Final Report for the IEA/ETSAP Project

"Modelling of hydrogen"

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1 Introduction

Hydrogen is a versatile, zero-carbon energy carrier. While electrification has been considered by many as the most appropriate strategy to decarbonise many energy services, hydrogen has received increasing attention in recent years, particularly for hard-to-decarbonise sectors such as heavy-duty vehicles, parts of industry, and shipping and aviation.

A wide range of energy models have been developed that explore the potential role of hydrogen energy systems (Blanco et al., in press). As energy system models are designed to explore supply-side decarbonisation across whole economies, for a range of energy sources, many of these models have long represented at least some hydrogen technologies. Yet studies have found a wide range of contradictory projections of future hydrogen use from studies using energy system models (Quarton et al., 2020, Hanley et al., 2018).

The reasons for these variations are not clear. Hydrogen systems are complex (Figure 1) and breadth and detail are thought to vary widely between models, for production technologies and particularly for delivery and end-use technologies. Some of the more technical challenges such as the hydrogen pressure and purity requirements of some technologies are considered by few models. There was also concern that technology cost and performance assumptions might not appropriate in some models.

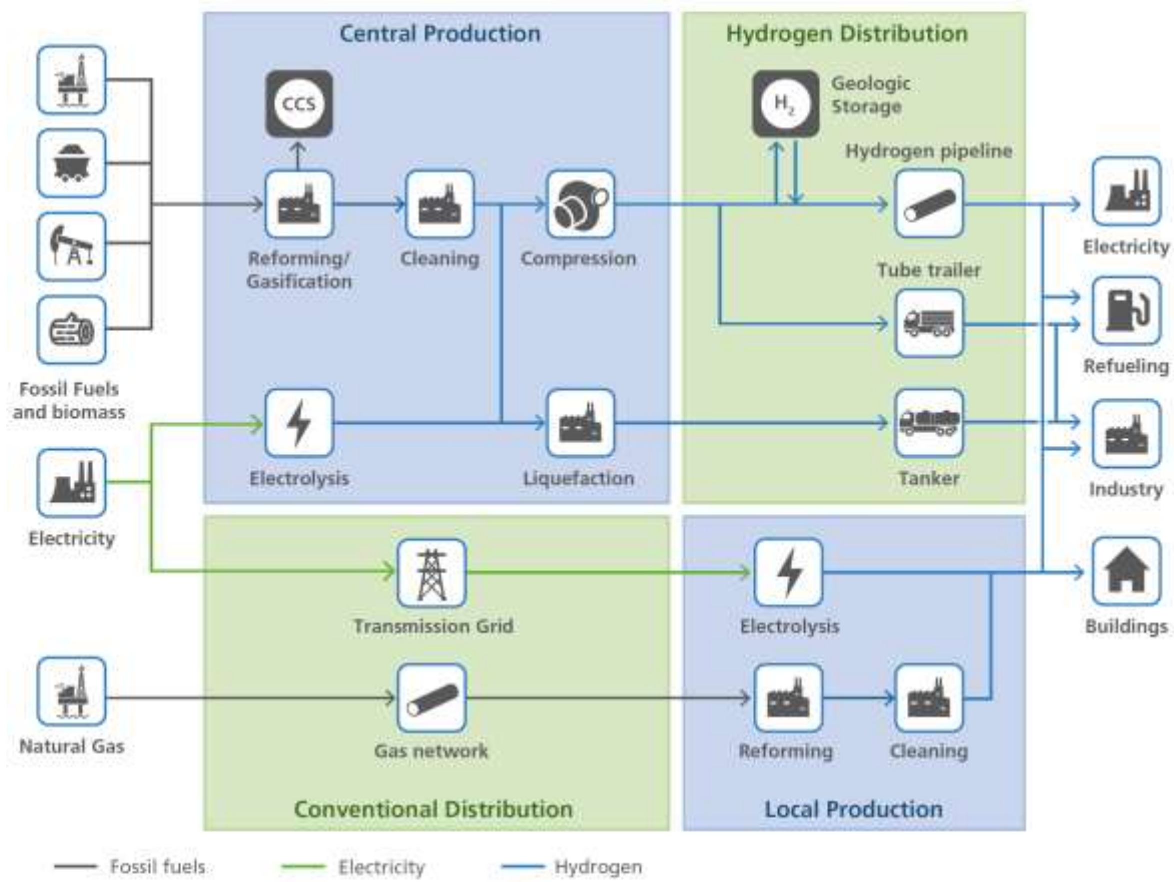

Figure 1. Schematic of a hydrogen reference energy system. From Staffell et al. (2019).

The aim of this project was to address these issues by comparing the representation of hydrogen energy systems across a range of TIMES energy system models from the IEA ETSAP community. A comparison of model outputs was also undertaken, and the insights discussed in a joint workshop with the IEA Hydrogen TCP. Finally, best-practice guidelines for representing hydrogen in energy system models were developed. This report presents these insights and guidelines.

2 Comparison of community model inputs

The comparison of model inputs focused on the technologies included in each model and the data assumptions for those technologies. It did not focus on other key aspects of the energy system identified by Dodds et al. (2015) such as spatial and temporal scales, the design of the reference energy system or user constraints affecting hydrogen (e.g. dynamic growth constraints).

2.1 Process for data collection

A call for participation was made to the ETSAP community. Eight national, one European and one global model were included in the comparison:

1. ETSAP-TIAM (Global) – Daniel Scamman, UCL
2. TIMES PanEU (EU) – Markus Blesl, IER
3. EnOp-TIMES (Belgium) – Jan Duerinck, VITO. EnOp-TIMES has a different scope to the other models as it focuses on the industrial sector rather than the whole economy.
4. TIMES_VTT (Finland) – Antti Lehttila, VTT
5. Irish TIMES (Ireland) – Shivika Mittal, UCC
6. JMRT Japan (Japan) – Hiroshi Hamasaki, Deloitte
7. TIMES-Norway (Norway) – Eva Rosenberg, IFE
8. TIMES-PT (Portugal) – Patrícia Fortes, Universidade Nova de Lisboa
9. STEM-Swiss (Switzerland) – Kannan Ramachandran, PSI
10. UK TIMES (UK) – Paul Dodds, UCL

Each team completed a worksheet, using the template in Appendix A, to document the hydrogen technologies and data assumptions. The initial model comparison was then discussed in a workshop at the ETSAP meeting in Paris in June 2019. Following that meeting, a number of additional questions were sent to each team and some data was updated. The results presented in this section were recorded at the end of this process. This means that they are relevant to the versions of these models at the end of 2019.

2.2 Hydrogen technology comparison

The comparison covered the whole hydrogen supply chain summarised in Figure 1. In this section, this is split into end uses, delivery and production.

End uses drive the use of hydrogen so are considered first. Until recently, hydrogen has been viewed primarily as a fuel for road transport and a number of fuel cell vehicles have been launched commercially in recent years. This is reflected in Table 1, in which all of the nine models that represent the transport sector include hydrogen technologies for road transport. In contrast, only three models consider hydrogen for rail transport and only one each for shipping and aviation. Table 2 examines wider energy system end-uses for hydrogen. Some of these were suggested at the workshop in Paris and so information on them was only requested when the data were revised following the workshop. As only five teams contributed a revision, there are gaps in the data. At least half of all models consider hydrogen applications for electricity generation, industrial decarbonisation and heating buildings. In contrast, few models represent direct reduced iron (DRI) for steel manufacturing or production of synthetic liquid organic fuels. One model represents hydrogen use in the dairy industry. So while most models represent a core set of hydrogen end-uses, emerging technologies are much less likely to be considered. No model has a comprehensive representation of all end-use technologies for transport or in the wider energy system.

	ETSAP-TIAM	TIMES PanEU	JMRT Japan	TIMES_VTT	STEM_CH	TIMES-Norway	UK TIMES	Irish TIMES	TIMES_PT	EnOp-TIMES	
Hydrogen use in road transport?	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	90%
Hydrogen use in rail transport?	No	No	No	No	Yes	No	Yes	No	Yes	No	30%
Hydrogen use in shipping?	No	No	No	No	No	Yes	No	No	No	No	10%
Hydrogen use in aviation?	Yes	No	No	No	No	No	No	No	No	No	10%

Table 1. Transport sector end-uses for which hydrogen technology options are represented in each model.

	ETSAP-TIAM	TIMES PanEU	JMRT Japan	TIMES_VTT	STEM_CH	TIMES-Norway	UK TIMES	Irish TIMES	TIMES_PT	EnOp-TIMES	
Non-energy industrial feedstock?	No	No	No	Yes	No	Yes	Yes	No	No	Yes	40%
Industry fuel for energy?	No	No	No	Yes	Yes	Yes	Yes	No	Yes	Yes	60%
Direct Reduced Iron (DRI)?	Yes				No	No	Yes		No		40%
Synthetic jet fuel?	No				Yes	No	No		Yes		40%
Other synthetic liquid fuels?	No				Yes	No	No		Yes		40%
Dairy industry?	No				Yes	No	No		No		20%
Building heat?	No	No	Yes	No	Yes	No	Yes	Yes	Yes	No	50%
Electricity generation?	No	Yes	Yes	Yes	Yes	No	Yes	Yes	Yes	No	70%

Table 2. End-uses outside of the transport sector for which hydrogen technology options are represented in each model.

A summary of hydrogen production and delivery options that are represented in each model is shown in Table 3. Most models represent both centralised and decentralised hydrogen production, and the infrastructure required to store and deliver hydrogen. Pressure and purity needs vary across the system, with road transport in particular requiring high-purity hydrogen at very high pressure. The costs of compressing hydrogen to the required pressure are included in almost 80% of models, but only a third consider purification costs (Table 4). A detailed breakdown of delivery technologies by model is shown in Table 5. Hydrogen delivery costs are a relatively small part of the total hydrogen cost (see Section 4.3 for further discussion of this assertion), and that is reflected in the level of detail in the models. While half of the models represent transmission pipelines and liquefied hydrogen road tankers, few consider other delivery options.

One delivery option in countries with substantial natural gas networks is to inject hydrogen into natural gas streams (Dodds and McDowall, 2013) or to repurpose existing natural gas pipes to use hydrogen (Dodds and Demoullin, 2013). Six of the models represent hydrogen injection (Table 6), with maximum injection rates ranging from 2%–15% in terms of energy content, which is around 6%–45%v/v. In practice, most hydrogen appliances are thought to be useable with 3%v/v hydrogen (1% energy content), while exceeding 20%v/v (6% energy content) would require new or altered appliances (Dodds and Demoullin, 2013).

	ETSAP-TIAM	TIMES PanEU	JMRT Japan	TIMES_VTT	STEM_CH	TIMES-Norway	UK TIMES	Irish TIMES	TIMES_PT	EnOp-TIMES	
Production plants	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes		100%
Decentralised production	Yes	Yes	No	Yes	Yes	Yes	Yes	Yes	Yes	Yes	90%
Delivery routes	Yes	No	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	80%
Storage	No	Yes	No	Yes	Yes	Yes	Yes	No	Yes	Yes	70%

Table 3. Hydrogen production and delivery system options implemented in each model.

	ETSAP-TIAM	TIMES PanEU	JMRT Japan	TIMES_VTT	STEM_CH	TIMES-Norway	UK TIMES	Irish TIMES	TIMES_PT	EnOp-TIMES	
Compression	No	No	Yes	Yes	Yes	Yes	Yes	Yes	Yes		78%
Purification	No	No	No	No	Yes	Yes	Yes	No	No		33%

Table 4. Representation of hydrogen compression and purification costs in each model.

	ETSAP-TIAM	TIMES PanEU	JMRT Japan	TIMES_VTT	STEM_CH	TIMES-Norway	UK TIMES	Irish TIMES	TIMES_PT	EnOp-TIMES	
Liquefaction	No	Yes	Yes	No	No	No	Yes	Yes	No	No	40%
Transmission pipeline HP	Yes	Yes	No	No	Yes	No	Yes	No	Yes	No	50%
Distribution pipeline HP	No	No	No	Yes	Yes	No	Yes	No	Yes	No	40%
Distribution pipeline LP	No	No	No	No	Yes	No	Yes	No	Yes	No	30%
Building pipes LP	No	No	No	No	No	No	Yes	No	No	No	10%
Road tanker	Yes	Yes	Yes	Yes	No	No	Yes	No	Yes	No	60%
Liquid H2 refuelling station	No	No	No	No	No	No	Yes	No	Yes	No	20%
Gas H2 refuelling station	No	No	No	No	No	No	Yes	No	Yes	No	20%
Gas H2 HRS onsite prod	No	No	No	No	No	No	Yes	No	No	No	10%
Gas field storage	No	No	No	No	No	No	Yes	No	No	No	10%
Salt cavern storage	No	Yes	No	No	No	No	Yes	No	Yes	No	30%

Table 5. Hydrogen delivery system technologies considered in each model.

	ETSAP-TIAM	TIMES PanEU	JMRT Japan	TIMES_VTT	STEM_CH	TIMES-Norway	UK TIMES	Irish TIMES	TIMES_PT	EnOp-TIMES	
Injection of small amounts of hydrogen into gas flows	Yes	Yes	No	Yes	Yes	No	Yes	No	Yes	No	60%
Maximum injection rate	15%	2%			4%		3%		7.2%		6%
Repurpose existing gas networks to deliver hydrogen	No	No	No	No	Yes	No	Yes	No	Yes	No	30%

Table 6. Options for using hydrogen in existing gas networks in each model.

The hydrogen production technologies represented in each model are listed in Table 7. All models consider electrolysers for hydrogen production from electricity. Most also include steam-methane reforming, both with and without carbon capture and storage (CCS). While biomass gasification is represented in seven models, only four consider biomass with CCS, despite this being potentially a key negative emissions technology in the future. Half of the models consider coal gasification but only a couple consider waste gasification, which is as yet unproven.

	ETSAP-TIAM	TIMES PanEU	JMRT Japan	TIMES_VTT	STEM_CH	TIMES-Norway	UK TIMES	Irish TIMES	TIMES_PT	EnOp-TIMES	
Biomass	Yes	Yes	No	Yes	Yes	No	Yes	Yes	Yes	No	70%
Biomass CCS	Yes	No	No	Yes	Yes	No	Yes	No	No	No	40%
Coal	Yes	Yes	No	Yes	No	No	Yes	Yes	No	No	50%
Coal CCS	Yes	Yes	No	Yes	No	No	Yes	Yes	No	No	50%
Waste	No	No	No	No	No	No	Yes	Yes	No	No	20%
Waste CCS	No	No	No	No	No	No	Yes	No	No	No	10%
Gas SMR	Yes	Yes	No	Yes	Yes	No	Yes	Yes	Yes	No	70%
Gas SMR CCS	Yes	Yes	No	Yes	Yes	No	Yes	No	Yes	No	60%
Electrolysis	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	100%

Table 7. Hydrogen production plant technologies considered in each model.

2.3 Hydrogen cost and performance data comparison

Capital cost assumptions for hydrogen production are shown in Figure 2 for the years 2020, 2030 and 2050. With the exception of biomass CCS, some models have costs at €500/kW or below for all technologies. Yet there are large cost ranges for each technology; for example, biomass gasification costs range from 400–3700 €/kW in 2020, and coal CCS from £600–3000 €/kW. Even gas SMR, which is widely used globally, has a factor of three difference between the lowest and highest capital cost assumption. Technology learning leading to reduced costs is assumed in several models. This is most apparent for biomass CCS, where costs reduce across most models, and for electrolysis, for which models assuming higher costs today project that they will reduce in the future.

Energy conversion efficiency assumptions for production technologies are shown in Figure 3. These have ranges of 5%–20% across the technologies and are assumed to increase slightly in the future through technological improvements, particularly for electrolysers.

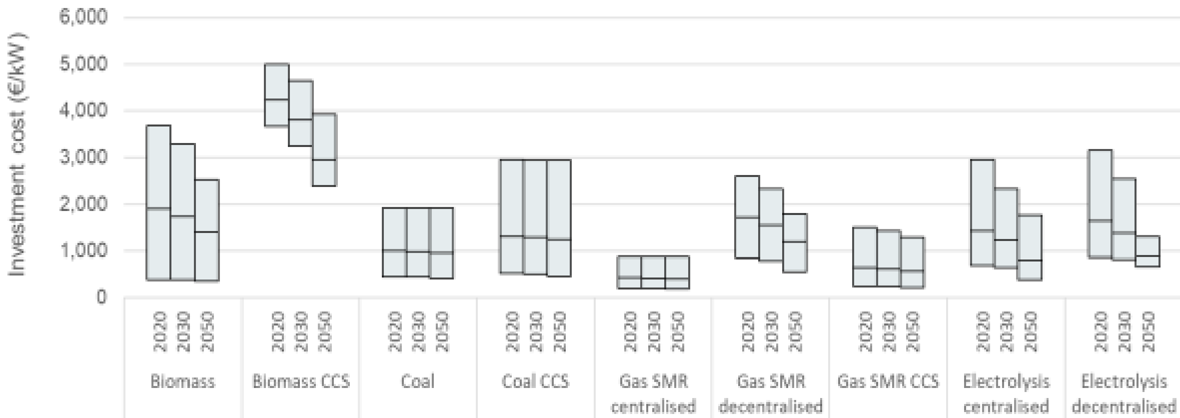

Figure 2. Comparison of hydrogen production investment cost assumptions by technology across the ten models. The model range and the mean cost are shown for the years 2020, 2030 and 2050, for real prices in the year 2018.

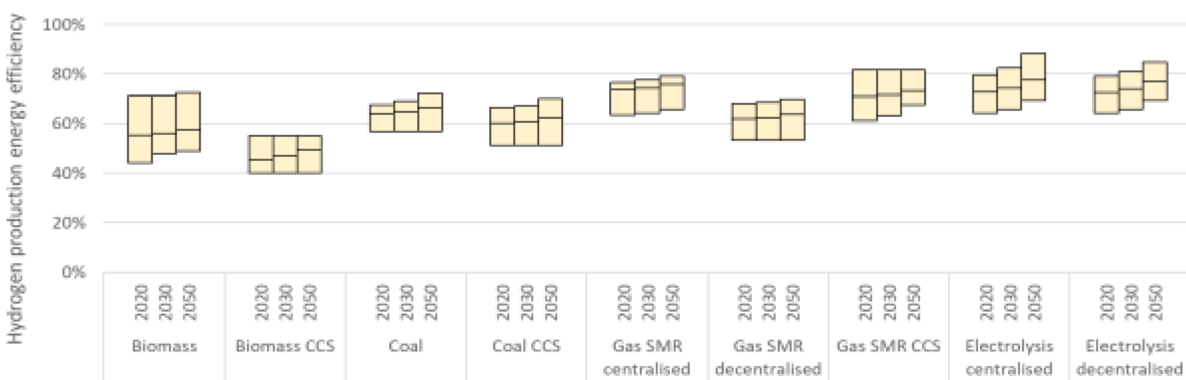

Figure 3. Comparison of hydrogen energy conversion efficiency assumptions by technology across the ten models. The model range and the mean conversion efficiency are shown for the years 2020, 2030 and 2050, for real prices in the year 2018.

Capital cost assumptions for delivery technologies are compared in Figure 4. A comparison is less meaningful than for production technologies for two reasons. First, fewer models include these technologies (Section 2.2), so only liquefaction and pipelines are considered in Figure 4. Second, pipeline costs are sensitive to the geography of supply and demand, which varies by country. Hence transmission pipeline costs range from 100–600 €/kW. As distribution pipelines are found in urban areas, they are less sensitive to geography than transmission pipelines but costs are affected by the urban population density. The cost ranges are smaller for both high-pressure (HP) and low-pressure (LP) distribution pipe networks. Liquefaction is a relatively mature technology and has high potential for cost reduction through economies of scale. Yet these are not apparent in the model data, with a wide range of costs in all three periods and only minor overall cost reductions assumed in the future.

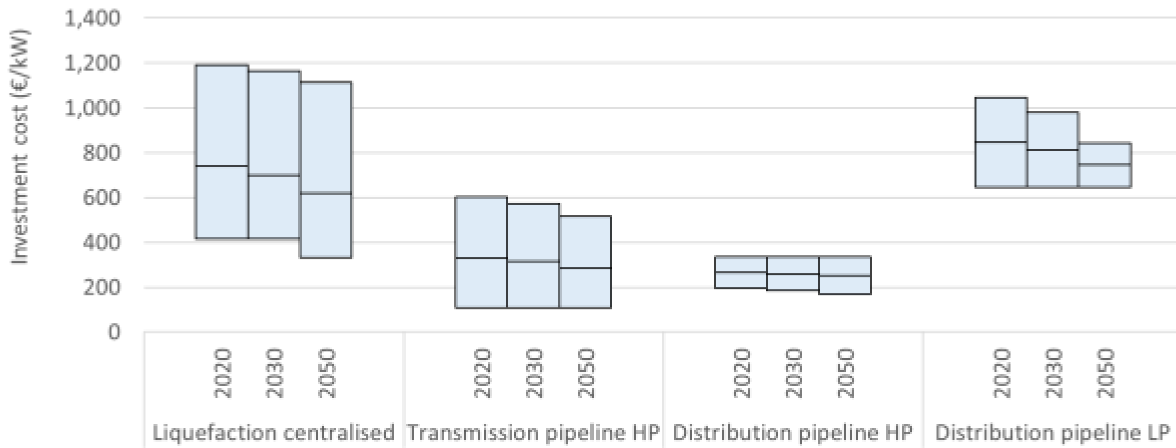

Figure 4. Comparison of hydrogen delivery infrastructure investment cost assumptions by technology across the ten models. The model range and the mean cost are shown for the years 2020, 2030 and 2050.

2.4 Discussion

Most models represent a core set of hydrogen end-uses, delivery and production technologies. However, the level of detail varies widely in the models, with most emerging technologies considered by only a few models. No model comprehensively represents all technologies.

Modelling hydrogen delivery is particularly challenging. Two broad approaches are used. The most common is for *components* of delivery routes (e.g. compression; pipelines; storage; refuelling) to be modelled separately, which enables varying capacities and changes in the choice of delivery systems over time. This is valuable for centralised hydrogen production because pipelines only become economic at high hydrogen demands, which is likely to happen later in a transition. An alternative approach, adopted for example in the JRC-EU-TIMES model, is to define *compound* technologies that include all parts of the delivery system (Sgobbi et al., 2016). The advantages of this approach are fewer technologies, which is an advantage in particular for larger models, and that the modelled delivery systems have internally-coherent costs. The disadvantages are that the number of delivery systems that can be modelled is limited, as each requires a separate technology, and there is no flexibility for parts of the delivery system to evolve over time.

There are substantial differences in investment costs and efficiencies between models. These might be at least partly a result of making different assumptions about the type and size of each technology. For example, cost disparities for liquefiers might reflect different assumptions about economies of scale, while the electrolysers category combines a number of different technologies (alkaline, proton electrolyte membrane (PEM) and solid oxide).

Only capital costs have been considered in this section. Another approach would have been to compare levelised costs, incorporating operating and fuel costs and energy conversion efficiencies. However, this is difficult for electrolysis in particular as the electricity cost varies between timeslices and the electrolyser capacity factor also varies. Gas prices can also vary substantially between regions.

It might be possible to use waste heat from hydrogen production for other purposes, for example low-temperature industrial heat or for heat networks, although improvements in technology efficiency over time would reduce the potential supply of heat. This option is not considered in any of the compared models.

Hydrogen-based energy carriers such as ammonia are not generally considered in energy system models. Yet ammonia is thought to have two potential roles in the energy system. First, it has been identified as a zero-carbon fuel for shipping, as the energy density is much higher than hydrogen. Second, several countries with low-cost solar and wind generation potential (e.g. Australia; Chile; Saudi Arabia) are considering producing cheap green hydrogen for export, but again this international trade is likely to be in the form of ammonia rather hydrogen due to the higher energy density. If countries were importing ammonia, then there would be an opportunity to power some technologies in industry, electricity generation and heavy transport using ammonia rather than hydrogen to reduce costs.

3 Comparison of community model outputs

An outcome of the workshop in Paris in June 2019 on model inputs was a need to identify key hydrogen technologies that would ideally be in all models. The suggested approach was to survey the community to understand which hydrogen technologies are deployed by models, as a more detailed representation of hydrogen technologies can be justified if it causes the model outputs to change. Each team in the project was invited to examine the uses of hydrogen in two broad scenarios:

1. "Optimal": the use of hydrogen in a typical cost-optimal decarbonisation scenario.
2. "High hydrogen": a decarbonisation scenario in which hydrogen use by 2050 is maximised. This hydrogen maximisation was typically achieved by minimum deployment and consumption constraints, but these were not prescribed in advance since each model is different. Instead, modellers were given latitude to decide how to maximise hydrogen use.

The aim was to consider how differences in inputs affect outputs. This is very difficult to assess quantitatively because each model has a different hydrogen energy system, numerous different data assumptions, and represents a different country. Also, "typical" decarbonisation varies between countries; for example, it could be an 80% reduction in emissions or a move to net zero CO_2 or net zero greenhouse gas emissions by 2050, and the target will affect the optimum level of hydrogen consumption.

Seven of the ten models also participated in a comparison of model outputs. These are listed in Table 8 and include the global ETSAP-TIAM model and six national models.

3.1 Hydrogen production and consumption in each model

Total hydrogen consumption in each model is very sensitive to population, so production per capita for each scenario is listed in Table 8. Four of the models have hydrogen production of 3.5–4.5 GJ/capita in the optimal scenario, which is substantially lower than the 8.5–12.5 GJ/capital production in the other three models. For most models, the increase in hydrogen production in the high hydrogen scenarios is a factor of 2–3 compared to the optimal scenario, except for the JMRT model. The high hydrogen scenarios have a much greater range than the optimal scenarios (7.5–37.7 GJ/capita) as a result of the

UK TIMES (37.7 GJ/capita) and the TIMES-PT (18.2 GJ/capita) having much higher production than the other models.

	Population	GJ/capita optimal	GJ/capita high hydrogen
Global ETSAP-TIAM	7600	4.1	8.2
JMRT (Japan)	126	8.5	10.1
UK TIMES	67	12.5	37.7
TIMES-Norway	5.4	3.5	11.4
STEM (Switzerland)	8.6	4.5	7.5
Irish TIMES	4.9	4.3	8.0
TIMES-PT (Portugal)	10	10.7	18.2

Table 8. Hydrogen production per capita in 2050 in the optimal and high hydrogen scenarios. Units: GJ/capita.

The rate of deployment of hydrogen industries in each model is compared in Figure 5 for the optimal scenario. Only two models have any demand in 2020. In 2030, demand does not exceed 25% of the 2050 demand in any model. By 2040, however, there is much divergence between models, with production ranging from 15% to 70% of the production in 2050; it is arguable whether the increase in production between 2040 and 2050 in some models is so high as to be technically infeasible.

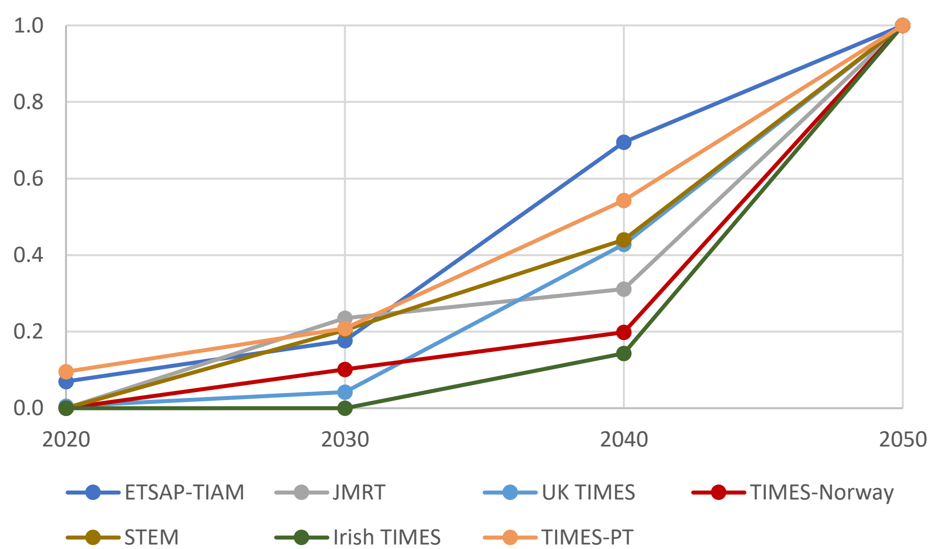

Figure 5. Normalised total hydrogen production in the optimal scenario, where production in 2050 for each model = 1.0.

The technologies used to produce hydrogen in each model in the optimal scenario are listed in Table 9. There are substantial differences across the models. Five models have production dominated by a single technology, of which four have different types of electrolysers and the other has steam-methane reforming. The other two models have production split across 4–5 technologies, with no single technology contributing more than 50% of total production. The proportion of hydrogen produced from electrolysis in each model over the period to 2050 is shown in Figure 6. Electrolysis dominates in three models by 2040. Only the UK TIMES model has no electrolysis by 2050. In the high hydrogen scenario, the options used are the same in each model, with the exception of UK TIMES which adds decentralised electrolysis to the portfolio. Even the proportions of each technology in each model are similar.

	ETSAP-TIAM	JMRT	UK TIMES	TIMES-Norway	STEM	Irish TIMES	TIMES-PT
Biomass	10%				0%		
Biomass CCS					29%		
Coal	14%						
Waste CCS			1%				
Gas SMR	46%				0%		
Gas SMR CCS			99%		24%		
Decentralised electrolysis						100%	3%
Centralised electrolysis	30%				47%		
Alkaline electrolyser		82%					1%
PEM electrolyser				100%			96%
Hydrogen from oil refineries		6%					
Hydrogen from iron and steel		12%					
Number of options used	**4**	**3**	**2**	**1**	**5**	**1**	**3**

Table 9. Fraction of hydrogen production by technology for the optimal scenario in 2050 as optimised by each model.

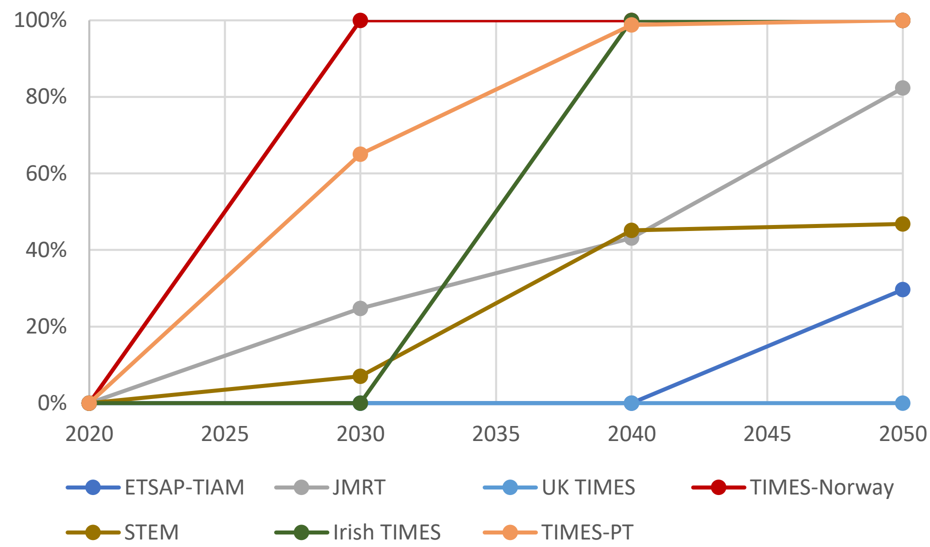

Figure 6. Fraction of hydrogen production from electrolysers in the optimal scenario in each model.

The proportion of hydrogen consumption in each sector in the optimal scenario is shown for each model in Table 10. Transport is the only sector with hydrogen consumption in all seven models. It accounts for almost half of consumption (45%) across the models. The industry sector also has substantial hydrogen use (29%), though only in five models, while remaining consumption is split across the other sectors. The JMRT model of Japan is the only one with substantial hydrogen consumption in buildings. Four models use hydrogen in three or fewer sectors in the optimal scenario; in contrast, UK TIMES uses hydrogen in six scenarios. The only model that uses hydrogen in additional sectors in the high hydrogen scenario is TIMES-PT, which extends consumption to buildings (residential and service).

It is useful to examine three sectors in more detail. Table 11 shows that heavy-duty vehicle (HDV) is the only transport sub-sector to have consumption across several models. Yet the two models without hydrogen use in HDVs, JMRT and UK TIMES, have the highest and third highest hydrogen production per capita overall (Table 8). Use of hydrogen in other sub-sectors varies across the models, with only bikes having no hydrogen consumption in 2050 in any model. Only two models have a role for hydrogen in cars, and only one each for trains, shipping and aviation. With the exception of STEM, each model has a dominant sub-sector that accounts for at least 75% of total hydrogen production for transport, but this dominant sub-sector tends to vary between models. It is surprising that there is so much variation between models within the sector. In the high scenario, consumption patterns are similar except for UK TIMES using hydrogen in light transport (cars, bikes, LDVs), and two models using hydrogen for shipping.

The use of hydrogen in industry has a quite different pattern (Table 12). The UK TIMES and TIMES-PT models use hydrogen across seven industrial sub-sectors. In contrast, the other models use hydrogen in two or fewer sub-sectors. It is possible that potential hydrogen use in many sub-sectors in those models is not represented in those models, and this assumption that it is not technically feasible then restricts cost-optimal hydrogen use in industry. There are very few changes in consumption patterns across the models in the high hydrogen scenario compared to the optimal scenario.

Two models use hydrogen in the process sector. These are for synthetic fuel production, which is not represented in many models, and in oil refineries, which in many models might be implicit as many refineries produce and consume hydrogen internally at present.

	ETSAP-TIAM	JMRT	UK TIMES	TIMES-Norway	STEM	Irish TIMES	TIMES-PT	Average
Agriculture			1%					
Services		55%	12%		3%		1%	10%
Industry	39%		65%	52%	6%		38%	29%
Residential		39%	4%					6%
Transport	61%	6%	2%	48%	52%	100%	44%	45%
Process					11%		17%	4%
Electricity			16%		27%			6%

Table 10. Fraction of hydrogen consumption in each sector for the optimal scenario in 2050 as optimised by each model. The STEM column does not sum to 100% due to rounding.

	ETSAP-TIAM	JMRT	UK TIMES	TIMES-Norway	STEM	Irish TIMES	TIMES-PT	Average
Car		100%			50%			21%
2-wheel and 3-wheel bikes								0%
Light-duty vehicle					8%			1%
Heavy-duty vehicle	4%			100%	38%	100%	4%	35%
Bus			15%		4%		96%	16%
Train			76%					11%
Shipping			10%					1%
Aviation	96%							14%

Table 11. Fraction of hydrogen consumption in the transport sector for the optimal scenario in 2050 as optimised by each model. The UK TIMES column does not sum to 100% due to rounding.

	ETSAP-TIAM	JMRT	UK TIMES	TIMES-Norway	STEM	Irish TIMES	TIMES-PT	Average
Iron and steel			8%	19%			3%	7%
Non-ferrous metals			1%				0%	0%
Cement								
Non-metallic minerals			25%				38%	16%
Chemicals			5%	81%	Not known		21%	27%
Paper			3%				4%	2%
Food and drink			18%	2.2			33%	13%
H2:CH4 blend	100%							25%
Other			40%				2%	11%

Table 12. Fraction of hydrogen consumption in the industry sector for the optimal scenario in 2050 as optimised by each model. The sub-sectoral breakdown is not known for the STEM model.

3.2 Discussion

Two of the models, UK TIMES and TIMES-PT, identify much greater roles for hydrogen than the others. Hydrogen is used more widely across the transport and particularly the industry sectors, but also in the other sectors, and overall production per capita is much higher. The only model that has a comparable production per capita is the JMRT model, which primarily uses hydrogen to decarbonise building heat. Section 2.2 noted that options for hydrogen end-uses are limited in many models outside the transport sector. The breadth of industrial opportunities for hydrogen in the UK TIMES and TIMES-PT models in Table 12 suggests that options for use across industry should ideally be represented. The use of hydrogen across a range of transport modes in Table 11 similarly shows the importance of representing hydrogen decarbonisation options across the whole transport sector. Novel technologies such as direct reduced iron (DRI) for steel production and synthetic jet fuel production from hydrogen could become important in deep decarbonisation pathways and should also be considered.

A wide range of production technologies are used in the scenarios, which suggests that each model should represent a wide range of technologies beyond electrolysers and natural gas SMR. While models of OECD countries tend to focus on CCS technologies for carbonaceous fuels, the use of unabated fossil fuels to produce hydrogen in the TIAM-UCL model show that these could still have a role in some countries, particularly those that are less developed or do not have suitable sequestration storage options for CO_2.

4 Guidelines for representing hydrogen in energy system models

This section presents best-practice guidelines for representing hydrogen supply chains in energy system models. It specifically considers improvements to the ETSAP-TIAM model. It focuses primarily on the *structure* of the reference energy system for hydrogen. A longer-term aim beyond this report is to improve the quality of parameter data through the collaboration with IEA Hydrogen, and so this is just touched upon here.

The level of detail that is implemented should reflect the geographical coverage of the model. National models can be much more detailed than global (multi-region) models as they are smaller and can consider local opportunities that might not be available in many countries (e.g. existing gas pipelines that can be repurposed for hydrogen; geology for underground hydrogen and CO_2 storage). An example of a detailed reference energy system for hydrogen is shown in Appendix B, but a simplified version of that system would likely be more appropriate for many models.

While a linear supply chain model might be considered, with centralised production feeding national then local distribution networks, in reality there could be a series of flows in both directions as shown in Figure 7. There are a number of options for hydrogen delivery infrastructure and these can be complex to implement, yet are likely to have a relatively small impact on overall costs compared to the costs of production and end-use technologies. Our advice is therefore to start with demand-side options, then production technologies, and finally to choose an appropriate approach to delivery costs.

While hydrogen is the focus of this report, it has become clear that ammonia produced from low-carbon hydrogen is more likely to be traded internationally and used as a shipping fuel, and could also be used elsewhere in the system. For these reasons, models of countries with seaports would ideally consider ammonia-fuelled technologies as well as hydrogen-fuelled technologies.

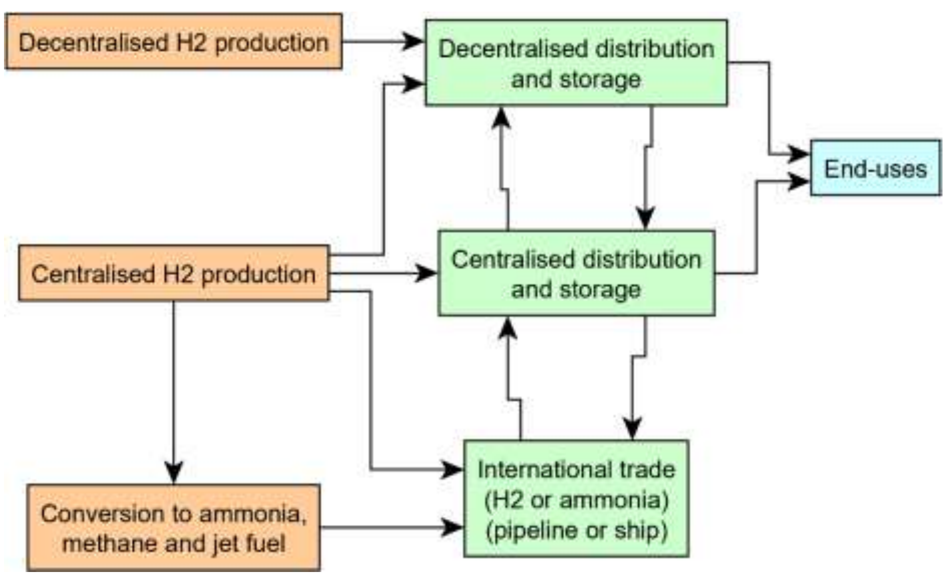

Figure 7. Simplified schematic of the implementation of hydrogen technology options in an energy system model.

4.1 Hydrogen end-uses

The potential for hydrogen to power end-use technologies, and the costs and implications, are not well understood across the community. There are many potential applications for hydrogen energy. Within the transport sector:

- Road: all types of light- and heavy-duty vehicles can use fuel cells and should be represented. Several companies have developed hydrogen internal combustion engines but it is uncertain whether these have a long-term future or will be stopgap technologies. Hybrid and plug-in hybrid fuel cell technologies should be considered.
- Rail: hydrogen offers an alternative to diesel, and also a hybrid option for trains on lines that are only partially electrified.
- Shipping: hydrogen could replace fuel oil in smaller boats, and ammonia or methanol used by international shipping. Power-to-liquids technologies could be important in the future.
- Air: hydrogen and ammonia could power jet engines in new aircraft, and hydrogen could also be used to produce synthetic aviation fuel (SAF) for existing aircraft.

Hydrogen is already widely used as an industrial feedstock, for example for ammonia production, and could be used to produce a wide range of synthetic fuels and high-value chemicals in the future with captured CO_2 (carbon capture and utilisation, or CCU) via the Fischer-Tropsch process. The possibilities and costs of these processes are not well understood. Hydrogen offers an option to decarbonise challenging demands such as high-temperature processes and iron reduction, but could more generally be used to replace most heat demands currently met by natural gas. New end-use technologies would be required. Modellers are recommended to consider potential uses across all industrial subsectors in a similar way to the UK TIMES and TIMES-PT models.

While renewables are expected to have a prominent role in future, there will be a need for low capital cost technologies providing peak electricity generation, and studies with the UK TIMES and ESME models have suggested that hydrogen turbines are likely to be the cheapest low-carbon option. Electricity generation using fuel cells would also be possible, particularly in areas with low demand that could take advantage of the scalability of fuel cells.

Countries with mature gas networks providing gas for heating (e.g. Japan; Germany) might be able to repurpose those networks to use hydrogen instead of natural gas. In the short-term, hydrogen injection could partially decarbonise the gas supply and could also provide a cheap option to use excess renewable generation. Both should be considered in models where appropriate.

Cost and performance data for end-use technologies are challenging to obtain as there are wide variations both within and particularly between countries. These variations reflect differences in societal trends and consumption patterns (e.g. cars are generally larger in the USA than Europe). As a rule of thumb, hydrogen combustion technology costs and performance should be similar to the equivalent natural gas technologies for buildings, industry and electricity generation. The future costs of fuel cell vehicles and non-road transport are more difficult to estimate. Costs should be derived using a consistent method for all comparable end-use technologies (e.g. various types of cars) to enable a coherent cost comparison within the model.

4.2 Hydrogen production

Based on the comparison of community model outputs, Section 3.2 argues that a range of production technologies should be included in the models. The minimum recommended set of technologies are:

- Electrolysers. Alkaline electrolysers operate at high capacity factors and low capital costs. PEM electrolysers offer highly-flexible operation to use excess renewable generation. Solid-oxide electrolysers have high efficiency and low electricity consumption. TIMES enables detailed modelling of electrolysers, for example by including the cost of replacement of the stack.
- Steam-methane reforming (SMR) with CCS. This could use both natural gas and biomethane. Non-CCS plants could be included for near-term deployment.
- Biomass gasification. Including CCS and non-CCS versions.

Modellers should also consider including coal, oil, bio-oil and waste plants, with and without CCS as appropriate. Emerging technologies such as the Kvaerner process and biological hydrogen production are difficult to represent as the long-term costs are not well understood.

Section 2.3 showed that cost and performance assumptions for hydrogen production technologies vary widely between models. Some cost and performance data ranges for production technologies are shown in Table 13 from a synthesis recently performed by the UK Government. Hydrogen production and electricity generation costs should have a consistent methodology to ensure the model is balanced.

		CAPEX (€/kW)			Fixed O&M (€/kW)			Efficiency			Elc
		2020	2030	2050	2020	2030	2050	2020	2030	2050	2050
Alkaline electrolyser	Low	796	539	468	33	32	31	66%	70%	74%	100%
	Central	938	732	670	34	33	32	77%	80%	82%	100%
	High	1288	1064	959	40	37	35	80%	83%	84%	100%
PEM electrolyser	Low	1041	473	366	35	34	33	62%	71%	76%	100%
	Central	1265	613	500	40	36	35	72%	79%	82%	100%
	High	2060	1327	979	47	40	38	81%	84%	87%	100%
Solid oxide electrolyser	Low	1475	746	575	57	53	52	70%	74%	77%	73%
	Central	1961	1127	751	60	56	54	74%	79%	86%	76%
	High	2820	1864	1418	61	58	57	87%	93%	96%	83%
SMR+CCS	Central	845	744	577	31	31	31	74%	74%	74%	0%
ATR+CCS	Central	992	894	677	29	29	29	80%	80%	80%	5%
ATR+GHR+CCS	Central	953	831	611	29	29	29	86%	86%	86%	4%
BECCS	Central	2845	2648	1196	109	102	46	65%	66%	69%	0%

Table 13. Cost and production data ranges for hydrogen production technologies. "CAPEX" is the capital expenditure (NCAP_COST). "Fixed O&M" are fixed operations and maintenance costs (NCAP_FOM). Real prices in the year 2018 are used. "Efficiency" is the overall energy conversion efficiency at the higher heating value (HHV) (ACT_EFF). "Elc" is the fraction of electricity in the energy inputs. "PEM" is proton exchange membrane. "SMR" is steam-methane reformer. "ATR" is autothermal reformer. "GHR" is gas-heated reformer. "BECCS" is biomass gasification with CCS. Source: adapted from BEIS (2021).

When comparing cost and performance data, it is important to understand whether energy is specified in terms of higher or lower heating value (HHV or LHV). Data in the literature has a range of approaches.

The level of production process detail should reflect the model temporal resolution. The value of flexible PEM electrolyser operation for integrating renewables will not be resolved by a model with low temporal resolution, so either a parameterisation of excess generation will be required (e.g. assuming a proportion of renewable output is excess generation that can only be captured by PEM electrolysers) or there will be little benefit from separately modelling alkaline and PEM electrolysers. Even a parameterisation is challenging as excess generation varies and increasing the capacity of PEM electrolysers to capture the excess will decrease the capacity factor of all deployed electrolysers. Another temporal resolution issue is that some technologies, such as some SMRs, have much reduced energy conversion efficiencies at part loads. Part-load efficiencies can be represented in TIMES models but the operation of such plants will only be represented accurately at high temporal resolution.

4.3 Hydrogen delivery systems

Delivery system data is challenging to find as costs are strongly influenced by topography (Schoots et al., 2010, van der Zwaan et al., 2011). This means that costs for one country might not be appropriate elsewhere.

The relative costs of delivery systems depend on both the geography and scale of demand (Yang and Ogden, 2007), and will change during a transition. For example, pipelines are the most cost-effective method of transporting large quantities of hydrogen, particularly over shorter distances, but require a substantial up-front investment and will have very high costs per unit energy in the early stages of a transition. For this reason, other delivery systems would likely be used early in a transition unless a substantial demand were created in a short space of time, for example by converting a large industrial cluster to use hydrogen. This issue could be circumvented by representing large pipeline systems using lumpy investments or small regions in a model, but such an approach would ideally be informed by an appraisal of how pipelines might develop during a transition (e.g. Moreno-Benito et al., 2017).

The relative importance and variability of infrastructure costs should be considered when deciding on the level of modelled detail for delivery infrastructure. Figure 8 shows that the cost of delivery infrastructure for fuel cell cars in a UK scenario was only around 10% of the total fuel cost, and the overall cost was anyway dominated by the capital and O&M costs of the car rather than the fuel used to power it. Expending substantial effort to model infrastructural systems for the transport sector would be difficult to justify in this case. Note, however, that fuel and infrastructural costs are likely to be substantially more important for stationary hydrogen technologies such as industry and heating, where end-use technologies are less costly.

Section 2.4 notes that two broad approaches are used to represent delivery systems: (i) representing separate *components* of delivery routes (e.g. compression; pipelines; storage; refuelling); or, (ii) defining *compound* technologies that include all parts of the delivery system. Both have advantages and disadvantages for model flexibility and accuracy. The choice of approach should reflect the model design.

It would be appropriate for models to include transmission pipelines, liquefaction and road tanker delivery, and possibly tube trailers. Injection of hydrogen into existing gas streams and repurposing of existing gas networks to deliver hydrogen would ideally be included where this is technically feasible.

Hydrogen pressure and purity are likely to vary throughout a delivery system and compression and purification costs could be substantial at some locations (e.g. refuelling stations), so should be taken into account. The infrastructure costs should be comparable to alternative non-hydrogen technologies; for example, capital costs for battery vehicle on-street and refuelling station chargers should be included if hydrogen refuelling station costs are included. International shipping of "green" renewable-derived ammonia, which can be cracked to hydrogen, is receiving increased attention. Models would ideally represent maritime imports of ammonia, where feasible, and the use of ammonia as a shipping fuel.

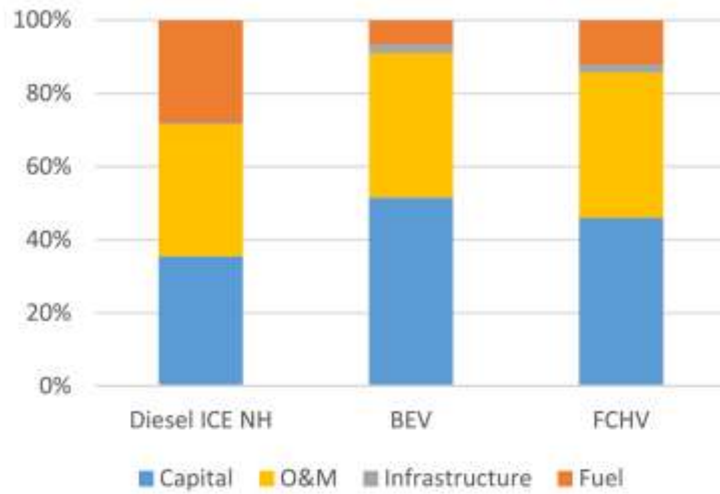

Figure 8. Breakdown of the total cost of ownership of ICE, battery and fuel cell cars using cost assumptions for the year 2050. "Capital" and "O&M" refer to the vehicle costs. "Fuel" is the cost of the fuel, excluding taxes, and "Infrastructure" is the delivery infrastructure used to deliver the fuel from the manufacturing/generating plant to the car. From: Dodds and Ekins (2014).

4.4 ETSAP-TIAM model improvement

The representation of hydrogen energy systems in the ETSAP-TIAM global energy system model was reviewed as part of this project with the aim of recommending future model improvements. ETSAP-TIAM was first released by IEA ETSAP to Contracting Parties in 2008. Several ETSAP members have created their own model version from the original model and have changed the model regions and resource and technology assumptions, including for hydrogen. These versions have not been made available to the wider ETSAP community. However, a new version of ETSAP-TIAM has been developed by an ETSAP-funded research project. The model design has been improved, and the base year updated from 2005 to 2018. The hydrogen RES was updated in this project, but there are opportunities for further improvements in the modelling of hydrogen.

The principal weakness of ETSAP-TIAM is the lack of end-use options for hydrogen. Hydrogen use is restricted to road and air transport, some parts of industry, and injection into gas streams. There is an opportunity to greatly extend the potential options across the transport and industry sectors, to electricity generation (turbines, fuel cells and even engines), power-to-liquids, and to heating buildings where this is a credible option.

Use of ammonia in shipping and trade of ammonia produced from green hydrogen has received much attention recently. Another priority for ETSAP-TIAM is to represent hydrogen trade by pipeline, where feasible, long-distance ammonia and hydrogen maritime trade, and potential uses of ammonia across the energy system.

Hydrogen delivery infrastructure is very limited in ETSAP-TIAM and could be improved to account for pressure and purity variations across the system. Hydrogen storage needs and opportunities are not considered at present. As timeslicing has been changed in ETSAP-TIAM to represent each of the four seasons separately, there is an opportunity to represent interseasonal hydrogen storage.

ETSAP-TIAM does have a range of hydrogen production technologies. The cost and performance data of these should be reviewed. A wider range of electrolysers could be included, for example high-temperature solid oxide electrolysers that have substantially lower electricity consumption.

5 Conclusions

There are many potential applications for hydrogen energy. The aim of this project was to identify best practice for representing hydrogen in energy system models. First, the representation of hydrogen energy systems in a range of TIMES energy system models from the IEA ETSAP community was compared. Next, a comparison of model outputs was undertaken. Finally, best-practice guidelines for representing hydrogen in energy system models were developed and presented in this report.

The level of modelling detail for hydrogen technologies varies widely between models. Most models contain a basic set of technologies (electrolysis; hydrogen for road transport). A few models represent a much wider range of hydrogen end-uses, both in the transport sector and across the wider energy system. These models tend to have higher hydrogen consumption in 2050 in low-carbon scenarios as some of these technologies are cost-competitive. If they are not represented in a model, the modeller is effectively making an assumption that they are not technically-feasible or not economically-viable. There is a need for modellers to review the breadth of end-use technologies represented in their models.

The outputs comparison suggests that models should represent a wide range of production technologies beyond electrolysers and natural gas SMR. Some technologies could usefully be further disaggregated in some models (e.g. PEM, alkaline and solid-oxide electrolysers), but this should take into consideration limitations arising from low temporal resolution. Work is still required to characterise key cost and performance data, hopefully in conjunction with IEA Hydrogen.

There is not a straightforward method to represent hydrogen delivery system infrastructure and there is much diversity between the models. Ammonia is emerging as a hydrogen-based energy vector that is likely to be particularly important for international trade, but is not generally considered by existing models and should be considered for future inclusion.

A comprehensive reference energy system for hydrogen is proposed in Appendix B. A lower level of detail is likely to be appropriate for most models, but this diagram is nevertheless useful to understand options and technical requirements across the energy system. Modellers can create coherent reference energy systems from this diagram that are appropriate for the regions that they are modelling.

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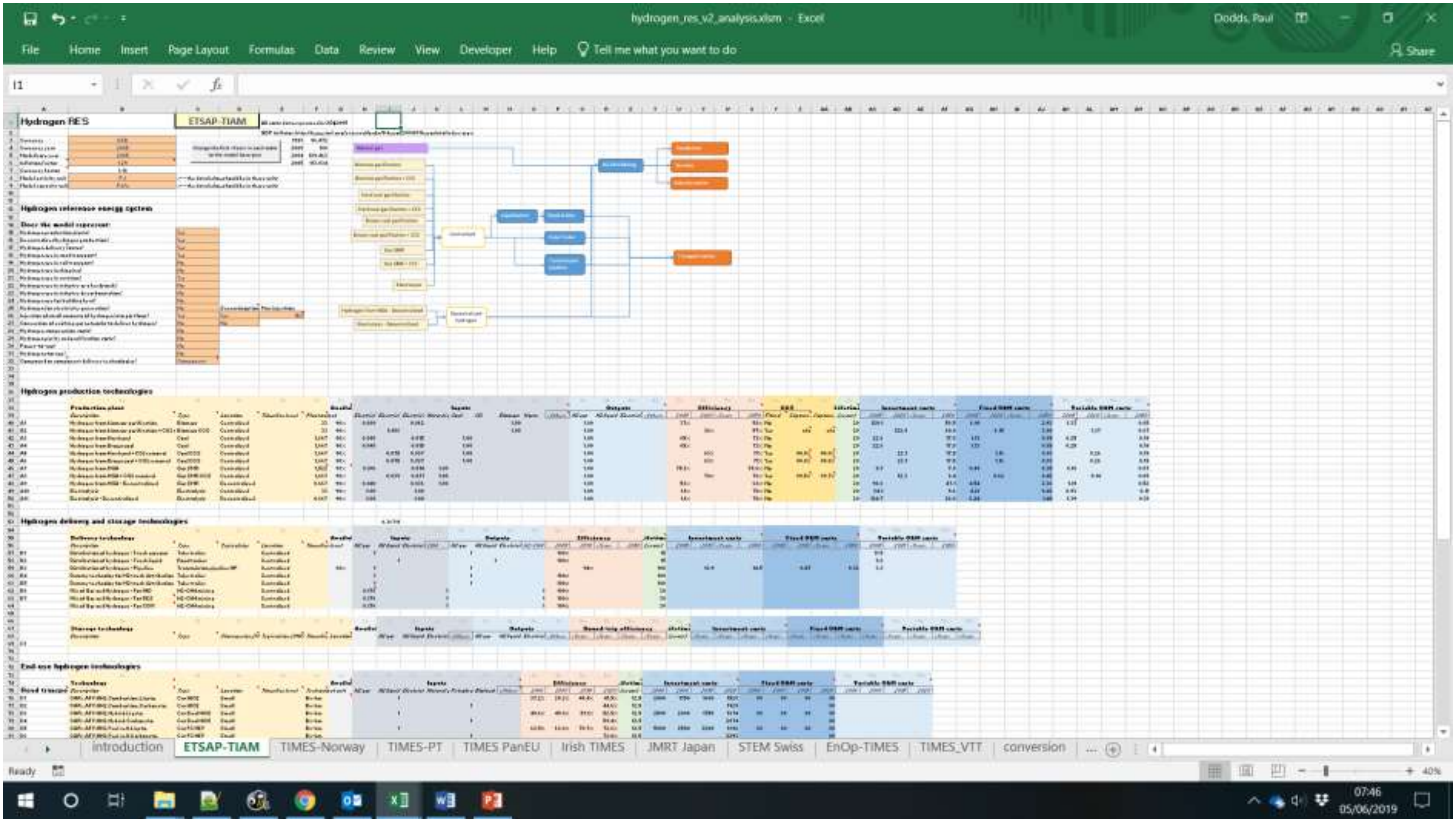
Appendix A: Example data collection input template

This image is available in a separate PDF on the ETSAP website.



Appendix B: Detailed hydrogen reference energy system example

This diagram is available in a high-resolution PDF on the ETSAP website.