costs through economies of scale are still required.^{39,40} Lastly, fuel cell costs are relatively high (around \$280 kW⁻¹ (ref. 41)), and manufacturing scale-up is required to make hydrogen competitive with other energy carriers.

Hydrogen can also be combined with captured CO₂ in carbon capture and utilisation (CCU) processes. CCU can produce useful energy carriers that are already in use and have existing infrastructures, such as methane, methanol and liquid hydrocarbons.^{42,43} The CO₂ used in CCU could be captured from fossil sources, but increased environmental benefit would be achieved if the CO₂ were captured from biomass or directly from the air.⁴⁴ The challenges for CCU are energy losses associated with the additional conversion step (20–35% (ref. 45)), and high costs compared to the fossil alternatives they would replace (e.g. CCU transport fuel may cost € per 30 GJ, compared to € per 15 GJ for petroleum-based fuels⁴⁶). Hydrogen can also be combined with nitrogen to produce ammonia, which has advantages for storage and transport, and can be used for heat and power generation.⁴⁷

3. Global energy scenarios and the representation of hydrogen

3.1 Energy scenarios

Energy scenarios can address the uncertainties surrounding the socio-technical evolution of energy sectors. Scenarios can be qualitative, relying on inputs from experts and stakeholders, or quantitative, usually based on energy systems models.⁴⁸ Scenario development aims to construct possible futures and the paths leading to them, and can guide strategic decision-making processes, for example for maintaining long-term energy supply-demand balances and optimising investment decisions. Consequently, these scenarios can be highly influential to the future of the technological “ecosystem” in different sectors. Due to the size and complexity of the energy systems being represented by energy scenarios, simplifying assumptions must be made, and these can have significant implications for the scenario results.

Several reviews of model-based scenarios and the modelling tools they use have been carried out, highlighting a variety of methods and results. Pfenninger *et al.*⁵⁸ reviewed energy systems models in the context of present-day energy systems, and identified several challenges that these models face, stemming from the increased complexity of modern energy systems. The review also provided recommendations for modelling practice, encouraging innovation with modelling methods, appropriate handling of uncertainty and modelling transparency. Meanwhile, Gambhir *et al.* reviewed energy scenario results, finding that the level of climate change ambition has a significant effect on the scenario results.⁵⁹ Lopion *et al.*⁶⁰ investigated trends in energy system models developed for national greenhouse gas reduction strategies, in the context of underlying research questions and their shift over



time, and found that there is an increasing need for high temporal and spatial resolutions.

As Hanley *et al.*¹⁷ found, the prominence of hydrogen varies significantly between energy scenarios. Whilst many of the scenarios Hanley *et al.* studied included some hydrogen in the transport sector, hydrogen prevalence in other sectors was low, except where hydrogen was a specific focus of the study. The scenarios that focus on hydrogen, such as the IEA Energy Technology Perspectives (ETP) 2 °C “high hydrogen” scenario,⁶¹ have begun a trend of greater hydrogen representation, and hydrogen prominence is growing in the most recent scenarios.

In this perspective, we discuss why there has been an historical absence of hydrogen in global energy scenarios, and why that is beginning to change. Many energy scenarios exist at regional and national levels, such as the EU Reference scenario,⁶² ASEAN Energy Outlook (SE Asia),⁶³ IDB Lights On scenario (Latin America),⁶⁴ EIA Annual Energy Outlook (USA),⁶⁵ China Renewable Energy Outlook,⁶⁶ the Japan Strategic Energy Plan,⁶⁷ and the Deep Decarbonization Pathways Project (various

countries).⁶⁸ However, in this perspective we focus on global scenarios with the greatest international impact.

The 12 studies that were considered are shown in Table 1. We focus on the scenarios from 10 model-based studies and also consider two hydrogen-focussed qualitative scenarios: the IEA Hydrogen and Fuel Cells Technology Roadmap³⁰ and the Hydrogen Council “Scaling Up” scenario,⁵⁷ as they provide a counterpoint for the potential for hydrogen, as perceived by experts and stakeholders.

3.2 Hydrogen representation in global energy scenarios

Between the 35 scenarios considered there is significant variation regarding which hydrogen technologies and end-use applications are considered, and the level of detail with which they are included. In Fig. 2, the level of representation of these hydrogen technologies is presented, including whether the technology is modelled, whether data assumptions are provided, and whether hydrogen contributes to the final results.

Table 1 Details of the studies and scenarios that were reviewed. Global studies from influential institutions were chosen, focussing on quantitative (model-based) scenarios. Two qualitative scenarios were also included

Study	Abbreviation	Model used	Scenario end year	Scenarios
World Energy Outlook (IEA) 2016 (ref. 49)	WEO 2016	World Energy Model + MoMo	2040	Current policies New policies 450 scenario
World Energy Outlook (IEA) 2017 (ref. 50)	WEO 2017	World Energy Model + MoMo	2040	Current policies New policies Sustainable development
World Energy Outlook (IEA) 2018 (ref. 14)	WEO 2018	World Energy Model + MoMo	2040	Current policies New policies Sustainable development
The Grand Transition (WEC) 2016 (ref. 15)	WEC	GMM	2060	The future is electric Hard Rock Unfinished Symphony Modern Jazz
REmap (IRENA) ⁵¹	REmap	E3ME	2050	Reference REmap
Energy Technology Perspectives (IEA) 2016 (ref. 52)	ETP 2016	ETP TIMES + MoMo	2050	6DS 4DS 2DS
Energy Technology Perspectives (IEA) 2017 (ref. 53)	ETP 2017	ETP TIMES + MoMo	2060	RTS 2DS B2DS
Energy Revolution (Greenpeace) ⁵⁴	ER	REMIX	2050	Reference E[R] ADV E[R]
Shell scenarios ^{16,55}	Shell	Shell World Energy Model	2100	Mountains Oceans Sky
Global Energy Assessment (IIASA) ⁵⁶	GEA	MESSAGE + IMAGE	2050	Supply (Conv. Trans) Mix (Conv. Trans) Efficiency (Conv. Trans) Supply (Adv. Trans) Mix (Adv. Trans) Efficiency (Adv. Trans)
Hydrogen Council (2017) ⁵⁷	H2 Council	Qualitative	2050	Hydrogen – scaling up
Technology Roadmap: Hydrogen and Fuel Cells (IEA) ³⁰	H2FC Roadmap	Qualitative	2050	2DS high H2



Legend

- No mention in the scenario
- Not modelled, but discussed
- Modelled, but no data assumptions provided
- Modelled, with data assumptions provided
- R** Included in the scenario results

Sector	Technology	Study																							
		World Energy Outlook (IEA) 2016		World Energy Outlook (IEA) 2017		World Energy Outlook (IEA) 2018		The Grand Transition (WEC) 2016		REmap (IRENA) 2018		Energy Technology Perspectives (IEA) 2016		Energy Technology Perspectives (IEA) 2017		Energy Revolution (Greenpeace) 2015		Shell scenarios 2018		Global Energy Assessment 2012		H2 Council 2017		H2FC Roadmap 2015	
		Scenario		Scenario		Scenario		Scenario		Scenario		Scenario		Scenario		Scenario		Scenario		Scenario		Scenario		Scenario	
Production	Electrolysis			R		R												R	R			R		R	
	From biomass																								
	Steam methane reforming																								
	Coal gasification																								
Storage	General storage																								
	Shipping (chemicals/liquid)																								
Transport	Trucks																								
	Pipelines																								
	Considered but not specified																								
	Re-conversion	Fuel Cell																							
Mobility	CCGT																								
	CHP																								
	LDVs																								
	MDVs/HDVs/trucks/buses																								
	H2 for alternative fuels																								
	Aviation																								
Industry	Shipping																								
	Considered but not specified																								
	Refining																								
Gas grid	Chemicals																								
	Not specified																								
Gas grid	Direct injection of H2																								
	Methanation																								

Fig. 2 Differing representation of hydrogen in scenarios from 12 global studies. Hydrogen representation is separated into seven sectors, covering the supply-side (production, storage, transportation), and applications of hydrogen (conversion to electricity, mobility, industry, gas grid). Colours refer to the level of representation in the scenario design; "R" denotes technologies that are included in the results of the scenario. See the legend for more details.

Whilst there are conflicts in the prominence of hydrogen between scenarios, what is common is that limited specific techno-economic information is provided. Often, concepts are discussed but with little detail, so it is difficult to understand how these concepts are represented and what assumptions have been made.

Regarding technologies, hydrogen production is covered in the most detail, and in this case techno-economic assumptions are often provided. Electrolysis is commonly considered, although the technology type is rarely specified (WEO 2018,¹⁴ Shell,^{16,55} GEA,⁵⁶ ER,⁵⁴ REmap⁶⁹). ETP 2017 specifically considers the more commercially developed alkaline electrolysis, whereas the H2 Council focus on PEM electrolysis, which many expect to overtake alkaline as the favoured technology.⁴⁰ The qualitative H2FC road map³⁰ is the only study to consider solid-oxide electrolysis.

Several studies discuss other production options, such as SMR, coal gasification and biomass-based production. These production options are typically mentioned when comparing hydrogen production costs (WEO 2018,¹⁴ H2FC Roadmap³⁰) or as a transitional step to fully decarbonised hydrogen (Shell^{16,55}). The techno-economic assumptions related to these technologies (mainly SMR, with or without CCS) are often presented, and it is observed that the costs of electrolysis and SMR + CCS are converging.³⁰

Other hydrogen infrastructures, such as transportation and storage, receive little coverage in most studies. A few studies discuss storage, but provide no data, suggesting it is not modelled (GEA,⁵⁶ ER,⁵⁴ H2 Council⁵⁷). Hydrogen transportation receives slightly more coverage, most commonly shipping for global transportation (WEO 2018,¹⁴ H2 Council,⁵⁷ GEA⁵⁶). In general, limited data is provided for transportation, so it is unclear what assumptions are made (*e.g.* how transportation is costed), or whether it is considered at all.

End-use applications are described in more detail in the scenarios. The most prominent end-use is mobility, which is considered in some form in all but WEO 2016 (ref. 49) and WEO 2017.⁵⁰ Fuel Cell Electric Vehicles (FCEVs) for light-duty passenger vehicles (LDVs) are predominant but heavier duty vehicles (HDVs, *e.g.* trucks and buses) are also discussed in more-recent studies (though rarely quantified). Instead, discussion is more focussed on societal issues, such as government policies. The qualitative studies^{30,57} provide more techno-economic data for HDVs. Finally, there is some interest in hydrogen for alternative fuels but limited details on techno-economic assumptions are provided (E[R],⁵⁴ ETP 2017,⁵³ H2 Council⁵⁷).

Beyond mobility, other applications for hydrogen are discussed in less detail. Several studies consider industrial applications, with refining applications such as steel and iron, and chemical applications such as ammonia production



being the most popular. Electrification of processes *via* electrolysis is mentioned (WEO 2018 (ref. 14)), but again with little detail. Interactions with the gas grid (either direct hydrogen injection or methanation) are often mentioned in discussion, but rarely quantified in the results (GEA;⁵⁶ WEO 2017,¹⁴ H2FC Roadmap,³⁰ H2 Council⁵⁷). Finally, conversion of hydrogen to electricity and heat is rarely mentioned. Where it is considered, the most common technologies are fuel cells, gas turbines and combined heat and power applications. The E[R] scenarios⁵⁴ are the only ones to include these applications in the scenario results.

3.3 Conflicting roles of hydrogen in global scenario results

The variability in representation of hydrogen in scenarios leads to conflicts in the level of contribution of hydrogen in the scenario results. Fig. 3 shows the contribution of hydrogen to final energy demand in 2050 in different sectors, for each of the scenarios that includes hydrogen in its results.

Overall, the scenarios indicate that hydrogen has the most potential in the mobility sector. Most scenarios have some level of hydrogen in this sector but they offer conflicting levels of contribution: in many cases this is less than 2% of transport energy demand in 2050 (*e.g.* WEC¹⁵ and ETP 2017 (ref. 53) scenarios); whereas the Greenpeace E[R] and Adv E[R] scenarios give contributions as high as 19% and 25%, respectively.⁵⁴

Similarly, the contribution of hydrogen in the industrial sector ranges between 0.7% of 2050 industrial demands (Shell Sky¹⁶) and 12% (H2 Council⁵⁷) but many scenarios do not include it at all.

The focus between these two sectors can also shift between scenarios: the Grand Transition scenarios suggest hydrogen should contribute to the mobility sector and not to industry whereas several of the Global Energy Assessment scenarios advocate the opposite.

The Greenpeace scenarios⁵⁴ are the only quantitative scenarios to include hydrogen in the results for the power and heating sectors and both qualitative scenarios also include it (H2FC Roadmap³⁰ and H2 Council⁵⁷).

4. Discussion: what must scenarios do to represent hydrogen fairly?

From the results in Section 3, and from previous reviews, there is clearly significant variation between scenarios concerning the prominence of hydrogen in energy systems. Although most of these scenarios rely on energy system models, the representation in these models is not sufficient to capture all of the advantages of hydrogen. In this section, we examine the key steps in quantitative scenario development, to understand why differing results may arise, and consider what scenario

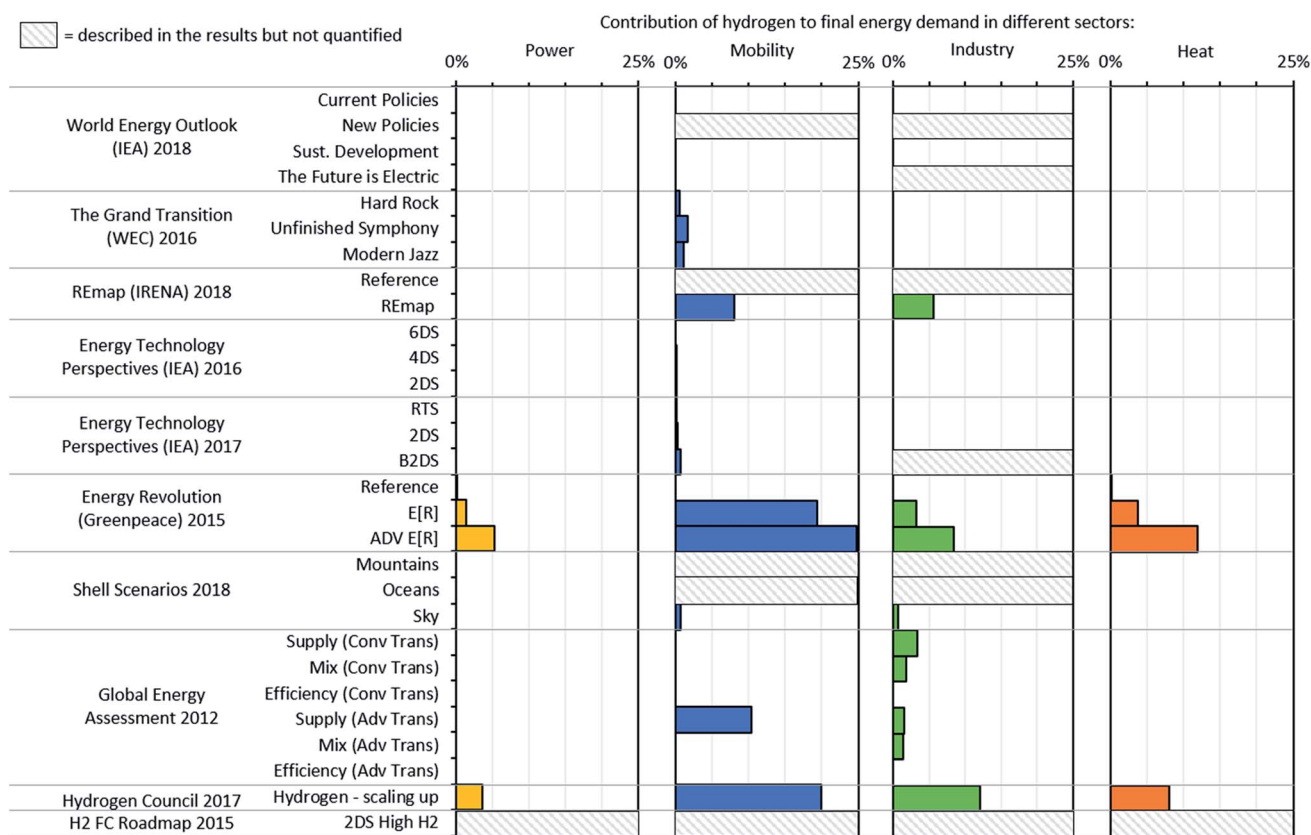


Fig. 3 Contribution of hydrogen to final energy demand in 2050 in power, mobility, industrial and heat sectors for a range of scenarios. Where studies state the inclusion of hydrogen in the results without precisely quantifying it, values have either been estimated by the author (IEA ETP 2016, Shell Sky and H2 Council scenarios), or the result has been denoted by a hashed box.



developers should be doing to make sure hydrogen, and other flexibility options (such as alternative storage technologies, demand-side response, electricity grid expansion and inter-connectivity⁷⁰), are appropriately represented.

4.1 Scenarios must use appropriate modelling tools

Energy systems models form the basis of most quantitative energy scenarios. A vast number of energy system modelling tools exist and can be categorised in different ways, including simulation *vs.* optimisation, top-down *vs.* bottom-up, *etc.* In a review of computing tools for energy systems, Connolly *et al.*⁷¹ identified 68 different energy system modelling tools. Lopion *et al.*⁶⁰ reviewed 24 energy system models in detail, also categorising them as above, and found a clear trend towards techno-economic bottom-up optimisation models in order to answer current research questions.

Each energy systems model is designed for its own unique purpose and has its own strengths and weaknesses. Some of the oldest models were developed in the second half of the 20th century to help understand energy systems in the context of the oil crisis and concerns over security of energy supply.⁵⁸ These models are the predecessors of many models in use today, where due to climate change, we face significantly different energy challenges. It is important that energy systems models in use today are appropriately designed to represent the challenges we face in the twenty-first century.

The most difficult task for modern day energy systems models is to capture the full degree of variability and complexity that exists in energy systems. Traditionally, energy systems were centralised and underpinned by fossil fuels. In the electricity sector for example, supply would be made up of either base-load or dispatchable generation. However, as more and more renewable sources such as solar and wind are introduced to aid decarbonisation, systems are becoming more spatially distributed, technologically diverse and temporally variable. Meanwhile, new technologies and increased interconnectivity are enabling more interaction between different energy sectors, known as “sector-coupling”.⁷² To ensure that energy system models not only provide an accurate representation of energy systems but also do not miss the potential of new technologies such as hydrogen-based technologies, they must capture the required level of temporal, spatial, technological, and inter-sectoral detail.

4.1.1 Models must capture sufficient temporal detail. Many large-scale energy models are unable to represent the time scales at which flexibility technologies such as electrolyzers, hydrogen storage and fuel cells are most useful. For example, traditional energy system models typically use representative time slices, such as day, night, and peak for a series of day types throughout the year. In some cases, within-day chronology is retained, meaning that it may be possible to model some level of intraday storage. However longer-term chronology is rarely retained, thus losing the ability to represent long-term storage,^{73,74} which is an area where hydrogen is seen to have strong potential.^{6,75} Novel methods for modelling seasonal storage are beginning to emerge^{76,77} but they have not been

applied to any of the global energy scenarios. Meanwhile, short-term dynamics, such as electricity dispatch on a sub-hour basis, are also not modelled by large-scale energy models. This means that another opportunity for hydrogen, as a short-term load balancer through electrolysis,^{78,79} is also missed. The effects of under-representing temporal detail in energy scenarios have been explored and it has been found that investment optimisations will underestimate the contribution of dispatchable power generation and instead favour baseload and intermittent renewables.⁸⁰ It is therefore likely that flexibility options such as those based on hydrogen are also being under-valued.

The challenge for large-scale energy systems models is to capture the full range of time scales necessary. The models are designed for long-term investment planning, and therefore require multi-decadal time horizons. However, the dynamics of the energy system at all time scales (including seasonal, weekly, daily, and sub-hourly) are important to how the system should be designed and operated.⁸¹ Approaches to improve the accuracy of the time-slicing method include using a higher resolution of time intervals; probabilistic representation of the loads and renewable energy supplies; and using real historical data for the time intervals.⁷³ However, each of these approaches suffers the same issue of failing to maintain chronology across the whole time horizon, hence some representation of flexibility is lost. Alternatively, energy systems models can be soft-coupled to power sector models, taking advantage of the latter's improved temporal representation.⁷³ However, this approach can increase overall complexity, as there are two separate models to maintain and run. Furthermore, due to the required iteration between the two models, there is no guarantee that an optimal solution will be obtained.

4.1.2 Models must capture sufficient spatial detail. As well as temporal flexibility, hydrogen can provide spatial flexibility to energy systems. Hydrogen transportation by road, pipeline and shipping provide opportunities for the transportation of energy that cannot be provided by other energy carriers (*e.g.* electricity). Large-scale (*e.g.* global) energy models usually have limited spatial detail, using average resource demands and supplies over large spatial regions.⁵⁸ Consequently, they do not capture the value of energy transportation at a smaller scale, such as across country. Furthermore, spatial variabilities in solar and wind generation will affect supply profiles across a region: this “spatial smoothing” cannot be fully represented with too coarse a spatial resolution.⁷³

One option for improving this modelling would be to include a higher spatial resolution but this would significantly increase the complexity of the model. Alternatively, models should seek to use representative data and relationships to value within-region energy transportation and distribution.

4.1.3 Models must appropriately represent technologies and inter-sectoral connectivity. Technological representation in large-scale energy models is often restricted to blanket details for each technology type, rather than representing individual technologies or plants.⁸⁰ Consequently, realistic operation of plants, taking their flexibility constraints into account, is not modelled. This is not helped by the lack of temporal resolution and chronology.



To improve technological representation, approaches include further modelling of ancillary markets (*e.g.* flexibility markets), and broader constraints that attempt to represent the overall behaviour of many individual technologies of a given type.⁷³

Finally, hydrogen is central to several sector-coupling options, including power-to-gas (for the gas grid),³⁷ power-to-heat,⁸² power-to-liquids,⁸³ and power-to-ammonia.⁸⁴ Energy systems models need to include the opportunity for transfers of energy between sectors, as this can unlock potential for cost and resource efficiency savings.

4.1.4 Models must represent the complexity of consumer behaviour. Uptake of new technologies is not only driven by cost or efficiency-based metrics for the entire energy system, but also by consumer choice, dependent on social factors and personal preference. For example, market adoption of FCEVs is sensitive to consumer perception of factors such as driving range, battery life, depreciation and capital cost. Furthermore, vehicle uptake is affected by consumer perception in the used vehicle market.

There are significant variations between models regarding how consumer choices are represented, for example the inclusion and relative importance of different utility factors representing consumer choice. Improvements in modelling can be achieved with more readily available data on elasticities and utility factors. Furthermore, a more detailed representation of different technology types (*e.g.* different weight and range categories for vehicles) will allow for a more accurate representation of consumer choice.

4.1.5 Models must remain manageable and user-friendly. Increasing computational power means that larger, more complex and more realistic models can be developed. However, this greater detail can introduce difficulty for the model users, in terms of managing the much larger datasets that are required as inputs and generated as outputs, analysing the results and communicating them to a general audience, such as policy makers and the general public. The challenge for energy systems models is therefore to use appropriate techniques such as those described above whilst preventing the model from becoming too difficult to use and to communicate. Although the detailed outputs of a complex model can be summarised using averages and high-level metrics, some of the important insights can only be understood from the details and presenting these in a manner that is easy to understand remains a key goal and challenge.

4.1.6 Model methodologies must be transparent. Due to the complexities in representing the details of energy systems, it is important that when scenarios are presented, the methodologies behind them are shared. The fact that these models are being used to predict what future energy systems may be, often many decades into the future, means that there is no real-life system against which the models can be validated. As most energy system models use optimisation and today's energy systems are far from optimal, it is difficult even to validate these models against current data. For this reason, it is important that the mathematical formulations behind the models be published so that they can be appropriately peer reviewed. However, this practice is very rare among the global energy scenarios:

none of the scenarios reviewed in Section 3 have published the mathematical formulations of their models. Indeed, most give no or very little information regarding the modelling approaches used and only the IEA ETP studies^{52,53} describe qualitatively the modelling framework that is used to generate the results (four soft-linked models are used, including ETP TIMES models for energy conversion and industry, the MoMo model for transport, and the Global buildings sector model for buildings). One might argue that if the results over a wide range of scenarios appear sensible, behave as expected and can be explained, then that is a sufficient test. However, since many modelling assumptions must be made even in complex models, different formulations of the same physical phenomena are possible and these can result in different but still sensible results.

One barrier to the publication of a model's mathematical formulation is the intellectual property rights of the organisation that developed the model. This is understandable, but the IP is more than just the mathematical constraints employed by the model. It is not practical to publish all of the know-how in the implementation and solution of the model (the minute details required to obtain robust and reliable solutions) and there are many other elements to the IP: data management, user interface, results management and analysis.

The main advantage of model transparency is that this allows other modellers to review the model, highlight any deficiencies and suggest improvements. This will provide researchers and policy makers with the confidence that the results of the scenarios are truly meaningful and that they can be taken forward with real enthusiasm. This can only really be possible by publishing the mathematical formulation of the model, as has been done in other similar areas (see *e.g.* ref. 85–90).

Finally, given that models each have their own strengths and weaknesses, transparency enables scenario developers to choose the model that is best suited to the application. Where energy scenarios are used to inform policy decisions, decision making cannot be considered fully transparent if the methodologies behind the modelling are not themselves transparent.

4.1.7 Challenges and pitfalls. We have argued that models must be much more detailed, and therefore complex, than are currently being used in global energy scenarios. Including features such as high spatial and temporal resolutions, uncertainty analysis, consumer behaviour and including a large range of technologies and energy carriers in a model is extremely challenging. Of course, the models should be made only as complex as is necessary to represent all of the features and details of hydrogen (and other) technologies that may play a role in the future energy system (such as rapid-response load balancing technologies). Modellers and scenario planners should follow a structured approach to developing new models similar to the one below:

1. Describe the purpose of the study carefully.
2. Define the scope so that the purpose can be achieved satisfactorily and with sufficient accuracy.



3. Build the simplest model that can accurately represent all of the features and interactions of the system defined in the scope.

4. Provide assumptions and limitations.

5. Discuss results in light of assumptions and limitations, acknowledging that the model is imperfect.

Deciding the necessary level of detail and accuracy is itself a difficult decision but this can be helped by performing smaller studies involving particular technologies to determine what level of spatial and temporal detail are required. The greatest difficulty for a modeller is when the required level of detail is so high that the model becomes computationally very demanding but further simplifications make the model no longer fit for purpose.

It is understandable that time pressure or intractability may tempt researchers into oversimplifying models in order to obtain results. This is a pitfall that needs to be avoided or at least taken with extreme caution. The results and conclusions obtained from an oversimplified model can be misleading and possibly erroneous. In the context of hydrogen, if a technology does not appear in the results then it is not possible to determine whether this is because of an inherent disadvantage of the technology or whether it is due to the inadequacy of the model to represent the technology's benefits.

Despite the challenges of including an unprecedented level of detail in energy system models, these are not insurmountable goals. As has been mentioned, techniques have already been developed that allow national energy systems to be optimised with high levels of spatial and temporal disaggregation. With increasing computing power and further research into advanced techniques and algorithms, more complex and detailed models will be possible in the near future. Scenario developers should be aiming to take advantage of these developments in order to obtain more reliable, and perhaps surprising, results.

4.2 Scenarios must be designed appropriately

Scenario design, including which sectors and technologies are included, what the level of ambition is, and what performance metrics are used, has a significant influence on scenario results. Scenario design will partly be determined by the capabilities of the model used. However, many decisions will also be made by the developer.

4.2.1 Scenarios must include all relevant sectors. As the results in Section 3 show, there is significant variation in the sectors that are included in different scenarios. Some sectors, such as mobility, are represented in almost all scenarios, but others have significant variability. For example, hydrogen is widely discussed as a key decarbonisation option for industry, as shown by its strong representation in the qualitative scenarios. Furthermore, in almost all quantitative scenarios where hydrogen in industry is included as an option, it contributes to the final results (*e.g.* ReMap, Shell and the Global Energy Assessment). However, several studies omit hydrogen in industry altogether, such as the early WEO and ETP scenarios, the WEC Grand Transition, and even the ambitious Energy

Revolution scenarios. Given that hydrogen does appear in the results of many of the scenarios that included it, it is reasonable to wonder if it would have also played a role in the other scenarios had they included it.

The other applications of hydrogen (re-conversion, gas grid) show similar variability between different scenarios and there is no consistent trend regarding which scenarios include which sectors. For studies that have re-produced scenarios in consecutive years (WEO, ETP), it is noticeable that the newer scenarios have a more comprehensive inclusion of sectors than the older scenarios. For example, WEO 2018 had at least some discussion of re-conversion, mobility, industry and the gas grid, whereas the previous iterations of the study (2016 and 2017) did not consider any of these sectors. Assuming that the modelling methods for these scenarios are not changed significantly from one year to the next, this again suggests that had these sectors been included earlier, they would have been seen in the scenario results. This shows the importance of including the sectors that have the most potential and suggests that awareness of the potential solutions of applications such as hydrogen is important for their prevalence in scenario results.

4.2.2 Scenarios must be technology rich: a technology not included will not appear in the results. As well as the importance of which sectors are included in a given scenario, it is important to consider which specific technologies are included. Again, Fig. 2 shows the variability in the hydrogen technologies that are included in each scenario. Fig. 2 would suggest that electrolysis is a key technology for hydrogen, as it is included in almost all scenarios. However, some scenarios even omit this technology. Despite referring to hydrogen as a transport fuel and the use of fuel cells, the WEC Grand Transition¹⁵ makes no reference to electrolysis or any other hydrogen production technology. The scenarios with a richer representation of hydrogen production technologies (*e.g.* fossil or biomass-based options as well as electrolysis) typically also include a greater representation of hydrogen in the scenario results.

A challenge for energy scenarios is to keep pace with and to estimate future technology developments so that they can be appropriately represented in scenarios for energy systems several decades in the future. For example, solid oxide electrolysis is a technology with significant interest due to its potential for higher efficiencies, reversible operation and co-electrolysis with carbon dioxide.³⁹ This is reflected in the technology's inclusion in the H2FC Roadmap.³⁹ However, the technology currently has a low level of commercial development, so is not included in any other scenarios.

Some of the most widely discussed advantages of hydrogen are its usefulness as an alternative energy vector, particularly for large-scale storage and transportation. However, these technologies are omitted from many scenarios. Hydrogen has a high volumetric energy compared to alternative energy storage options, so it is seen to have potential for large scale energy storage applications, for example for balancing electricity supplies and demands in systems with large penetrations of intermittent renewable energy. This potential is reflected in the qualitative scenarios, as well as the Shell and GEA scenarios, however no other scenarios include hydrogen storage.



Similarly, another advantage of hydrogen is that it can be transported easily at a range of scales. Unlike electricity, hydrogen can be shipped across long distances internationally, creating the potential for global supply chains.⁹¹ Pipelines also provide the opportunity for hydrogen transportation, and there is interest in both purpose-built hydrogen pipelines and repurposing existing natural gas grids.³⁷ At a smaller scale, hydrogen can also be transported on road by truck. Like storage, hydrogen transportation is hardly included in any of the scenarios.

The omission of these key hydrogen infrastructures is significant, as they are central to what makes hydrogen a potentially valuable energy carrier in future systems. Whilst the technologies for hydrogen production and consumption may not be the most efficient or the lowest cost, benefits arise from the efficiency with which hydrogen can be stored and transported, and hence these infrastructures should be included in energy scenarios.

4.2.3 Scenarios must have an appropriate level of ambition. In addition to the technologies and sectors included in the scenario, the level of scenario ambition also influences the prevalence of hydrogen in the results. Most scenarios investigate how an energy system may evolve over time, under existing or expected policies, and can be described as “explorative”; whereas other scenarios impose strict targets on the final energy system and can be referred to as “normative”. Reduction of greenhouse gas emissions is a typical target in normative scenarios. While some explorative global energy scenarios can even show an increase in global greenhouse gas (GHG) emissions, normative scenarios often target drastic cuts in GHG emissions, including nearly net-zero emission scenarios.

Scenarios with higher levels of GHG reduction ambition show a tendency towards a greater prevalence of hydrogen in their results. Drawing quantitative correlations between GHG

reductions and hydrogen prevalence is challenging, due to the tendency for scenarios to discuss hydrogen usage without providing specific data. However, Fig. 4 shows estimated hydrogen usage as percentage of total final energy demand in several scenarios, compared with the GHG emissions reduction in the scenario. A negative GHG emissions reduction represents an increase in emissions over the scenario time horizon.

Ambitious GHG reduction targets are achieved to some extent with increased uptake of intermittent renewables such as wind and solar. Consequently, energy system flexibility is required to balance electricity supplies and demands. With intermediate decarbonisation objectives, such as an 80% reduction in emissions, this “backup” can be provided by fossil fuels. However, in close to “net-zero” scenarios, nearly any usage of fossil fuels must be balanced by carbon sequestration. Where carbon sequestration is unattractive (due to technical, economic or social factors), alternatives such as hydrogen for energy storage become much more attractive.

Furthermore, with more variable renewable electricity generators on the grid in ambitious GHG scenarios, there is increased complexity in energy markets, for example with increased occurrence of near-zero power prices arising from excess electricity generation. In these situations, there is greater potential for alternative technologies such as power-to-gas to find viable business cases.^{92,93}

Finally, scenarios with less ambitious decarbonisation objectives do not always consider the decarbonisation of the more challenging sectors, such as industry or long-haul transport. Certain hydrogen pathways, such as power-to-fuels, are particularly attractive in these sectors.⁹⁴

4.2.4 Scenarios must consider other objectives. Besides the level of decarbonisation and renewables integration ambition, many other objectives and constraints, such as political interest, social acceptance and national strategies, may be included in

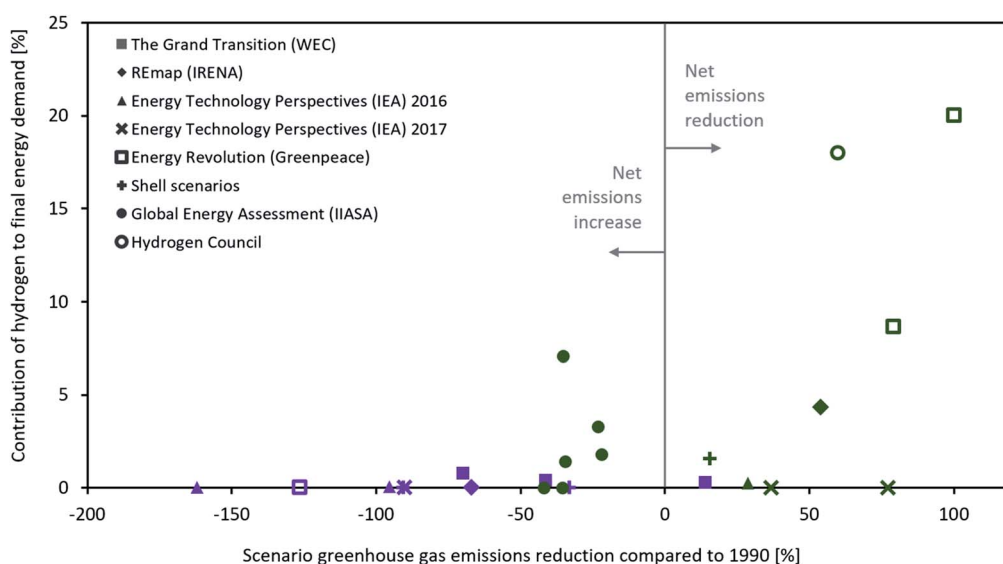


Fig. 4 Effect of greenhouse gas (GHG) emissions reduction on hydrogen prevalence in energy scenarios. A negative GHG emissions reduction represents an increase in emissions over the scenario time horizon. Explorative scenarios are displayed in purple, while normative are displayed in green.



Table 2 Cost estimates for key hydrogen technologies for present day and 2050

Technology	Units	Capex		Ref.
		Today	2050	
Electrolyser (alkaline)	€ per kW _{el}	800–1700	400–700	39, 97 and 98
Electrolyser (PEM)	€ per kW _{el}	1300–3200	300–700	39, 97 and 98
SMR (with CC)	€ per kW _{H₂} (HHV)	600–1300	400–600	11, 30, 98 and 99
H ₂ storage (vehicle on-board)	€ per kW h _{H₂} (HHV)	13–20	8 (target)	100
Fuel cell (vehicle on-board)	€ per kW _{el}	38–152	34 (target)	100
H ₂ storage (UG compressed)	€ per kW h _{H₂} (HHV)	0.1–2.0	0.1–2.0	98, 99 and 101
Fuel cell (stationary)	€ per kW _{el}	640–2900	330–1500	30 and 102

a scenario that will affect its outcomes. For example, nuclear power is a politically controversial technology that many countries are choosing to phase out.⁹⁵ Other potentially controversial technologies include CCS, and even onshore wind power. Meanwhile there are also resource-based constraints: *e.g.* some regions have limited biomass potential, limiting this option for future energy systems aiming for energy independence. These choices shape the scenario design and the evolution of the energy system. As these become more constrained, it is possible that hydrogen pathways will emerge as one of the remaining degrees of freedom to achieve ambitious climate targets.

4.3 Scenarios must use consistent and substantiated data assumptions

As well as broad scenario design, the thousands of data parameters that are input into each scenario will influence the scenario results.

Typical input data for technologies in energy systems models will include cost data (*e.g.* capital and operating costs) and performance data (*e.g.* operating rates, efficiencies, environmental impacts, *etc.*). For any technology there will be an uncertainty range in these data, depending on how, when and where the technology is installed and operated. As an example, some cost estimates for key hydrogen technologies are shown in Table 2, showing the wide uncertainty range in the literature. Energy scenarios are not able to capture this range in every detail, due to the large number of variables already being considered, and consequently must carry out some “averaging”.

Energy scenarios also need to capture the changes in cost and performance data that will occur over time. Rapid progress in energy technologies has been seen before, for example in solar PV³ and lithium-ion batteries.⁹⁶ This sort of progress is dependent on the scale of production. Learning curves can be used to estimate improvements in cost and technical performance with increased production rates but estimating the rates of uptake of technologies is challenging, particularly as these can be influenced by government policy.

Large-scale energy scenarios are typically based on policies that are already in place and free-market decisions. For the future, usually broad policies (*e.g.* system wide GHG targets) are used rather than sector specific. Technology agnostic measures are usually preferred, to promote the development of the most competitive options, and ensure that governments do not choose technologies with higher costs for society. However, due

to the learning curve effect, some technologies that are not economically attractive in the early stages of deployment may deliver a lower long-term cost. This requires additional incentives to go beyond this “valley of death” region to be able to reach that long-term target.¹⁰³

For example, although electrolysis is a relatively well established technology, studies that find hydrogen from electrolysis to be competitive with conventional hydrogen production or even fossil fuel alternatives usually rely on reductions in cost resulting from significant scale-up of production (*e.g.* ref. 97), which most likely would only occur with strong government support. Similarly, for technologies at the R&D level, incentives need to be technology specific since this will determine the research strategy and priorities. In turn, this R&D can lead to cost and efficiency improvements, which will influence the prominence of the technology in energy scenarios. Experience from the power sector has shown that a mix of technology specific and technology neutral policies achieve the best results in promoting low carbon options.¹⁰⁴

Model-based scenario studies should model a full range of technology and policy assumptions. Ideally, sensitivity analysis would be used to understand the significance of different data uncertainties on scenario results. This analysis may also provide insights into the relative value of R&D for different technologies and sectors. Of course, sensitivity analyses can be expensive when applied to large, complex models, hence there is an argument for simpler models, with a more thorough treatment of data uncertainty.¹⁰⁵ Despite this, the models should not be simplified to the point where they no longer represent the energy system with sufficient accuracy, as this will result in unrealistic sensitivities, especially when non-linear effects are involved. The simplified model should only be used for sensitivity analysis and the more-detailed model used to explore interesting “corner” points identified in the analysis – to check that the analysis is correct.

As a minimum, studies should share the data assumptions that were made in their analysis but unfortunately even this is rare. The IEA H2FC Roadmap³⁰ and IASA Global Energy Assessment^{56,106} contain detailed descriptions of the technical and economic performance of most hydrogen technologies throughout the supply chain. However, as Fig. 2 shows, several studies include hydrogen in their scenario results but little or no information at all is given on the data assumptions made (*e.g.* WEC,¹⁵ Shell¹⁶).



5. Conclusions

Energy systems are becoming more technologically diverse, spatially distributed and temporally variable. Consequently, there is an opportunity for new “flexibility” options, such as hydrogen, to play a role. In the authors' view, the greatest opportunities for hydrogen lie in the industrial and heavy-duty transport sectors, where hydrogen's high energy density and low greenhouse gas emissions could make it the preferred energy carrier. With the establishment of large-scale hydrogen production, transportation and storage infrastructure for these sectors, there will be many opportunities to use hydrogen for additional flexibility in other sectors, such as the power sector.

However, the exact role that new technologies such as hydrogen will have is unclear, and it is the purpose of energy scenarios to help to indicate what the role might be. In the authors' view, global energy scenarios, especially those based on energy system models, have been pessimistic with respect to hydrogen. This is beginning to change but coverage of hydrogen is still often restricted to a few main applications, such as mobility.

The main challenge for energy systems models is that many of the opportunities for new technologies such as hydrogen are in spaces that previously have not existed in energy systems, for example in energy storage (both at short and long time scales) and for sector-coupling. Energy systems models have traditionally not been good at representing the fine details, such as temporal variability. Capturing these details, whilst also encompassing the big picture of a long-term global energy transition is computationally and practically complex, and therefore a big challenge for the modelling community. Nonetheless, techniques are emerging to handle these complexities, and computational power is improving all the time, enabling more ambitious projects. We believe that overcoming these challenges will be necessary to determine with confidence the role that hydrogen should play in the future energy mix.

Meanwhile, if global energy scenarios are currently unable to represent all of the fine details and nuances of future energy systems, it is essential that they acknowledge this and do not present their scenario results with overconfidence. Much greater sharing of the methodologies and input assumptions behind energy scenarios is needed, so that the implications of the results can be correctly interpreted. Scenario developers should also constantly improve their practice, informed by findings from elsewhere. Numerous alternative approaches have been developed for exploring the role of new technologies in future energy systems, including qualitative scenarios and more detailed energy systems modelling at smaller scales. All of this research is valuable and should be taken into account with as much esteem as global energy scenarios.

Authors' contribution

All authors conceptualised the study at an initial workshop. CJQ & SS coordinated and drafted the paper. OT & LW performed the review of global energy scenarios. HH provided the analysis of scenario ambition and hydrogen prevalence. CM, NJS & HB

helped structure the paper, contributed to the draft and provided feedback. JL and MR provided feedback and additional arguments.

Conflicts of interest

There are no conflicts of interest to declare.

Acknowledgements

The present work was carried out within the framework of Task 38 of the Hydrogen Technology Collaboration Programme of the International Energy Agency. The task is coordinated by the Institute for techno-economics of energy systems (I-tésé) of the CEA, supported by the ADEME. CJQ and SS would like to acknowledge the Department of Business, Energy and Industrial Strategy (BEIS) and the Engineering and Physical Sciences Research Council (EPSRC) for funding his studentship. Thanks also to Dr Ian Llewelyn and Dr Jose M. Bermudez from BEIS for their very valuable inputs and feedback on this work. OT acknowledges the funding provided by Air Liquide to support her PhD thesis (framework of her contribution to this article). MR acknowledges the Helmholtz Association under the Joint Initiative “Energy System 2050 – A Contribution of the Research Field Energy” and Detlef Stolten for very important contributions and insights. SS would like to thank the EPSRC for partial funding of her research through the BEFEW project (Grant No. EP/P018165/1).

References

- 1 Committee on Climate Change, *Net Zero, The UK's contribution to stopping global warming*, <http://www.theccc.org.uk/publication/net-zero-the-uks-contribution-to-stopping-global-warming/>, 2019.
- 2 D. G. Victor, D. Zhou, E. Ahmed, P. K. Dadhich, J. G. J. Olivier, H.-H. Rogner, K. Sheikho and M. Yamaguchi, Introductory Chapter, in *Climate Change 2014: Mitigation of Climate Change. Contribution of Working Group III to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change*, Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, 2014.
- 3 International Renewable Energy Agency, *Renewable Power Generation Costs in 2017*, <http://www.irena.org/publications/2018/Jan/Renewable-power-generation-costs-in-2017>, Abu Dhabi, 2018.
- 4 H. Ibrahim, A. Ilinca and J. Perron, Energy storage systems – Characteristics and comparisons, *Renewable Sustainable Energy Rev.*, 2008, **12**(5), 1221–1250.
- 5 A. Gallo, J. Simões-Moreira, H. Costa, M. Santos and E. Moutinho dos Santos, Energy storage in the energy transition context: A technology review, *Renewable Sustainable Energy Rev.*, 2016, **65**, 800–822.
- 6 A. Abdon, X. Zhang, D. Parra, M. K. Patel, C. Bauer and J. Worlitschek, Techno-economic and environmental



- assessment of stationary electricity storage technologies for different time scales, *Energy*, 2017, **139**, 1173–1187.
- 7 R. Schlögl, The Revolution Continues: Energiewende 2.0, *Angew. Chem., Int. Ed.*, 2015, **54**(15), 4436–4439.
 - 8 H. Lund, P. Alberg Østergaard, D. Connolly and B. Vad Mathiesen, Smart energy and smart energy systems, *Energy*, 2017, **137**, 556–565.
 - 9 A. Prinzhofer, I. Moretti, J. Francolin, C. Pacheco, A. D'Agostino, J. Werly and F. Rupin, Natural hydrogen continuous emission from sedimentary basins: The example of a Brazilian H₂-emitting structure, *Int. J. Hydrogen Energy*, 2019, **44**(12), 5676–5685.
 - 10 S. Schiebahn, T. Grube, M. Robinius, V. Tietze, B. Kumar and D. Stolten, Power to gas: Technological overview, systems analysis and economic assessment for a case study in Germany, *Int. J. Hydrogen Energy*, 2015, **40**, 4285–4294.
 - 11 IEA Greenhouse Gas R&D Programme, *Techno-Economic Evaluation of SMR Base Standalone (Merchant) Hydrogen Plant with CCS*, <https://ieaghg.org/component/content/article/49-publications/technical-reports/784-2017-02-smr-based-h2-plant-with-ccs>, 2017.
 - 12 M. Ball and M. Weeda, The hydrogen economy – Vision or reality?, *Int. J. Hydrogen Energy*, 2015, **40**, 7903–7919.
 - 13 N. Brandon and Z. Kurban, Clean energy and the hydrogen economy, *Philos. Trans. R. Soc., A*, 2017, **375**, 20160400.
 - 14 International Energy Agency, *World Energy Outlook 2018*, <http://www.iea.org/weo2018/>, 2018.
 - 15 World Energy Council, *World Energy Scenarios 2016 – The Grand Transition*, <http://www.worldenergy.org/publications/entry/world-energy-scenarios-2016-the-grand-transition>, 2016.
 - 16 Shell, *Shell Scenarios, Sky, Meeting the goals of the Paris agreement*, http://www.shell.com/promos/business-customers-promos/download-latest-scenario-sky/_jcr_content.stream/1530643931055/eca19f7fc0d20adbe8330d3b0b27bcc9ef72198f5/shell-scenario-sky.pdf, 2018.
 - 17 E. S. Hanley, J. Deane and B. Ó. Gallachóir, The role of hydrogen in low carbon energy futures – A review of existing perspectives, *Renewable Sustainable Energy Rev.*, 2018, **82**, 3027–3045.
 - 18 B. Pivovar, N. Rustagi and S. Satyapal, Hydrogen at Scale (H₂@Scale) key to a clean, economic, and sustainable energy system, *Electrochem. Soc. Interface*, 2018, **27**, 47–52.
 - 19 F. Zhang, P. Zhao, M. Niu and J. Maddy, The survey of key technologies in hydrogen energy storage, *Int. J. Hydrogen Energy*, 2016, **41**, 14535–14552.
 - 20 P. Nikolaidis and A. Poullikkas, A comparative overview of hydrogen production processes, *Renewable Sustainable Energy Rev.*, 2017, **67**, 597–611.
 - 21 C. Philibert, *Renewable Energy for Industry: From green energy to green materials and fuels*, International Energy Agency, 2017.
 - 22 R. Ramachandran and R. K. Menon, An overview of industrial uses of hydrogen, *Int. J. Hydrogen Energy*, 1998, **23**(7), 593–598.
 - 23 P. E. Dodds and S. Demoullin, Conversion of the UK gas system to transport hydrogen, *Int. J. Hydrogen Energy*, 2013, **38**, 7189–7200.
 - 24 R. Tarkowski, Underground hydrogen storage: Characteristics and prospects, *Renewable Sustainable Energy Rev.*, 2019, **105**, 86–94.
 - 25 A. B. Gallo, J. R. Simões-Moreira, H. K. M. Costa, M. M. Santos and E. Moutinho dos Santos, Energy storage in the energy transition context: A technology review, *Renewable Sustainable Energy Rev.*, 2016, **65**, 800–822.
 - 26 Energiepark Mainz, Energiepark Mainz, <http://www.energiepark-mainz.de/en/>, accessed 04 September 2019.
 - 27 Electricity Generating Authority of Thailand, *EGAT to develop the first wind hydrogen hybrid in Asia to support the future of renewable energy*, 11 April 2018, <http://www.egat.co.th/en/news-announcement/news-release/egat-will-develop-the-first-wind-hydrogen-hybrid-in-asia-to-support-the-future-of-renewable-energy>, accessed 04 September 2019.
 - 28 Ministerial Council on Renewable Energy, *Hydrogen and Related Issues, Basic Hydrogen Strategy*, http://www.meti.go.jp/english/press/2017/pdf/1226_003b.pdf, 2017.
 - 29 G. Anandarajah, W. McDowall and P. Ekins, Decarbonising road transport with hydrogen and electricity: Long term global technology learning scenarios, *Int. J. Hydrogen Energy*, 2013, **38**, 3419–3432.
 - 30 International Energy Agency, *Technology Roadmap: Hydrogen and Fuel Cells*, <http://www.iea.org/publications/freepublications/publication/TechnologyRoadmapHydrogenandFuelCells.pdf>, 2015.
 - 31 E. Ruffini and M. Wei, Future costs of fuel cell electric vehicles in California using a learning rate approach, *Energy*, 2018, **150**, 329–341.
 - 32 H2stations.org, Hydrogen Refuelling Stations Worldwide, <http://www.netinform.de/h2/h2stations/default.aspx>, accessed 11 September 2019.
 - 33 T. Hua, R. Ahluwalia, L. Eudy, G. Singer, B. Jermer, N. Asselin-Miller, S. Wessel, T. Patterson and J. Marcinkoski, Status of hydrogen fuel cell electric buses worldwide, *J. Power Sources*, 2014, **269**, 975–993.
 - 34 B. Verheul, *Overview of hydrogen and fuel cell developments in China*, Holland Innovation Network China, <http://www.nederlandwereldwijd.nl/binaries/nederlandwereldwijd/documenten/publicaties/2019/03/01/waterstof-in-china/Holland+Innovation+Network+in+China+-+Hydrogen+developments.+January+2019.pdf>, 2019.
 - 35 Alstom, *Alstom Coradia iLint*, <http://www.alstom.com/our-solutions/rolling-stock/coradia-ilint-worlds-1st-hydrogen-powered-train>, accessed 04 September 2019.
 - 36 Hydrogen Europe, *Hydrogen in Industry*, 2019, <https://hydrogeneurope.eu/hydrogen-industry>, accessed 14 June 2019.
 - 37 C. Quarton and S. Samsatli, Power-to-gas for injection into the gas grid: What can we learn from real-life projects,



- economic assessments and systems modelling?, *Renewable Sustainable Energy Rev.*, 2018, **98**, 302–316.
- 38 Central Intelligence Agency, *CIA World Factbook*, 2019, <http://www.cia.gov/library/publications/the-world-factbook/fields/383.html>, accessed 14 June 2019.
- 39 A. Buttler and H. Spliethoff, Current status of water electrolysis for energy storage, grid balancing and sector coupling via power-to-gas and power-to-liquids: a review, *Renewable Sustainable Energy Rev.*, 2018, **82**, 2440–2454.
- 40 O. Schmidt, A. Gambhir, I. Staffell, A. Hawkes, J. Nelson and S. Few, Future cost and performance of water electrolysis: An expert elicitation study, *Int. J. Hydrogen Energy*, 2017, **42**, 30470–30492.
- 41 G. Morrison, J. Stevens and F. Joseck, Relative economic competitiveness of light-duty battery electric and fuel cell electric vehicles, *Transportation Research Part C: Emerging Technologies*, 2018, **87**, 183–196.
- 42 S. M. Jarvis and S. Samsatli, Technologies and infrastructures underpinning future CO₂ value chains: A comprehensive review and comparative analysis, *Renewable Sustainable Energy Rev.*, 2018, **85**, 46–68.
- 43 C. J. Querton and S. Samsatli, The value of hydrogen and carbon capture, storage and utilisation in decarbonising energy: Insights from integrated value chain optimisation, *Appl. Energy*, 2019, DOI: 10.1016/j.apenergy.2019.113936.
- 44 H. Daggash, C. Heuberger and N. Mac Dowell, The role and value of negative emissions technologies in decarbonising the UK energy system, *Int. J. Greenhouse Gas Control*, 2019, **81**, 181–198.
- 45 S. Brynolf, M. Taljegard, M. Grahn and J. Hansson, Electrofuels for the transport sector: A review of production costs, *Renewable Sustainable Energy Rev.*, 2018, **81**, 1887–1905.
- 46 D. Connolly, B. Mathiesen and I. Ridjan, A comparison between renewable transport fuels that can supplement or replace biofuels in a 100% renewable energy system, *Energy*, 2014, **73**, 110–125.
- 47 Institute for Sustainable Process Technology, *Power to Ammonia*, <http://www.topsectorenergie.nl/sites/default/files/uploads/Energie%20en%20Industrie/Power%20to%20Ammonia%202017.pdf>, 2017.
- 48 A. Ernst, K. H. Biss, H. Shamon, D. Schumann and H. U. Heinrichs, Benefits and challenges of participatory methods in qualitative energy scenario development, *Technol. Forecast. Soc. Change*, 2018, **127**, 245–257.
- 49 International Energy Agency, *World Energy Outlook 2016*, <http://www.iea.org/newsroom/news/2016/november/world-energy-outlook-2016.html>, 2016.
- 50 International Energy Agency, *World Energy Outlook 2017*, <http://www.iea.org/weo2017/>, 2017.
- 51 International Renewable Energy Agency, *Accelerating the Energy Transition through Innovation, a working paper based on global REmap analysis*, http://www.irena.org/-/media/Files/IRENA/Agency/Publication/2017/Jun/IRENA_Energy_Transition_Innovation_2017.pdf, Abu Dhabi, 2017.
- 52 International Energy Agency, *Energy Technology Perspectives 2016*, <http://www.iea.org/etp2016/>, 2016.
- 53 International Energy Agency, *Energy Technology Perspectives 2017*, <http://www.iea.org/etp2017/>, 2017.
- 54 Greenpeace, *Energy [R]evolution, A sustainable World Energy Outlook 2015, 100% Renewable Energy for all*, <http://www.greenpeace.org/archive-international/en/campaigns/climate-change/energyrevolution/>, 2015.
- 55 Shell, *New Lens Scenarios, A shift in perspective for a world in transition*, http://www.shell.com/energy-and-innovation/the-energy-future/scenarios/new-lenses-on-the-future/_jcr_content/par/relatedtopics.stream/1519787235340/77705819d8c8c77394d9540947e811b8c35bda83/scenarios-newdoc-english.pdf?, 2018.
- 56 International Institute for Applied Systems Analysis, *Global Energy Assessment: Toward a Sustainable Future*, http://www.iiasa.ac.at/web/home/research/Flagship-Projects/Global-Energy-Assessment/Chapters_Home.en.html, 2012.
- 57 Hydrogen Council, *Hydrogen scaling up, A sustainable pathway for the global energy transition*, <http://www.hydrogencouncil.com/wp-content/uploads/2017/11/Hydrogen-scaling-up-Hydrogen-Council.pdf>, 2017.
- 58 S. Pfenninger, A. Hawkes and J. Keirstead, Energy systems modeling for twenty-first century energy challenges, *Renewable Sustainable Energy Rev.*, 2014, **33**, 74–86.
- 59 A. Gambhir, J. Rogelj, G. Luderer, S. Few and T. Napp, Energy system changes in 1.5 °C, well below 2 °C and 2 °C scenarios, *Energy Strategy Reviews*, 2019, **23**, 69–80.
- 60 P. Lopion, P. Markewitz, M. Robinius and D. Stolten, A review of current challenges and trends in energy systems modeling, *Renewable Sustainable Energy Rev.*, 2018, **96**, 156–166.
- 61 International Energy Agency, *Energy Technology Perspectives 2012: Pathways to a Clean Energy System*, http://www.iea.org/publications/freepublications/publication/ETP2012_free.pdf, 2012.
- 62 European Commission, *EU Reference Scenario*, https://ec.europa.eu/energy/sites/ener/files/documents/20160713%20draft_publication_REF2016_v13.pdf, 2016.
- 63 ASEAN Centre for Energy, *The 5th ASEAN Energy Outlook 2015–2040*, <http://www.aseanenergy.org/resources/the-5th-asean-energy-outlook/>, 2017.
- 64 L. H. Balza, R. Espinasa and T. Serebrisky, *Lights on? Energy needs in Latin America and the Caribbean to 2040*, Inter-American Development Bank, 2016.
- 65 U.S. Energy Information Administration, *Annual Energy Outlook 2019*, <http://www.eia.gov/outlooks/aeo/>, 2019.
- 66 China National Renewable Energy Centre, *China Renewable Energy Outlook 2018*, <http://boostre.cnrec.org.cn/index.php/2018/11/27/china-renewable-energy-outlook-2018/?lang=en>, 2018.
- 67 Government of Japan, *Strategic Energy Plan*, http://www.meti.go.jp/english/press/2018/pdf/0703_002c.pdf, 2018.
- 68 Deep Decarbonization Pathways Project, *Pathways to deep decarbonization 2015 report*, SDSN – IDDRI, <http://>



- deepdecarbonization.org/wp-content/uploads/2016/03/DDPP_2015_REPORT.pdf, 2015.
- 69 International Renewable Energy Agency, *Global Energy Transformation*, http://www.irena.org/-/media/Files/IRENA/Agency/Publication/2018/Apr/IRENA_Report_GET_2018.pdf, 2018.
- 70 P. D. Lund, J. Lindgren, J. Mikkola and J. Salpakari, Review of energy system flexibility measures to enable high levels of variable renewable electricity, *Renewable Sustainable Energy Rev.*, 2015, **45**, 785–807.
- 71 D. Connolly, H. Lund, B. Mathiesen and M. Leahy, A review of computer tools for analysing the integration of renewable energy into various energy systems, *Appl. Energy*, 2010, **87**, 1059–1082.
- 72 M. Robinius, A. Otto, P. Heuser, L. Welder, K. Syranidis, D. S. Ryberg, T. Grube, P. Markewitz, R. Peters and D. Stolten, Linking the Power and Transport Sectors – Part 1: The Principle of Sector Coupling, *Energies*, 2017, **10**, 956.
- 73 S. Collins, J. P. Deane, K. Poncelet, E. Panos, R. C. Pietzcker, E. Delarue and B. P. Ó. Gallachóir, Integrating short term variations of the power system into integrated energy system models: A methodological review, *Renewable Sustainable Energy Rev.*, 2017, **76**, 839–856.
- 74 L. Kotzur, P. Markewitz, M. Robinius and D. Stolten, Impact of different time series aggregation methods on optimal energy system design, *Renewable Energy*, 2018, **117**, 474–487.
- 75 S. Samsatli and N. J. Samsatli, The role of renewable hydrogen and inter-seasonal storage in decarbonising heat – Comprehensive optimisation of future renewable energy value chains, *Appl. Energy*, 2019, **233–234**, 854–893.
- 76 S. Samsatli and N. J. Samsatli, A general spatio-temporal model of energy systems with a detailed account of transport and storage, *Comput. Chem. Eng.*, 2015, **80**, 155–176.
- 77 L. Kotzur, P. Markewitz, M. Robinius and D. Stolten, Time series aggregation for energy system design: Modeling seasonal storage, *Appl. Energy*, 2018, **213**, 123–135.
- 78 Fuel Cells Bulletin, ITM achieves rapid response electrolysis in P2G energy storage, *Fuel Cell. Bull.*, 2016, **2016**(1), 9.
- 79 Fuel Cells Bulletin, Hydrogenics wraps up Ontario utility-scale grid stabilization trial, *Fuel Cell. Bull.*, 2011, **2011**(7), 9.
- 80 K. Poncelet, E. Delarue, D. Six, J. Duerinck and W. D'haeseleer, Impact of the level of temporal and operational detail in energy-system planning models, *Appl. Energy*, 2016, **162**, 631–643.
- 81 S. Samsatli, I. Staffell and N. J. Samsatli, Optimal design and operation of integrated wind-hydrogen-electricity networks for decarbonising the domestic transport sector in Great Britain, *Int. J. Hydrogen Energy*, 2016, **41**, 447–475.
- 82 L. G. Ehrlich, J. Klamka and A. Wolf, The potential of decentralized power-to-heat as a flexibility option for the German electricity system: A microeconomic perspective, *Energy Policy*, 2015, **87**, 417–428.
- 83 H. Blanco, W. Nijs, J. Ruf and A. Faaij, Potential for hydrogen and Power-to-Liquid in a low-carbon EU energy system using cost optimization, *Appl. Energy*, 2018, **232**, 617–639.
- 84 J. Ikäheimo, J. Kiviluoma, R. Weiss and H. Holttinen, Power-to-ammonia in future North European 100% renewable power and heat system, *Int. J. Hydrogen Energy*, 2018, **43**, 17295–17308.
- 85 D. Henning, S. Amiri and K. Holmgren, Modelling and optimisation of electricity, steam and district heating production for a local Swedish utility, *Eur. J. Oper. Res.*, 2006, **175**(2), 1224–1247.
- 86 B. H. Bakken, H. I. Skjelbred and O. Wolfgang, eTransport: Investment planning in energy supply systems with multiple energy carriers, *Energy*, 2007, **32**(9), 1676–1689.
- 87 A. Bischi, L. Taccari, E. Martelli, E. Amaldi, G. Manzolini, P. Silva, S. Campanari and E. Macchi, A detailed MILP optimization model for combined cooling, heat and power system operation planning, *Energy*, 2014, **74**, 12–26.
- 88 S. Samsatli, N. J. Samsatli and N. Shah, BVCM: a comprehensive and flexible toolkit for whole-system biomass value chain analysis and optimisation – mathematical formulation, *Appl. Energy*, 2015, **147**, 131–160.
- 89 S. Samsatli and N. J. Samsatli, A multi-objective MILP model for the design and operation of future integrated multi-vector energy networks capturing detailed spatio-temporal dependencies, *Appl. Energy*, 2018, **220**, 893–920.
- 90 S. Samsatli and N. J. Samsatli, A general mixed integer linear programming model for the design and operation of integrated urban energy systems, *J. Cleaner Prod.*, 2018, **191**, 458–479.
- 91 A. Chapman, T. Fraser and K. Itaoka, Hydrogen import pathway comparison framework incorporating cost and social preference: Case studies from Australia to Japan, *Int. J. Energy Res.*, 2017, **41**, 2374–2391.
- 92 G. Guandalini, S. Campanari and M. C. Romano, Power-to-gas plants and gas turbines for improved wind energy dispatchability: Energy and economic assessment, *Appl. Energy*, 2015, **147**, 117–130.
- 93 D. Parra, X. Zhang, C. Bauer and M. K. Patel, An integrated techno-economic and life cycle environmental assessment of power-to-gas systems, *Appl. Energy*, 2017, **193**, 440–454.
- 94 S. J. Davis, N. S. Lewis, M. Shaner, S. Aggarwal, D. Arent, I. L. Azevedo, S. M. Benson, T. Bradley, J. Brouwer, Y.-M. Chiang, C. T. M. Clack, A. Cohen, S. Doig, J. Edmonds, *et al.*, Net-zero emissions energy systems, *Science*, 2018, **360**, 6396.
- 95 World Nuclear Association, *Nuclear Power in the World Today*, February 2019, <http://www.world-nuclear.org/information-library/current-and-future-generation/nuclear-power-in-the-world-today.aspx>, accessed 17 June 2019.
- 96 B. Nykvist and M. Nilsson, Rapidly falling costs of battery packs for electric vehicles, *Nat. Clim. Change*, 2015, **5**, 329–332.
- 97 G. Glenk and S. Reichelstein, Economics of converting renewable power to hydrogen, *Nat. Energy*, 2019, **4**, 216–222.



- 98 I. Walker, B. Madden and F. Tahir, *Hydrogen Supply Chain Evidence Base*, Element Energy Ltd, <http://www.gov.uk/government/publications/hydrogen-supply-chain-evidence-base>, 2018.
- 99 Northern Gas Networks, Equinor and Cadent, H21 North of England, <http://www.northerngasnetworks.co.uk/event/h21-launches-national/>, 2018.
- 100 S. Satyapal, *U.S. Department of Energy Hydrogen and Fuel Cell Technology Overview, FC EXPO*, 2018, http://www.energy.gov/sites/prod/files/2018/03/f49/fcto_doe_h2_fc_overview_satyapal_fc_expo_2018_0.pdf, 2018.
- 101 HyUnder, *Assessment of the Potential, the Actors and Relevant Business Cases for Large Scale and Long Term Storage of Renewable Electricity by Hydrogen Underground Storage in Europe*, <http://hyunder.eu/publications/>, 2014.
- 102 L. Welder, P. Stenzel, N. Ebersbach, P. Markewitz, M. Robinius, B. Emonts and D. Stolten, Design and evaluation of hydrogen electricity reconversion pathways in national energy systems using spatially and temporally resolved energy system optimization, *Int. J. Hydrogen Energy*, 2019, **44**, 9594–9607.
- 103 C. Azar and B. A. Sandén, The elusive quest for technology-neutral policies, *Environmental Innovation and Societal Transitions*, 2011, **1**, 135–139.
- 104 S. de Mello and H. Paulo, Cost-effectiveness as energy policy mechanisms: The paradox of technology-neutral and technology-specific policies in the short and long term, *Renewable Sustainable Energy Rev.*, 2016, **58**, 1216–1222.
- 105 S. Pfenninger, L. Hirth, I. Schlecht, E. Schmid, F. Wiese, T. Brown, C. Davis, M. Gidden, H. Heinrichs, C. Heuberger, S. Hilpert, U. Krien, C. Matke, A. Nebel, R. Morrison, B. Müller, *et al.*, Opening the black box of energy modelling: Strategies and lessons learned, *Energy Strategy Reviews*, 2018, **19**, 63–71.
- 106 International Institute for Applied Systems Analysis, *Global Energy Assessment Scenario Database*, 11 November 2013, <http://www.iiasa.ac.at/web/home/research/researchPrograms/Energy/Global-Energy-Assessment-Database.en.html>, accessed 6 September 2019.

