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How to incentivise hydrogen energy technologies for net zero: Whole-system value chain optimisation of policy scenarios

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Abstract

Policy intervention is essential for enabling energy decarbonisation, and historic examples such as wind and solar power show how well-designed policy can lead to long term system benefits. Hydrogen technologies are emerging technologies that, with sufficient policy support, can also become established and provide valuable energy services. In this study, the policies available for supporting emerging energy technologies and encouraging system decarbonisation are analysed, and their relevance to hydrogen technologies is considered. Value chain optimisation is used to assess the effectiveness of these policies in a system undergoing transition to net-zero emissions. The optimisation results show that both carbon budgets and carbon taxation approaches can be effective in achieving net-zero emissions, but that the details of the policy design can significantly influence overall costs and emissions. The results also show that in a net-zero energy system, hydrogen technologies have a role in industry without needing specific policy support, but policy intervention is needed for hydrogen to become established in other sectors (such as domestic and commercial heating). Both feed-in tariffs and obligations for hydrogen injection were found to be effective at increasing hydrogen uptake, although with an increase in overall system cost of £11–14 for each additional MWh of hydrogen in the system. This study shows the benefits of using value chain optimisation to analyse energy policies and technologies. It also emphasises the importance of careful policy design in order to achieve the best overall system outcomes.

Keywords: Hydrogen; Energy policy; Net zero; Integrated multi-vector energy networks; Value chain optimisation; Value Web Model

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Nomenclature

Abbreviations

AIMMS	Advanced Interactive Multidimensional Modeling System
BEIS	Department for Business, Energy and Industrial Strategy (UK Government)
CCGT	Combined Cycle Gas Turbine
CCS	CO ₂ Capture and Storage
CfD	Contracts for Difference
CHP	Combined Heat and Power
CO ₂	Carbon Dioxide
COP	Coefficient of Performance
CPF	Carbon Price Floor
ETS	Emissions Trading System
FIT	Feed in Tariff
GB	Great Britain
GHG	Greenhouse Gas
H ₂	Hydrogen
HP	High Pressure
ICE	Internal Combustion Engine
IEA	International Energy Agency
LCFS	Low Carbon Fuel Standard
LP	Low Pressure
OCGT	Open Cycle Gas Turbine
RHI	Renewable Heat Incentive
RO	Renewables Obligation
RPS	Renewable Portfolio Standard
RTFO	Renewable Transport Fuel Obligation
SMR	Steam Methane Reforming
tCO ₂	Tonnes of Carbon Dioxide
UoR	Unit of Resource
VWM	Value Web Model

*Mathematical notation*¹

Indices and sets

$b \in \mathbb{B}$	Transport infrastructures
$c \in \mathbb{C} \subset \mathbb{R}$	Biomass resources (“crops”)
$d \in \mathbb{D}$	Daily interval types (e.g. weekday, weekend)

¹This section covers the new equations and constraints presented in this article. The complete mathematical formulation of the model, and the nomenclature, can be found in a previous paper by Samsatli and Samsatli [1] and also in the supplementary material for this paper.

$i \in \mathbb{I}$	System impacts (e.g. costs, CO ₂ emissions)
$h \in \mathbb{H}$	Hourly (sub-day) intervals
$l \in \mathbb{L}$	Linepack technologies
$m \in \mathbb{M}$	Transport technologies
$p \in \mathbb{P}$	Conversion technologies
$\mathbb{P}^C \subseteq \mathbb{P}$	Commercial/industrial conversion technologies
$\mathbb{P}^D \subseteq \mathbb{P}$	Domestic conversion technologies
$\mathbb{P}^{\text{inj}} \subseteq \mathbb{P}$	Conversion technologies that represent hydrogen injection into the gas grid (either partial or complete conversion)
$\mathbb{P}^H \subseteq \mathbb{P}$	Conversion technologies that produce hydrogen
$r \in \mathbb{R}$	Resources
$s \in \mathbb{S}$	Storage technologies
$sl \in \mathbb{SL}$	Solar PV installation types (e.g. solar farm and rooftop)
$t \in \mathbb{T}$	Seasonal time intervals
$w \in \mathbb{W}$	Wind turbine type (e.g. onshore and offshore)
$y \in \mathbb{Y}$	Long term planning time intervals (e.g. decadal)
$z \in \mathbb{Z}$	Spatial zones

Parameters

$B_y^{\text{CO}_2}$	Annual CO ₂ budget during planning period y [MtCO ₂ /yr]
c_{city}^{Bio}	System impact of producing a unit of biomass crop c in season t of planning period y [£/t or tCO ₂ /t] (impacts of planting, cultivating and harvesting the crop)
c_{rhdty}^M	System impact of importing a unit of resource r during hour h , day type d , season t and planning period y [£/MWh or tCO ₂ /MWh]
c_{rhdty}^U	System impact of producing a unit of resource r during hour h , day type d , season t and planning period y (e.g. domestic natural gas production) [£/MWh or tCO ₂ /MWh]
c_{rhdty}^X	System impact of exporting a unit of resource r during hour h , day type d , season t and planning period y [£/MWh or tCO ₂ /MWh]
C_{*iy}	System impact of the capital investment in a technology in planning period y [£ or tCO ₂]. $*$ represents transport infrastructures b , linepack technologies l , conversion technologies p , storage technologies s , solar PV installations sl or wind turbines w
$d_{zz'}$	Distance between the centres of spatial zones z and z' [km]
D_{iy}^{OM}	Factor for discounting operating (annual) impacts i incurred in planning period y back to the beginning of the time horizon
D_{*iy}^C	Factor for discounting capital investments made in planning period y back to the beginning of the time horizon (i.e. the start of the first planning period). $*$ represents transport infrastructures b , linepack technologies l , conversion technologies p , storage technologies s , solar PV installations sl or wind turbines w
H_y^{min}	Minimum allowable annual level of hydrogen injection into the gas grid in planning period y [MWh/yr]
n_h^{hd}	Duration of sub-day interval h [h]
n_d^{dw}	Number of occurrences of day type d in a week (e.g. 5 for a weekday, 2 for a weekend)

n_t^{wt}	Number of repeated weeks in season t
n_y^{yy}	Number of repeated years in planning period y
N_{slzy}^{ES}	Number of pre-existing solar PV installations of type sl in zone z in planning period y (accounts for estimated retirement dates)
N_{wzy}^{EW}	Number of pre-existing wind turbines of type w in zone z in planning period y (accounts for estimated retirement dates)
$V_y^{\text{CO}_2}$	Taxation rate (cost impact) for one tonne of CO_2 emissions during planning period y [$\text{£}/\text{tCO}_2$]
V_y^{FIT}	Feed-in tariff payment (cost impact) for one MWh of hydrogen injected into the gas grid during planning period y [$\text{£}/\text{MWh}$]
$\alpha_{\text{H}_2,py}$	Conversion factor of hydrogen ($r = \text{H}_2$) by technology p in planning period y
β_b	Directionality parameter for transport infrastructures b : = -1 if one-way unidirectional (can only be built and operated in one direction); = 0 if two-way unidirectional (unidirectional infrastructure but can be built in both directions); = 1 if bidirectional (only one infrastructure needed that can be operated in either direction)
β_{piz}	Factor representing variations in the impact i of production technology p in spatial zone z
κ_{piy}	Factor representing variations in the impact i of production technology p in planning interval y (e.g. to represent cost learning reductions over time)
$\phi_{\star iy}$	Annual O&M (fixed) impact of a technology in planning period y [$\text{£}/\text{yr}$ or tCO_2/yr]. \star represents linepack technologies l , conversion technologies p , storage technologies s , solar PV installations sl or wind turbines w
$\varphi_{\star iy}$	Variable operating impact of a technology in planning period y [$\text{£}/\text{MWh}$ or tCO_2/MWh]. \star represents linepack technologies l , conversion technologies p , solar PV installations sl or wind turbines w
$\varphi_{\star siy}^*$	Variable operating impact of a task for storage facility s in planning period y [$\text{£}/\text{UoR}$ or tCO_2/UoR]. \star represents either the “get”, “hold” or “put” task
$\hat{\varphi}_{miy}^{\text{Q}}$	Distance-dependent variable operating impact of transport process l in planning period y [$\text{£}/\text{km}/\text{MWh}$ or $\text{tCO}_2/\text{km}/\text{MWh}$]
$\bar{\varphi}_{miy}^{\text{Q}}$	Distance-independent variable operating impact of transport process l in planning period y [$\text{£}/\text{MWh}$ or tCO_2/MWh] (e.g. flat rate freight charges)
ω_i	Weighting factor for including performance indicator i in the objective function

Variables

$\mathcal{J}_{iy}^{\text{total}}$	Total net present impact of performance indicator i in planning period y
$\mathcal{J}_{\text{Cost},y}^{\text{CO}_2\text{tax}}$	Total net present cost impact of CO_2 taxation in planning period y [£M]
$\mathcal{J}_{\text{Cost},y}^{\text{FIT}}$	Total net present cost impact of hydrogen feed-in tariffs in planning period y [£M]
$\mathcal{J}_{\text{CO}_2,y}^{\text{total}}$	Total net present CO_2 impact of all technologies and resources in planning period y [MtCO_2]
H_y^{inj}	Total hydrogen injected into gas grids per year in planning period y [MWh/yr]
H_y^{prod}	Total hydrogen produced by hydrogen-producing technologies per year in planning period y [MWh/yr]

\mathcal{L}_{lzhdy}^*	Operation rate of a task by linepack system l in zone z during hour h of day type d in season t of planning period y [MWh/h]. \star represents either the “get”, “hold” or “put” task
M_{rzhdy}	Import rate of resource r in zone z during hour h of day type d in season t of planning period y [MWh/h]
$N_{\star zy}$	Total number of a technology in zone z during planning period y . \star represents transport infrastructures b , linepack technologies l , conversion technologies p , storage technologies s , solar PV installations sl or wind turbines w
$NI_{\star zy}$	Number of new technologies invested in at the beginning of planning period y in zone z . \star represents transport infrastructures b , linepack technologies l , conversion technologies p , storage technologies s , solar PV installations sl or wind turbines w
P_y^{P,CO_2}	Total emissions of (uncaptured) CO ₂ by conversion technologies in planning period y [tCO ₂]
\mathcal{P}_{pzhdy}	Total rate of operation of conversion technology p in zone z during hour h of day type d in season t of planning period y [MW]
$\mathcal{Q}_{mzz'hdy}$	Operation rate of transport technology m from zone z to zone z' during hour h of day type d in season t of planning period y [MWh/h]
\mathcal{S}_{szhdy}^*	Operation rate of task by storage s in zone z during hour h of day type d in season t of planning period y [MWh/h]. \star represents either the “get”, “hold” or “put” task
U_{rzhdy}	Utilisation of natural resource r in zone z during hour h of day type d in season t of planning period y [MWh/h]
X_{rzhdy}	Export rate of resource r in zone z during hour h of day type d in season t of planning period y [MWh/h]
Z	Objective function

Post-optimisation metrics

$C^{CO_2,avg}$	Average increase in net present system cost per tonne of CO ₂ saved, compared to a reference case [£/tCO ₂]
$C_y^{CO_2,marg}$	Marginal change in net present system cost that would arise for a change in the CO ₂ budget of 1 tCO ₂ in planning period y [£/tCO ₂]
H^{REF}	Total quantity of hydrogen produced across the entire scenario time horizon in the reference case [MWh]
$I_{CO_2}^{REF}$	Total CO ₂ impact across the entire scenario time horizon in the reference case [MtCO ₂]
I_{Cost}^{REF}	Total cost impact across the entire scenario time horizon in the reference case [£M]
$T_y^{CO_2}$	Estimated trading price of CO ₂ allowances during planning period y

1. Introduction

Energy systems are likely to require new energy technologies and carriers, such as hydrogen, in order to decarbonise, but government intervention is likely to be necessary to help these technologies establish themselves. Well-designed government intervention requires an understanding of both the optimal pathway to

decarbonisation and the efficacy of the policy options available. In this study, different policies for bringing about decarbonisation and supporting new energy technologies are considered and modelled through value chain optimisation, focussing in particular on the role of hydrogen.

There is increasing consensus that energy systems will need to reach net-zero emissions in order to prevent the worst effects of climate change [2]. Whilst this may be technically possible, it will require government intervention to support low-carbon technologies and shift away from existing greenhouse gas (GHG) emitting technologies. However, it is important that the energy transition is both equitable and cost-effective, so the design of any government intervention must be considered carefully.

For energy systems to eliminate GHG emissions, various technology solutions will be needed, including both well-established technologies, such as wind turbines and solar photovoltaic (PV), and emerging technologies. Hydrogen is one emerging solution that may have an important role in helping to decarbonise energy systems [3]. Hydrogen is an alternative energy carrier to electricity or fossil fuels, and can be converted to heat or electricity without generating GHG emissions. If hydrogen is produced via electrolysis (powered by renewable electricity), from bioenergy, or from fossil fuels with carbon capture and storage (CCS), then the production of hydrogen is also low-carbon. There are many possible applications for hydrogen, including heating in homes and industry; as a transport fuel; for bulk electricity storage; and as a chemical feedstock [4].

However, it is unclear exactly how hydrogen should be used to maximise its benefit to decarbonising energy systems, and key hydrogen technologies (e.g. electrolyzers and fuel cells) are yet to mature sufficiently to make significant contributions to energy systems. Governments can support these technologies, and doing so now could save GHG emissions and costs in the long run. However, government intervention must be carefully designed to ensure that the energy transition is both cost-effective and equitable.

This study provides a detailed analysis of policy incentives for hydrogen, and considers hydrogen technologies within the electricity, heat and industrial sectors. A range of policies are evaluated, including capital grants, hydrogen feed-in tariffs, and obligations on hydrogen uptake. Additionally, different CO₂ taxation and CO₂ budget policy strategies are evaluated.

The assessment includes value chain optimisation of a national energy system using the Value Web Model (VWM), which was developed by Samsatli and Samsatli [1]. This study builds on the work of Quarton and Samsatli [5], in which the VWM was used to assess the potential for hydrogen injection into the gas grid. A number of new developments are included in this work compared to previous studies with the VWM, which will lead to novel insights:

1. A 40 year time horizon is modelled, including the transition of a present-day system to net-zero emissions. Value chains with net-negative CO₂ emissions are also modelled for the first time, in order to help the system achieve net-zero emissions.
2. A full suite of policies is modelled, for supporting both the decarbonisation of the system (CO₂ taxation and CO₂ budgets) and the uptake of hydrogen technologies (capital grants, feed-in tariffs and obligations). This study represents the first time that value chain optimisation has been used for such a comparison of different policy interventions, enabling a holistic analysis of the different pathways to net-zero and comparing them in their optimal configurations.
3. A new set of post-optimisation metrics is developed, for example hydrogen policy cost-effectiveness, to enable better interpretation of the optimisation results.

4. Various sensitivity studies are conducted, for example considering the effect of the model discount rate, to assess the robustness of the model and results, and to develop new energy system insights.

The remainder of this paper is structured as follows. Section 2.2 provides a literature review of modelling to evaluate energy policy options, followed by an analysis of the available policies for encouraging an energy transition. The scenario modelling method is then described in Section 3, including details of the Value Web Model used for the value chain optimisation, and details of the scenarios that were modelled. Section 4 presents and discusses the results of these scenarios, and finally conclusions are given in Section 5.

2. Literature review

2.1. Modelling to evaluate energy policy options

Scenario modelling can be valuable for assessing the effectiveness of energy policies, by modelling scenarios in which different policies are imposed and measuring the consequences using metrics such as technology uptake, costs, and environmental impacts [6]. Chai and Zhang [7] used modelling to compare energy policies within the China energy system, emphasising that increased spending was needed throughout the research, development and demonstration stages for emerging energy technologies. Meanwhile, Martinsen [8] assessed the interactions between domestic policies and global learning rates on the uptake of new technologies in Norway, through MARKAL-based modelling, finding that domestic subsidies could encourage uptake of technologies, but have limited impact on emissions. Global energy scenario studies, such as the World Energy Outlook [9], also model energy policies but generally have little comparison of policy options. Often these studies use explorative scenarios, which focus on policies that are already in place or planned, and they can therefore underestimate the uptake of emerging technologies [6].

Whilst general policy studies are valuable, hydrogen has unique characteristics, so needs specialist consideration. Many energy policy studies focus on the electricity sector, and hydrogen can contribute here, but it could also span other sectors including heat, industry and transport. Furthermore, hydrogen is an energy carrier that has multiple technologies and infrastructures associated with it, such as electrolyzers, fuel cells, hydrogen storage and hydrogen transportation infrastructures, therefore the challenge may be to establish multiple different technologies concurrently: a chicken-and-egg problem [10].

Various reviews have assessed the potential of hydrogen and provided recommendations for future policies. Ball and Weeda [10], for example, state the need for robust policy support of hydrogen, both in the level and longevity of the support provided. The Hydrogen Council argue that hydrogen can scale up and become cost competitive in many sectors, but only with significant support, including regulatory support, infrastructure investment, financial support and new market creation [11]. The IEA have argued that policies are needed to stimulate commercial demand for hydrogen, mitigate risks, and promote research and development [4].

Several studies have modelled hydrogen within energy systems but with little consideration of policies beyond decarbonisation constraints. Panos et al. [12] and Blanco et al. [13] both used TIMES-based models, of the Switzerland and EU energy systems respectively, to model hydrogen and other technologies under varying decarbonisation constraints. McPherson et al. [14] used MESSAGE to model electricity storage options

(including hydrogen) in scenarios with and without a CO₂ tax, finding that increased levels of R&D for flexibility technologies were needed in scenarios without CO₂ taxes. Cerniauskas et al. [15] optimised hydrogen supply chains to compare the competitiveness of hydrogen with incumbent energy carriers under various CO₂ tax rates. In a roadmap study for hydrogen in the Flanders region of Belgium, Thomas et al. [16] modelled various hydrogen case studies, and made recommendations for future hydrogen policies, but did not model them.

Net-zero has only recently become an ambition for many energy systems, and is likely to affect hydrogen uptake, however it was not modelled in any of the studies mentioned above. Panos et al. [12] and Blanco et al. [13] both identified that more stringent decarbonisation constraints typically lead to a greater role for hydrogen in the scenario results. For many of the hardest-to-eliminate emissions, for example in industry or long-haul transport, hydrogen is the low-carbon alternative with the most potential [17]. Therefore, moving to an ambition of net-zero emissions is most likely to increase the demand for hydrogen, so this should be accounted for in modelling studies.

Some studies have modelled hydrogen-specific incentives but all have focussed on Feed-In Tariffs (FITs). Scamman et al. [18] modelled a range of business case studies for power-to-hydrogen and injection into the gas grid with varying FITs, capital grants and electricity prices, finding that with appropriate support now, learning rates would make power-to-gas self-sustaining by 2030. Budny et al. [19] also modelled some business case studies, focussing on storage and access to balancing markets in Germany, but found that high FITs were necessary to achieve profitability. Finally, Quarton and Samsatli [5] assessed the prospects of hydrogen injection into the gas grid in the UK through value chain optimisation, finding FITs of £20/MWh to be sufficient to incentivise low levels of partial injection in the present-day system.

In this study, the approach used by Quarton and Samsatli [5] was developed further, for the first time accounting for a range of policies beyond FITs, including capital grants, and obligations on hydrogen uptake. Additionally, different policy strategies for achieving a net-zero energy system were considered, including CO₂ taxation and CO₂ budgets.

2.2. Policies to incentivise energy technologies

In the following subsections, the policy tools available to governments for encouraging energy transitions are examined. Figure 1 presents an overview of the policy types considered in this section, including the stage of technology development at which they are typically used. Policies are separated into two categories: policies for penalising existing technologies and policies for supporting emerging technologies. More details on these policies, including actual examples and discussion of how they may be applied to hydrogen, are given in the following subsections.

2.3. Penalising existing technologies

A key challenge for energy policy is to correct for energy market failures, such as negative externalities [20]. For example, well-established, low-cost technologies often have adverse environmental impacts which can be penalised by policy intervention. This may either encourage these technologies to innovate (e.g to reduce CO₂ emissions), or create a more level playing field for emerging technologies.

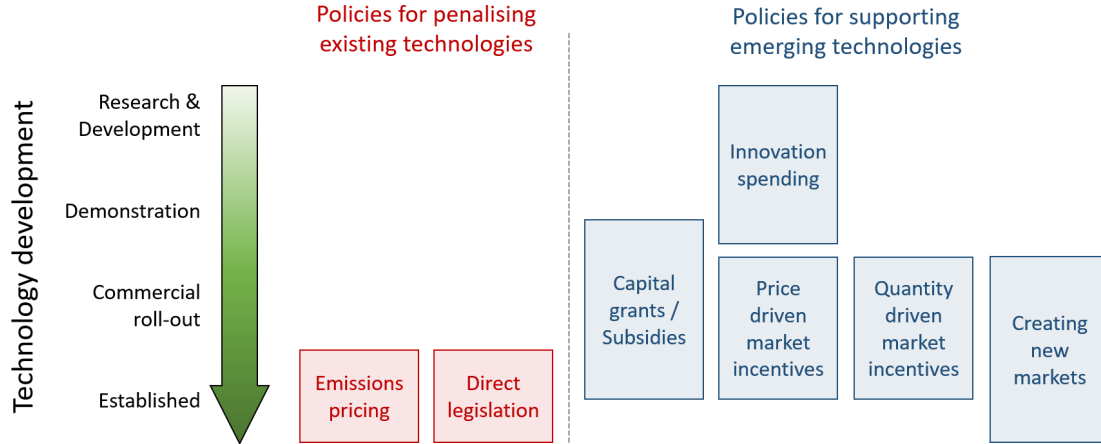


Figure 1: Policy options for either penalising existing energy technologies or supporting emerging technologies. The vertical positions of the policy types indicate the stage of technology development at which they are typically applied.

Table 5: Categorisation and examples of policies aimed at penalising existing energy technologies

Category	Location	Policy	Examples	Sector/Application	Ref.
<i>Emissions pricing</i>					
Carbon tax	British Columbia	Carbon tax		All *	[21]
Carbon cap and trade	EU	Emissions Trading System (ETS)		Industry, Electricity	[22]
<i>Direct legislation</i>					
	Various	Vehicles emission standards		Transport	[23]
	Various	Ban on sales of vehicles with internal-combustion engines		Transport	[24]
	UK	Coal & wet wood ban (Clean Air Strategy)		Heat	[25]

* Greenhouse gas emissions from all combustion of fossil fuels are included, excluding a few minor exemptions [21].

Table 5 summarises the policy types that are considered in this section, with some real-life examples. Typically these policies are used to penalise well-developed technologies, but could also be used for less-developed technologies.

2.3.1. Emissions pricing

Emissions pricing is widely discussed for incentivising emissions reductions, and there are some examples of successful emissions pricing policies. A detailed discussion of the wider economic merits and drawbacks of emissions pricing is beyond the scope of this study but many valuable reviews have been written on the subject. For example: Narassimhan et al. [22] reviewed the practical aspects of the emission trading systems in several global regions; Sumner et al. [26] examined the effectiveness of policies aimed at reducing carbon emissions; Goulder and Schein [27] compared the benefits and the impacts of carbon taxes against cap and trade approaches; and Zhang and Wang [28] reviewed different policies for carbon mitigation in 144 countries around the world. This section describes the main options for emissions pricing and discusses how they might influence emerging energy technologies, in particular hydrogen.

Emissions pricing aims to account for the negative externality that is GHG emissions by imposing an addi-

tional cost on emitters [27]. Whilst this does not directly influence emerging technologies, it makes incumbent, high-emission technologies more expensive, which may allow low-carbon alternatives to enter the market, or encourage emitters to invest in decarbonisation. Two common approaches for emissions pricing are carbon taxation or carbon cap-and-trade.

With a carbon tax, governments collect tax for each tonne of CO₂ emitted by each organisation within the taxation system [26]. Carbon taxes are relatively straightforward to implement and generate a revenue stream for the government, but they are also a relatively blunt tool and could be regressive if the collected revenue is not re-distributed equitably [28].

In British Columbia a carbon tax has been implemented relatively successfully: in 2015, Murray and Rivers [21] estimated that the tax had helped to reduce emissions by between 5% and 15%, with negligible impacts on the wider economy. The scheme was designed to be revenue-neutral, with tax revenues being redistributed through various fiscal measures, to limit the social impacts. Carbon taxes have also been introduced in Sweden, New Zealand, and Chile [28].

Carbon cap-and-trade (also known as carbon trading or emissions trading) is an alternative to carbon taxation, where an allowable level of emissions across the whole system is determined, and emissions allowances are allocated to all organisations within the system [22]. Allowances can be traded so that emitters can either reduce their own emissions or purchase allowances from others. The total number of allowances can be reduced over time, reducing overall emissions. An advantage of carbon-trading schemes is that the market determines the most cost-effective way to eliminate emissions, with the price of emissions allowances (CO₂ trading price) being influenced by the rate at which decarbonisation is achieved. However, the scheme must be carefully managed to ensure that the CO₂ trading price is sufficiently high and to prevent emissions leakage into other countries outside the scheme [27].

Examples of carbon-trading schemes include the EU Emissions Trading System (ETS), and schemes in Switzerland, South Korea, California, and China [22]. Early carbon-trading implementations faced some operational issues, such as overestimation of allowable emissions, but more recent implementations (e.g. in California and South Korea) have learned lessons from these issues and been designed more carefully [22].

In some cases, carbon taxes are used in combination with carbon-trading schemes, to cover aspects not accounted for by the trading scheme. In the UK, for example, the Carbon Price Floor (CPF) sets a minimum limit for the CO₂ trading price. If the price falls below the CPF, the price difference is collected as tax [29]. In France, a carbon tax is imposed on emissions that fall outside of the EU cap-and-trade scheme, such as transport and domestic heating [21].

2.3.2. Legislation

Direct legislation can be used to specify standards for technologies (e.g. allowable emissions levels), or whether certain technologies are allowed to operate at all (e.g. banning the worst-polluting technologies). In the transport sector, many governments have requirements for allowable levels of emissions for vehicles [23], and several governments have announced plans to ban the sales of internal-combustion engine (ICE) vehicles altogether [24]. Similar measures exist in other sectors: in the UK, for example, the sale of coal and wet wood for use in domestic heating has been banned on air-quality grounds [25].

Table 6: Categorisation and examples of policies for supporting emerging energy technologies

Category	Location	Policy	Sector/Application	Ref.
<i>Technology development</i>				
Innovation spending	USA	DOE Hydrogen and Fuel Cells program	Various	[30]
	Japan	Basic Hydrogen Strategy	Various	[31]
	EU	Fuel Cells and Hydrogen Joint Technology Initiative	Various	[32]
<i>Technology roll-out</i>				
Capital grant/subsidy	Various	Support for wind and solar installations	Renewable electricity	[33]
	UK	Hydrogen for Transport Programme	Hydrogen refuelling	[34]
	California	Alternative and Renewable Fuel and Vehicle Technology Program	Hydrogen refuelling	[35]
<i>Technology competitiveness</i>				
Price-driven	Germany	Feed-in tariff (FIT)	Renewable electricity	[36]
	UK	Contracts for Difference (CfD)	Low-carbon electricity	[37]
Quantity-driven	UK	Renewable Heat Incentive (RHI)	Heat / Gas	[38]
	UK	Renewables Obligation (RO)	Renewable electricity	[39]
	UK	Renewable Transport Fuel Obligation (RTFO)	Transport fuel	[40]
New markets	California	Low Carbon Fuel Standard (LCFS)	Transport fuel	[41]
	Various*	Balancing markets	Electricity	[42]

* For example, the majority of EU countries have their own balancing markets, each with unique regulations [42].

These policies could influence hydrogen technologies. Hydrogen fuel cell vehicles are an alternative to ICE vehicles, for example, so they are likely to benefit from the ban on ICE vehicles. Similar effects would be achieved in other sectors: in the heat sector, for example, low-carbon technologies would benefit if natural-gas boilers were banned.

A challenge for policies intended to penalise existing technologies, whether through emissions pricing or direct legislation, is vested interests. Penalised technologies are likely to have stakeholders who stand to lose if these technologies are made less competitive or banned altogether, and these stakeholders may attempt to influence legislation to reduce its potency. Consequently, policies in this category may require a strong mandate for the government to overcome these vested interests.

2.4. Supporting emerging technologies

Support for new energy technologies can be provided throughout the technology life-cycle, including: technology development and demonstration; commercial roll-out; and aiding the technology’s market competitiveness. Supporting new technologies may help them develop and become competitive in their own right, or correct for market externalities. The policy categories considered in this section, along with examples, are given in Table 6.

2.4.1. Supporting technology development

Government investment in technology innovation is important to help new technologies to develop, and should be provided to support the research, development and demonstration stages of the technology. The

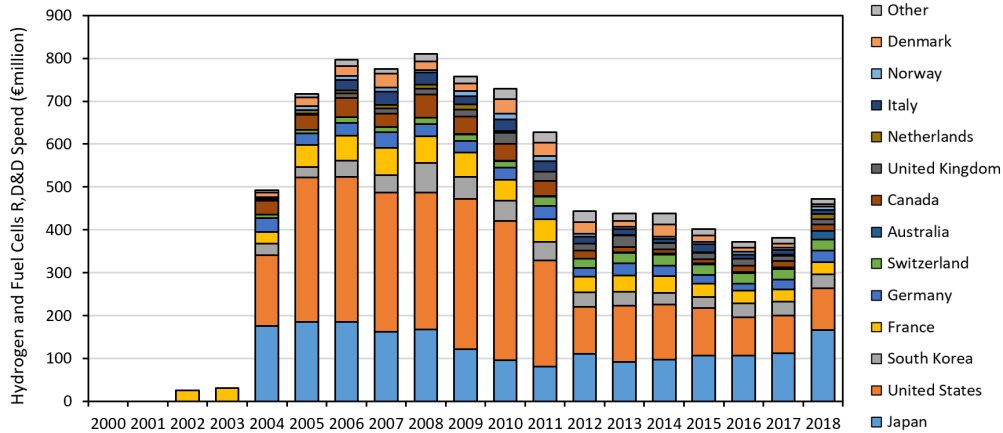


Figure 2: Historic research, development and demonstration spending on hydrogen and fuel cells in IEA countries. Data from [43].

private sector may also invest in innovation, voluntarily or under government obligation, depending on the specific technology and present market need. Investment in innovation can help to develop prototypes, scale-up to demonstration and later commercial scale, improve performance, and reduce costs.

Most developed countries have energy innovation programmes, many including hydrogen. In 2018, International Energy Agency (IEA) member states spent €15.4 billion on energy research, development and demonstration projects, of which €478 million was spent on hydrogen and fuel cell projects [43]. Figure 2 shows historic innovation spending on hydrogen and fuel cells in IEA countries. Notable programmes include the US Department of Energy’s Hydrogen and Fuel Cells programme [44], including the H2@Scale project [45], various schemes as part of Japan’s “Basic Hydrogen Strategy” [31], and the Fuel Cells and Hydrogen Joint Technology Initiative, part of the EU Horizon 2020 Framework [32].

For the energy transition, continued innovation spending will be valuable to hydrogen technologies at various stages of development. Many hydrogen technologies have been shown to be technically viable, but need further development and demonstration to prove functionality, scale-up, and achieve efficiency and cost improvements: example technologies include large-scale electrolysis and fuel cells, hydrogen gas turbines, hydrogen storage, hydrogen injection into gas grids, and use in long-haul and heavy duty transport [4]. Meanwhile there may be other technologies at earlier stages of development that have the potential for significant future contributions [46].

2.4.2. Supporting technology roll-out

Capital grants or direct spending on a technology can be used to cover some or all of the upfront costs of installation: to encourage technology learning, or simply to aid roll-out of the technology so that it can provide system benefits (e.g. lower emissions) [33]. Capital grants and similar financial support have been used in numerous countries to support renewable-energy technologies; early examples include subsidies for wind turbines in the USA and Europe in the 1980s [47] and for solar PV in Japan in the 1990s [48].

This type of scheme already exists for hydrogen vehicle refuelling stations, including schemes in the UK [34], California [35], and Germany [49]. This approach is valuable because hydrogen vehicles rely on a

well-established refuelling infrastructure: by helping to install the infrastructure, the purchase of hydrogen vehicles will be encouraged. Alternatively, grants for the purchase of the vehicle itself can be offered: such schemes already exist in the UK [50], Germany [51], California [52], Japan [53], South Korea [54], and China [55].

As with hydrogen for transport, hydrogen for heating relies on a hydrogen distribution infrastructure, so investment support for new hydrogen distribution infrastructure, or conversion of existing natural gas infrastructure to hydrogen, would reduce the obstacles to uptake of hydrogen for heating. Governments could also support the up-front cost of converting homes to hydrogen (e.g. new hydrogen boilers).

2.4.3. Supporting technology competitiveness

Whilst early support of technology development is necessary, support within markets may also be needed for technologies to establish themselves [20]. Penalising existing technologies can assist this by creating a more level playing field for emerging technologies, but is unable to target specific emerging technologies, so more developed (i.e. lower cost) technologies may be favoured. Therefore more direct support of emerging technologies through intervention into existing markets may be preferred: for example with price-driven incentives (adjusting market prices) or quantity-driven incentives (imposing requirements on the quantities of energy supplied by certain technologies). Alternatively, new markets can be created that aim to reward specific technology offerings.

2.4.3.1. Price-driven incentives.

Feed-in tariffs (FITs) are a type of price-driven incentive that have widely been used in electricity markets to incentivise renewable generators, usually by guaranteeing a certain price for the renewable electricity. A prominent example of a FIT scheme was implemented in Germany to incentivise wind, solar PV, and biomass electricity generation by obliging electricity utilities to buy all generation from qualifying renewable generators at a pre-determined price [56]. Different price-driven incentives have been used worldwide with different formats but performing similar functions. For example the contract for difference (CfD) scheme in the UK involves long term contracts with generators for a fixed price (the “strike” price). When the market price is below the strike price, the government pays the difference, but if the market price exceeds the strike price, the generator must pay the difference back [37].

Price-driven schemes also exist beyond the electricity sector. Under the Renewable Heat Incentive (RHI) in the UK, the government pays an incentive of around £22-49 for each MWh of biomethane injected into the natural gas grid [57], and similar schemes exist in other EU countries [58]. Price-driven incentives can also support the energy consumer instead of the energy producer, for example making payments for each unit of heat generated by qualifying heating technologies [38].

A challenge for price-driven incentives is determining the incentive level. In the original German FIT scheme, the same fixed price was used for all qualifying generators [39], but this may enable projects with costs lower than this fixed price to capture surplus profit, whilst higher cost (e.g. less developed) projects may still struggle to compete [59]. Therefore a technology-specific tariff may be preferred, as was later adopted in Germany [56]. Alternatively, auctions can be used to determine tariffs: in the UK CfD scheme, qualifying

renewable generators bid with the rate they would receive for their electricity generation, and contracts are awarded to the lowest bids [37]. In this way, generator surplus profit should in theory be reduced [36]. This scheme also includes separate technology “pots”, so that less developed technologies do not compete with more developed technologies [37].

Although no examples of price-driven hydrogen incentives for producers are currently in use, similar models to those described above would be feasible for hydrogen. For example, studies have considered FITs for hydrogen injection into gas grids (e.g. using whole-system value chain optimisation [5] and a feasibility analysis [18]), which could resemble the biomethane injection tariffs described above. Other price-driven hydrogen incentives are less obvious, as hydrogen is a separate energy carrier, so does not compete directly with existing energy carriers. The European Commission is considering a price-driven incentive to support low-carbon hydrogen in industry, using a contract-for-difference approach, linked to the carbon price [60]. Alternatively, payments could be made for the production of fuels synthesised from low-carbon hydrogen, such as synthetic methane, methanol, or Fischer-Tropsch hydrocarbons [61]. On the consumer side, price incentives could reduce the retail price of hydrogen as it competes with alternatives, for example transport fuels.

2.4.3.2. Quantity-driven incentives.

Quantity-driven incentives, also known as Renewable Portfolio Standards (RPS), typically compel the market to purchase a quantity of the supported resource, allowing the market to determine the most cost-effective way of doing so [59]. Such schemes are often used in conjunction with tradeable certificates, which can be traded between generators who have not reached their quota and those who have (and hence have surplus certificates). There may also be the option for generators to buy-out if they have missed the quota, by paying a pre-defined penalty price.

RPS schemes have been used in the electricity sector in various countries, including the UK and Italy [39], and Australia and China [62], but can also be used in other sectors. For example, as part of the Renewable Transport Fuel Obligation in the UK, large-scale suppliers of transport fuel must show that a percentage of the fuel they supply has come from renewable and sustainable sources, and tradeable certificates are used [40]. The Zero Emission Vehicle mandate, in use in 11 states in the USA, works on a similar principle, mandating that vehicle manufacturers supply a certain proportion of low emission vehicles, with a tradeable credit system [63].

Alternatively, quantity-driven schemes can specify a different parameter to control, such as CO₂ intensity. In California, for example, the Low Carbon Fuel Standard (LCFS) ensures that suppliers of transport fuel have a maximum allowable CO₂ intensity across all of the fuel they supply: credits are available for fuels with lower CO₂ intensities (and are also issued for electric and hydrogen charging and refuelling infrastructure), and can be traded to offset fuels with higher CO₂ intensities [41]. A CO₂ intensity scheme may not achieve the same results as a conventional RPS scheme: for example, a conventional RPS may not distinguish between wind and solar electricity generation, despite the two technologies having different levels of embedded CO₂.

Whereas price-driven incentives determine the level of incentive in advance, quantity-driven incentives can allow markets to determine how the quota is met, and the value of the qualifying generation (e.g. the trading

price of certificates) [59]. This should minimise producer surplus profit, provided the certificate trading price settles at the marginal cost of production from qualifying sources. However, as with price-driven incentives, this may not be effective if some qualifying technologies have lower costs than others (e.g. because they are more developed) [39], so may need to be managed with separate technology categories (with separate certificates and quotas).

Accountability is important with quantity-driven schemes, as there have been instances where the quotas have never been met, either due to no enforceability (e.g. in China [62]) or a low buy-out penalty price (e.g. the UK Renewables Obligation [39]). Quantity-driven schemes may also present more investment risk, for example if the certificate market is unstable, which could increase overall costs. Finally, Haas et al. [39] suggest that quantity-driven incentives with certificate schemes may be more administratively complex and therefore more costly to implement.

As with price-driven incentives, quantity-driven incentives are most easily applicable to hydrogen in markets where it can compete directly with alternatives. For example in transport, hydrogen is already included within the LCFS used in California and elsewhere. Quantity-driven incentives could be implemented in gas markets if an obligation were imposed on gas suppliers to inject a minimum amount of hydrogen into their gas grids. Tradeable certificates could also be used, with different values depending on the CO₂ intensity of the injected hydrogen. Alternatively, a CO₂-intensity based scheme could be used, where gas suppliers are required to achieve an average CO₂ intensity for all injected gas; this approach would support both hydrogen and biomethane injection. Applications of quantity-driven incentives to support hydrogen in other sectors are less obvious but may be more achievable than price-driven incentives; examples could include an obligation for industries to switch to hydrogen where possible (e.g. in steel production and refining [4]), or a minimum required level of renewable hydrogen in industries that currently use fossil hydrogen.

In theory, quantity-driven incentives, especially those using tradeable certificates, may achieve lower system costs than price-driven incentives, as they encourage more competition between supported technologies. However, examinations of various EU schemes for supporting renewable electricity suggest that price-driven incentives have achieved greater technology uptake at lower cost [39]. This may be due to the greater stability and lower regulatory and market risks of price-driven incentives, and may explain why some countries that initially adopted quantity-driven incentives, such as the UK and Italy, have more recently moved to price-driven systems. For either price-driven or quantity-driven incentives, technology-specific schemes are seen to be more cost effective than technology-neutral ones, as they help to minimise the surplus profit for the operators of lower cost technologies [59].

2.4.3.3. Creating new markets.

If emerging technologies are unable to compete with incumbent technologies within existing markets, new markets can be created that value different characteristics. For hydrogen, markets that reward flexibility may be valuable. Flexibility is becoming increasingly important as intermittent renewables contribute more to energy systems, but conventional energy markets do not necessarily value this, instead focussing on a fixed price per unit of energy delivered [64]. Energy storage and transportation technologies, including hydrogen, could provide valuable services to energy systems but need markets to recognise this value.

Flexibility is most valuable in the electricity sector, due to the increasing penetration of intermittent renewables and the need for supplies and demands to be balanced instantaneously; in other sectors there are often already flexibility solutions in place, such as gas grid linepack flexibility [6]. Electricity flexibility is needed for a range of functions, including security of supply through backup capacity, rapid power ramping, supplying peak energy demands, and managing power quality [65]; markets must be found that value these services. In many countries the electricity transmission system operator already offers payments for flexibility services [42]. Typically, services are categorised based on response speed, ramp rate and response duration; payments may be a fixed payment per MW of capacity, per hour that the service is available, in addition to a payment for each MWh of energy used. Procurement of these services varies: in the UK, suppliers are selected from bids based on cost and the nature of the service being offered [66]. Localised flexibility markets are also begin to develop, via distribution network operators or independent platforms, that could enable small producers and even consumers to provide flexibility to the grid [67].

Hydrogen technologies could access these flexibility markets in various ways. Hydrogen is relatively easy to store, so could be used in dispatchable hydrogen turbines or fuel cells to provide rapid response [68]. Furthermore, hydrogen technologies can also be used for frequency control, either through turbines as synchronous generators, or with PEM fuel cells and electrolyzers [69]. Power-to-gas with injection into the gas grid can link the electricity system to the gas system, creating opportunities to exploit the flexibility of the gas grid for electricity grid services [6].

Another example of new markets for hydrogen is in the chemicals and industrial sectors. Globally, around 33% of hydrogen usage is in refining, 27% is used for ammonia, and 10% is used for methanol, but more than 99% of this hydrogen is produced from fossil fuels, and the supply chains are not typically viewed as part of the energy system [4]. There could be opportunities for greater sector-coupling, with hydrogen for chemical and industrial uses being supplied from the energy system, for example from power-to-gas.

3. Methods

The aim of this study was to examine the role of hydrogen throughout a transition from the present day to a net-zero energy system in 2050, applying a variety of decarbonisation and hydrogen-focussed policies. This was done by modelling different policy scenarios using value chain optimisation and comparing the optimal energy system configuration under each policy. The value chain optimisation methodology and details of the modelled energy system are given in Section 3.1. The design of the different policy scenarios, along with how they are modelled, is discussed in Section 3.2. Section 3.3 describes the computational statistics of the optimisation model. Finally, Section 3.4 provides a description of how the optimisation results were analysed to obtain important metrics and insights.

3.1. Energy value chain optimisation

3.1.1. Value Web Model

The scenario modelling was performed using the Value Web Model (VWM), which is a mixed integer linear programming optimisation model for designing, and determining the operation of, integrated multi-vector

energy networks. The mathematical formulation was developed by Samsatli and Samsatli [1] and has recently been applied to develop low-carbon scenarios for: interseasonal storage and renewable hydrogen for heat [70]; energy networks at the city level [71]; hydrogen and carbon capture, storage and utilisation [72]; and gas grid linepack, power-to-gas and hydrogen injection into gas grids [5]. The full model nomenclature and mathematical formulation are presented in the supplementary material. The following paragraphs provide an overview of the model.

The VWM can simultaneously determine both the design of energy value chains and how they should be operated in order to minimise the model objective function. In this study, the objective function, Z , is defined as follows:

$$Z = \sum_{iy} \omega_i \mathcal{S}_{iy}^{\text{total}} \quad (1)$$

Here, $\mathcal{S}_{iy}^{\text{total}}$ is the total impact of all resources and technologies in the model. The index i specifies the performance indicator that is represented: in this study the indicators that were included were $i = \text{Cost}$ and $i = \text{CO}_2$. The parameter ω_i is a weighting factor to specify the relative importance of each performance indicator in the objective function: in this study the objective was to minimise overall system cost (so $\omega_{\text{Cost}} = 1$ and $\omega_{\text{CO}_2} = 0$). The index y represents each decadal planning interval that was modelled.

The definition of $\mathcal{S}_{iy}^{\text{total}}$ has 23 separate terms, so in the interest of space it is not presented in this section but a full description can be found in the supplementary material. In summary, the terms include the following components:

- Capital, fixed operating and variable operating impacts of all conversion, storage and transportation technologies;
- Impacts associated with the utilisation of natural resources (e.g. production of natural gas or growth of biomass);
- Impacts of any resource imports or exports; and
- Impacts of any policy interventions, such as CO₂ taxation.

Impacts may be either positive or negative (for example negative CO₂ impacts in the case of biomass growth or offshore CO₂ sequestration).

Optimisation decisions include which energy resources should be utilised and when, which energy technologies should be installed, where and when, and how they should be operated. The VWM is a spatio-temporal model, meaning that it can account for the spatial distribution and temporal variation of a number of properties. These include: resource availabilities and energy demands that vary in both space and time, decisions about where to locate new technologies and when to invest in them (i.e. long term energy system planning over multiple decades) as well as how to operate them on a seasonal, day-to-day and hourly basis. The spatial and temporal representation of the model allows it to include a detailed account of energy storage and transportation/transmission of resources.

This approach to modelling energy systems is valuable, as it is able to represent large-scale details, such as the overall decarbonisation pathway and system costs, whilst also representing detailed aspects of the energy system (which affect the overall performance of the system). For example, specific results such as how a single technology is operated over the course of a day can be examined. Different modelling constraints can be imposed to represent policy interventions on the system, for example controlling CO₂ or subsidising particular technologies. Hence the effects of these policy interventions on the system design, operation, costs, and environmental impacts can be assessed.

3.1.2. Representation of energy value chains

The VWM can represent entire energy value chains, from primary resource to end-use. The value chains are represented using a range of energy resources (e.g. electricity, hydrogen and natural gas) and technologies (e.g. conversion technologies, storage technologies and transmission technologies). Figure 3 shows a schematic of the resources and technologies that are included in the scenario studies and how they are interconnected.

In general, there are three different types of resource that can be modelled in the VWM. Primary resources, such as wind or natural gas, have limited availabilities (e.g. dependent on wind speed profiles and land area) and can be extracted for use in the energy system. Some primary resources, such as wind and solar, require “resource utilisation” technologies (wind turbines and solar PV) to extract and use the available energy. Some resources represent final energy services, such as electricity and heat, and have spatio-temporal demands that must be satisfied. Finally, the other resources represent intermediates or wastes, such as some energy carriers and CO₂ (which can be a waste if it is emitted to the atmosphere, or an intermediate if it is captured stored or utilised).

As illustrated in Figure 3, conversion technologies take certain resources as inputs and produce others as outputs. Conversion technologies are governed by various constraints including the efficiencies, and other requirements, with which they convert the input resources to the outputs, maximum and minimum operating rates, and costs.

Also included in the VWM are storage technologies, that store given resources over one or more time intervals. Storage technologies are governed by constraints including maximum and minimum storage inventory, resource requirements, etc.

Finally, transmission technologies enable the transportation of resources between spatial zones: two representative spatial zones, z and z' , are shown in Figure 3, but in practice any number of zones may be modelled. Some transmission technologies also include some storage functionality, in order to represent gas pipeline linepack.

In addition to these resource and technology constraints, further constraints in the VWM keep track of overall system costs, environmental impacts and other factors such as land use.

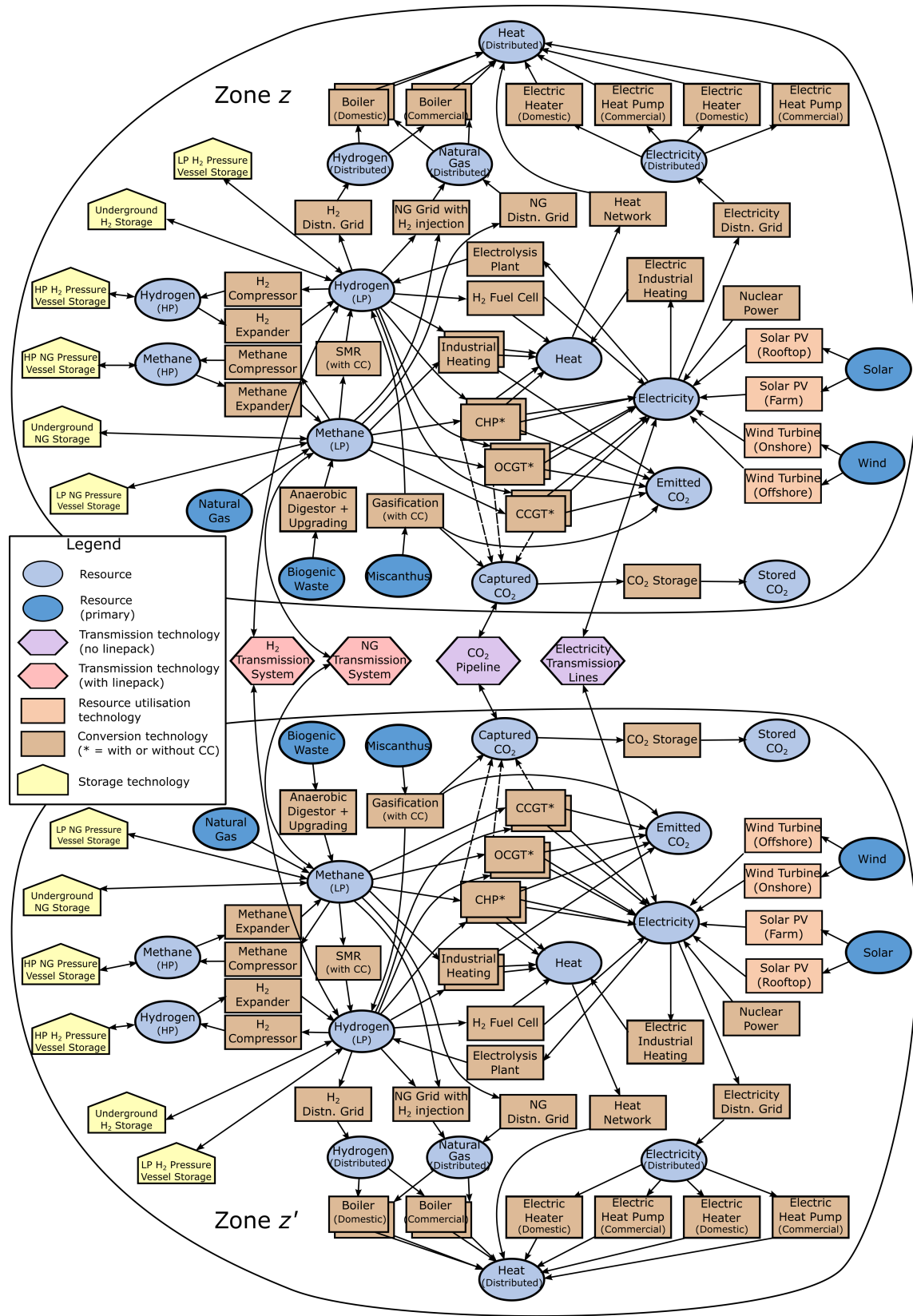


Figure 3: Diagram showing the resources and technologies considered in this study. Primary resources are available that may be converted by conversion technologies to eventually produce resources that satisfy energy demands. Transportation technologies can be used to move resources between zones; two representative spatial zones, z and z' , are shown in the diagram. Finally, storage technologies can store resources over one or more time interval.

3.1.3. Resources and technologies included in this study

The resources and technologies in Figure 3 were all included in the scenario modelling for this study. The input data for these technologies was based on the data in [73] and are presented in detail in the supplementary material. Uptake of hydrogen technologies was the focus of this study, so various hydrogen technologies were modelled. Alternative energy resources and technologies were also included, such as electricity and natural gas.

For hydrogen production, three value chains were modelled in this study: reforming of methane, electrolysis (also known as power-to-gas), and gasification of biomass. Inclusion of a bioenergy production route allows for the potential for negative CO₂ emissions, if the CO₂ emitted through gasification is captured and sequestered in CO₂ storage. Design of bioenergy value chains is complex, with different pathways available including generation of electricity and heat, and the environmental impact of the value chain can depend heavily on the biomass feedstock and conversion processes used [74]. Evaluation of these issues, specific to bioenergy, is beyond the scope of this study. Here, a representative biomass to hydrogen value chain was modelled in order to explore its possible interaction with other hydrogen value chains. The supplementary material provides more details of the these value chains.

For utilisation of hydrogen, the following technologies were modelled: combined cycle gas turbines (CCGTs) and open cycle gas turbines (OCGTs) for the conversion of hydrogen to electricity; fuel cells and combined heat and power (CHP) plants for conversion to electricity and heat; and a range of heating technologies including domestic and commercial boilers, and generic industrial heating technologies.

Hydrogen storage technologies were also modelled. For larger scale storage, hydrogen can be stored underground in salt caverns and depleted oil and gas fields. Alternatively, hydrogen can be stored above-ground in pressure vessels including “low pressure” (up to 80 bar) and “high pressure” (up to 500 bar) options. Hydrogen transmission pipelines with linepack storage capacity were also modelled.

Injection of hydrogen into existing gas distribution grids was also modelled, either partially or via complete conversion of the gas grid to hydrogen. Partial injection refers to the blending of hydrogen with natural gas, up to a certain limit (20% by volume in this study). This process involves minimal alterations to existing natural gas distribution grids, but requires injection equipment to ensure that the maximum allowable level of injection is not exceeded. Alternatively, “100%” hydrogen injection involves the conversion of natural gas distribution grids to hydrogen, so that they can no longer be used for natural gas. The practicalities of both of these injection options, as well as further details of how they are represented in the VWM, are provided by Quarton and Samsatli [5].

As Figure 3 shows, various other value chains were also modelled, beyond hydrogen. Methane-based value chains were modelled, including production of either natural gas or bio-methane from biogenic waste. The methane can then be used in SMR to produce hydrogen, in CCGTs or OCGTs to produce electricity, in CHP plants, or in various heating technologies in the domestic, commercial and industrial sectors. For the larger installations (e.g. gas turbines and SMR), the CO₂ emissions can be captured and transported to offshore CO₂ storage sites. As well as using gas turbines, electricity can be produced from wind, solar or nuclear power. The electricity can subsequently be used to satisfy electricity demands, or for heating in the domestic, commercial and industrial sectors.

3.2. Scenario design

Scenarios were modelled using the VWM in order to explore the impact of different policies on both the transition of national energy system to net-zero by 2050, and the uptake of hydrogen technologies within that system. Overall, 15 different scenarios were modelled, each with a unique configuration of decarbonisation policies and hydrogen incentives. Additionally, 23 sensitivity scenarios were modelled, exploring the effects of certain data assumptions. The policy scenarios were designed based on the information that was gathered in Section 2.2, and are separated into two groups:

1. Scenarios with policies for penalising existing technologies, in order to achieve energy system decarbonisation, and
2. Scenarios with additional policies for hydrogen technologies (whilst still including policies to achieve decarbonisation).

More details of these scenario groups are given in the following subsections.

The scenarios were designed to represent the Great Britain (GB) energy system. Demands for heat and electricity in the domestic, commercial and industrial sectors were modelled, that must be satisfied at all times. Any of the technologies shown in Figure 3 could be installed to convert primary resources into the final energy demands, although subject to their operational constraints, and incurring costs for installation and operation. Additionally, existing installed capacities of several technologies were modelled, including natural gas transmission and distribution infrastructures.

In this study GB was represented with 16 spatial zones, based on the National Grid Seven Year Statement zones [75]. Temporally, three seasons were modelled: “summer”, “winter”, and a short “peak” season (for the most extreme energy demands). Within each season, days were represented with four sub-day intervals, representing sub-day variability in resource availabilities and demands. Finally, four decadal planning intervals were modelled, allowing new investment decisions at the beginning of each decade, and long-term trends in energy demands and technology costs. The model input data used in this study, including technology data and spatio-temporal resource availabilities and demands, was based on [73], the details of which are provided in the supplementary material.

As the scenarios that were modelled represent the GB energy system, the currency used for modelling was British pound sterling (£). In the remainder of this paper, cost data are reported in pounds. In 2019 the average exchange rate between British pounds and U.S. dollars was $\text{£}1 = \text{\$}1.28$ [76].

3.2.1. Scenarios with policies for decarbonisation

Table 7 gives a summary of the first set of scenarios, with policies to penalise existing technologies and achieve decarbonisation. The modelled scenarios include: one in which CO₂ was not constrained; a set of three with different CO₂ budget trajectories; and a set of three with different CO₂ tax trajectories. Apart from the “CO₂ unconstrained” scenario, the goal of the scenarios is to decarbonise by 2050 at minimum overall system cost. Although the decarbonisation target is to reach net-zero emissions, whether or not this is achieved depends on the policies that are imposed (e.g. a CO₂ tax does not guarantee the system will reach net zero by 2050, as discussed in Section 2.3.1).

Table 7: Details of the first set of scenarios, focussing on policies for decarbonisation. The CO₂ tax rates shown are model input values, and are therefore un-discounted.

Scenario subset	CO ₂ constraint/impact	2020 - 2030	2030 - 2040	2040 - 2050	2050 - 2060
CO ₂ unconstrained	None	-	-	-	-
CO ₂ budgets	CO ₂ budget (MtCO ₂ /yr):				
	1) “Late”	236	236	236	0
	2) “Steady”	236	160	80	0
	3) “Early”	236	100	50	0
CO ₂ tax	CO ₂ tax (£/tCO ₂):				
	1) “Low”	54	116	177	240
	2) “Medium”	54	132	209	290
	3) “High”	54	148	241	340

3.2.1.1. CO₂ unconstrained scenario.

In the “CO₂ unconstrained” scenario, no constraints or other policies are applied to CO₂ emissions, so the optimisation simply seeks to meet all energy demands at minimal cost, irrespective of environmental impact. This scenario gives an indication of the overall system costs and emissions in a case with no policy intervention.

3.2.1.2. CO₂ budgets scenarios.

In the “CO₂ budgets” scenarios, a constraint was applied that limits the total allowable emissions in each decade:

$$\mathcal{I}_{\text{CO}_2, y}^{\text{total}} \leq B_y^{\text{CO}_2} n_y^{\text{yy}} \quad \forall y \in \mathbb{Y} \quad (2)$$

In this equation, $\mathcal{I}_{\text{CO}_2, y}^{\text{total}}$ (the total impact $\mathcal{I}_{iy}^{\text{total}}$ for $i = \text{CO}_2$) is the total CO₂ impact (net CO₂ emissions, in MtCO₂) in the entire system during planning period y ; $B_y^{\text{CO}_2}$ is the CO₂ budget (in MtCO₂/yr) in period y ; and n_y^{yy} is the number of years in period y .

Three CO₂ budget scenarios were modelled with different budget trajectories, shown in Table 7. All cases have a budget of 236 MtCO₂/yr in the first decade, estimated from the fourth and fifth carbon budgets set by the Committee on Climate Change [77] for the sectors that are included in this study. The budget for the final decade was set to 0 MtCO₂/yr in all cases. Each case has different budgets for the intervening decades: the “steady” case represents a consistent reduction of around 80 MtCO₂/yr per decade, whilst the other cases represent either slower or faster decarbonisation trajectories that still reach net-zero emissions by 2050.

With minimal policy intervention, the “late” case theoretically gives the cost-optimal pathway for achieving net-zero emissions in 2050-2060. Comparison of the three cases shows the effects of different decarbonisation trajectories on the overall energy system design, CO₂ emissions, and costs. These scenarios are also analogous to a CO₂ cap-and-trade scheme, assuming that the entire energy system is included in the scheme.

3.2.1.3. CO₂ tax scenarios.

Three scenarios were modelled with CO₂ taxes imposed on all CO₂ emissions across the system, whilst negative emissions (e.g. from bioenergy with CCS) are rewarded at the same rate. The net cost to the system of the CO₂ tax is defined as follows:

$$\mathcal{J}_{\text{Cost},y}^{\text{CO}_2\text{tax}} = \mathcal{J}_{\text{CO}_2,y}^{\text{total}} V_y^{\text{CO}_2} \frac{D_{\text{Cost},y}^{\text{OM}}}{D_{\text{CO}_2,y}^{\text{OM}}} \quad \forall y \in \mathbb{Y} \quad (3)$$

In this equation the total system CO₂ impact, $\mathcal{J}_{\text{CO}_2,y}^{\text{total}}$, is multiplied by the CO₂ tax rate, $V_y^{\text{CO}_2}$, which has a pre-defined value for each decadal interval y . The final factor in Equation 3 relates to discounting of cost and CO₂ impacts. All annual impacts in $\mathcal{J}_{iy}^{\text{total}}$ in the model include a discount factor D_{iy}^{OM} , which discounts annual impacts in period y back to the present day (for example to represent the time value of money). However, CO₂ impacts are generally not discounted (but could be in principle, for example to penalise earlier emissions, which remain in the atmosphere for longer, causing more climate damage). Therefore, the quotient $D_{\text{Cost},y}^{\text{OM}}/D_{\text{CO}_2,y}^{\text{OM}}$ is included to convert the discounting of CO₂ into discounting of cost.

The net cost of the CO₂ tax, $\mathcal{J}_{\text{Cost},y}^{\text{CO}_2\text{tax}}$, is included in the optimisation objective function (which is a sum of all system costs), so will incentivise a reduction in CO₂ emissions. However, CO₂ emissions are not controlled directly, so achieving net-zero emissions is not guaranteed, but depends on whether the tax rate is a sufficient incentive to decarbonise.

In each scenario, the CO₂ tax rate is increased in each decade, reaching its maximum in the final decade. The tax rates that are modelled ($V_y^{\text{CO}_2}$) are given in Table 7 and are un-discounted values. The initial tax rate of £54/tCO₂ is taken from the National Grid FES 2019 “High” CO₂ price scenario; the rates in subsequent decades rise linearly [78].

3.2.2. Scenarios with policies for incentivising hydrogen

The second set of scenarios includes policies for supporting hydrogen technologies, to explore their effectiveness for encouraging hydrogen uptake. All scenarios in this set also include CO₂ budgets, equal to the budgets in the “steady” CO₂ budgets case in Table 7, to ensure that the system still reaches net-zero emissions by 2050. The policies that were modelled focus on the use of hydrogen in gas distribution grids, to be subsequently used for domestic and commercial heat.

Table 8 gives details of the scenarios. The policies that were modelled are based on the information in Section 2.2, and include: a set of scenarios with obligations for hydrogen injection (quantity-driven incentives); a set of scenarios with feed-in tariffs for hydrogen injection (price-driven incentives); and a set of scenarios with capital grants for hydrogen boilers.

3.2.2.1. Hydrogen injection obligations.

The first set of hydrogen-focussed scenarios use a quantity-driven incentive. A constraint is imposed stating that the total amount of hydrogen injected into gas grids in a given decade y must exceed the minimum required level:

Table 8: Details of the second set of scenarios, focussing on policies for incentivising hydrogen. The hydrogen FITs shown are model input values and are therefore un-discounted.

Scenario subset	H ₂ constraint/incentive	2020 - 2030	2030 - 2040	2040 - 2050	2050 - 2060
H ₂ injection obligations	Minimum H ₂ injection (TWh/yr):				
	1) “Low”	0	25	50	100
	2) “Medium”	0	50	100	200
	3) “High”	0	75	150	300
H ₂ injection FITs	H ₂ injection FITs (£/MWh):				
	1) £10/MWh	0	10	10	10
	2) £30/MWh	0	30	30	30
	3) £50/MWh	0	50	50	50
H ₂ boiler grants	H ₂ boilers capital grant (% of capex):				
	1) 50%	0	50	50	50
	2) 100%	0	100	100	100

$$H_y^{\text{inj}} \geq H_y^{\text{min}} \quad \forall y \in \mathbb{Y} \quad (4)$$

Where H_y^{min} is the minimum required level of hydrogen injection (the hydrogen injection obligation, in TWh/yr), and H_y^{inj} is the total amount of hydrogen injected into gas grids per year in period y , given by:

$$H_y^{\text{inj}} = 10^{-6} \sum_{zhdtp \in \mathbb{P}^{\text{inj}}} (n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} \mathcal{P}_{pzhdty} \alpha_{\text{H}_2,py}) \quad \forall y \in \mathbb{Y} \quad (5)$$

In this equation, hydrogen injection may be via partial injection, or completely converted gas grids: these technologies make up the subset $p \in \mathbb{P}^{\text{inj}}$. \mathcal{P}_{pzhdty} is the total operating rate of all technologies of type p in spatial zone z during a given time interval (hour h of day type d in season t of decade y). $\alpha_{\text{H}_2,py}$ is the rate at which a single technology p consumes or produces hydrogen: therefore the product of \mathcal{P}_{pzhdty} and $\alpha_{\text{H}_2,py}$ (for $p \in \mathbb{P}^{\text{inj}}$) is the total rate of injection of hydrogen in a given time interval (in MW). Finally, the parameter n_h^{hd} gives the duration of each hourly interval h , n_d^{dw} gives the number of day types d in a week, and n_t^{wt} gives the number of weeks in season t .

The optimisation seeks the system with the lowest overall cost that meets this constraint. In practice, these scenarios could represent a tradeable obligation certificate scheme, where each gas supplier has an obligation to inject a level of hydrogen into the gas grid. Three scenarios are included in this set, with required injection levels in the final decade of 100 TWh/yr, 200 TWh/yr and 300 TWh/yr respectively. There is no minimum level in the first decade, and the minimum level rises progressively in the following decades. For comparison, the energy supplied to the GB natural gas distribution grid in 2019 was approximately 480 TWh [79].

3.2.2.2. Hydrogen injection feed-in tariffs.

The second set of scenarios use a price-driven incentive: a feed-in tariff (FIT) is paid for each MWh of hydrogen injected into the gas distribution grid. The FIT is paid for either partial injection or 100% injection into converted natural gas distribution grids. The FIT payment acts as a revenue to the system, therefore

has a negative value when included in the optimisation objective function, which is the minimisation of total cost. The total cost impact of FIT payments can thus be defined as follows:

$$\mathcal{J}_{Cost,y}^{FIT} = -H_y^{inj} V_y^{FIT} D_{Cost,y}^{OM} \quad \forall y \in \mathbb{Y} \quad (6)$$

In this equation, H_y^{inj} is the total hydrogen injected per year in period y , as defined in Equation 5, V_y^{FIT} is the value of a FIT payment (in £/MWh), and $D_{Cost,y}^{OM}$ is the discount factor that discounts the annual costs/payments in period y back to the present day. In the model, the FIT payments are seen as a system revenue and are included in the optimisation objective function. In reality, this FIT payment would be an additional revenue to the gas supplier, and would be paid by the government (or eventually added to consumer gas bills).

Three scenarios were modelled with different FITs. In each scenario, no FIT is paid in the first decade, followed by a constant FIT in the three remaining decades. The modelled FITs were chosen based on previous work, where FITs of up to £50/MWh were found to be sufficient to incentivise partial hydrogen injection into gas grids [5]. In this study, the FIT has been extended to also apply to 100% hydrogen injection.

3.2.2.3. Hydrogen boiler capital grants.

Finally, scenarios were modelled with direct capital grants for domestic and commercial hydrogen boilers. Within the VWM, this policy was modelled as a reduction in the capital cost of the boiler technologies (which would thus reduce the overall cost in the optimisation objective function). In practice, this cost would be covered by the government. In both cases, the grants are available in the third and fourth decades. The grant is worth 50% of the boiler capex in the first case, and 100% of the boiler capex in the second case.

3.2.3. Sensitivity scenarios

In addition to the scenarios presented above, a series of sensitivity scenarios were modelled, exploring the effects of two key assumptions. The full details of these scenarios are provided in the supplementary material.

3.2.3.1. Discount rate.

Given that the optimisation process includes decisions and costs over several decades, the net present cost approach is used, where future costs are discounted to the present day. This discounting reflects the time value of money and means that future impacts have a lower weighting in the overall objective function than present-day impacts.

The discount rate may affect scenario results. For example, Emmerling et al. [80] assessed the impacts of discount rates ranging between 1% and 8% on decarbonisation outcomes in integrated assessment models and found that lower discount rates resulted in more action sooner and less need for NETs in the future. For related reasons, Stern [81] proposed that a discount rate of 0.1% be used when modelling the economics of climate change.

A discount rate of 3.5% was used for cost impacts in the main scenarios in this study, in line with UK government guidance [82]. However, sensitivity scenarios were also modelled with discount rates of 0.1% and 8%. As the discount rate is most likely to affect decarbonisation decisions, such as when to invest in decarbonisation and the impacts of CO₂ prices, the discount rate sensitivities were performed for the “decarbonisation” scenarios detailed in Table 7.

3.2.3.2. Electric heat pump coefficient of performance.

Electric heat pumps are seen as a valuable option for heat decarbonisation due to their high coefficient of performance (COP); Quarton and Samsatli [5], for example, found that electric heat pumps may be preferred to conversion of gas grids to hydrogen due to the greater energy efficiency from production end-use. However, there is some uncertainty in the COP that may be achievable by electric heat pumps. In the main scenarios in this study, COPs of 2.5 and 4 were assumed for domestic heat pumps and commercial heat pumps, respectively. Sensitivity scenarios were modelled with a COP of 2 for both domestic and commercial heat pumps, to determine whether this lower COP would affect electric heat pump uptakes and, consequently, hydrogen uptake. These sensitivities were performed for the scenarios with hydrogen-focussed policies detailed in Table 8.

3.3. Implementation

The VWM was implemented in AIMMS (Advanced Interactive Multidimensional Modeling System) and solved with the CPLEX solver. Each scenario includes approximately 200,000 variables, of which around 4,000 are integer variables, and 330,000 constraints. The optimisation was performed on a workstation with 10 cores and 128 GB RAM. Each scenario took around 30 hours to solve with an optimality tolerance of 2%.

3.4. Interpretation of cost results

All scenarios in this study consider the transition of the GB energy system over four decades from 2020 with the optimisation objective of minimising system net present cost. The system cost includes all of the costs incurred in the utilisation of the resources and installation and operation of the technologies shown in Figure 3, thus representing the overall cost to society, including both costs incurred by energy producers (e.g. installation and operation of a power plant), and costs incurred by consumers (e.g. installation and operation of a boiler in the home or business). Although system cost is useful for comparing the overall cost of different scenarios, additional metrics are described in this section that can be used to explore costs in more detail, including the costs for particular policies or individuals.

Some of the implications of discount rates for optimisation modelling were described in Section 3.2.3. Discounting of future costs also has implications when comparing model results and policies from different decades. In this study, unless otherwise stated, the cost results that are reported are the present-day, discounted costs. However, un-discounted values are reported in some cases where they are more relevant.

3.4.1. Average CO₂ cost

The average CO₂ cost metric was used to compare costs and CO₂ emissions between scenarios. For a given scenario, the overall system costs and emissions are compared to a reference case (the unconstrained CO₂ case), to give the additional cost for each tonne of CO₂ that is saved:

$$C^{\text{CO}_2, \text{avg}} = \frac{\sum_y \mathcal{J}_{\text{Cost}, y}^{\text{total}} - I_{\text{Cost}}^{\text{REF}}}{I_{\text{CO}_2}^{\text{REF}} - \sum_y \mathcal{J}_{\text{CO}_2, y}^{\text{total}}} \quad (7)$$

In this equation $\mathcal{J}_{\text{Cost}, y}^{\text{total}}$ and $\mathcal{J}_{\text{CO}_2, y}^{\text{total}}$ are the total cost and CO₂ impacts in each decade y for the scenario in question, discounted to present day values; in Equation 7 they are summed over all decades y to give total values for the entire time horizon. $I_{\text{Cost}}^{\text{REF}}$ and $I_{\text{CO}_2}^{\text{REF}}$ are the equivalent total cost and CO₂ impacts over the entire time horizon for the reference case (the unconstrained CO₂ case). As a result, a value for the average cost of CO₂ savings is obtained, which has units of £/tCO₂ and is discounted to the present day.

3.4.2. Hydrogen policy cost-effectiveness

A similar metric to the average CO₂ cost was used to assess the cost-effectiveness of policies for incentivising hydrogen. This metric compares overall system costs and hydrogen uptake between a given scenario and a reference scenario. Hydrogen uptake is measured in terms of total hydrogen production and is calculated as follows:

$$H_y^{\text{prod}} = \sum_{z h d t, p \in \mathbb{P}^{\text{H}}} (n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} \mathcal{P}_{p z h d t y} \alpha_{\text{H}_2, p y}) \quad \forall y \in \mathbb{Y} \quad (8)$$

This equation has a similar definition to Equation 5 but is summed over *all* hydrogen-producing technologies, denoted by the subset $p \in \mathbb{P}^{\text{H}}$. Hence, total hydrogen production in decade y is calculated by summing the hydrogen produced by each technology p in spatial zone z , during time interval $h d t$.

In this case, the reference scenario is the “steady” CO₂ budgets scenario, which reaches net-zero emissions by 2050 and has no specific hydrogen incentives. The hydrogen policy cost-effectiveness is defined as the increase in overall system cost compared to the reference case, for each additional MWh of hydrogen produced over the course of the time horizon. It is given by the following equation:

$$C^{\text{H}_2, \text{avg}} = \frac{\sum_y \mathcal{J}_{\text{Cost}, y}^{\text{total}} - I_{\text{Cost}}^{\text{REF}}}{\sum_y H_y^{\text{prod}} - H^{\text{REF}}} \quad (9)$$

where H^{REF} is the total hydrogen produced over the time horizon in the reference case. $C^{\text{H}_2, \text{avg}}$ signifies the effect on the discounted overall system cost of the increased hydrogen usage in the system (units of £/MWh).

3.4.3. Marginal CO₂ cost

A marginal CO₂ cost metric was used to represent the change in overall system cost for a change in total system emissions of 1 tCO₂, calculated using the shadow price property within AIMMS. The shadow price of a constraint within AIMMS is defined as “the marginal change in the objective value with respect to a change in the right-hand side (i.e. the constant part) of the constraint” and is calculated by the optimisation solver [83].

Therefore for this study, the shadow price of the CO₂ budget constraint (shown in Equation 2) in a given decade y gives the change in the overall system cost (the objective function) that arises if the allowable level of emissions in a decade is increased by 1 tCO₂. This value is described as the marginal cost of CO₂, $C_y^{\text{CO}_2, \text{marg}}$. As a different CO₂ budget can be imposed in each decade, $C_y^{\text{CO}_2, \text{marg}}$ has a different value for each decade.

Scenarios with enforced CO₂ budgets may represent a CO₂ cap-and-trade scheme, assuming that: all CO₂ emissions across the entire system (e.g. including domestic emissions) are included in the scheme; there is perfect operation of the scheme; and emissions allowances can be efficiently traded between emitters. The marginal CO₂ cost, $C_y^{\text{CO}_2, \text{marg}}$, represents the cost of an emitter reducing their emissions by 1 tCO₂, discounted to present day values. The price at which an emitter would be willing to purchase a CO₂ allowance is likely to be equal to this value, although un-discounted in order to represent the actual price paid at that time. Therefore the estimated CO₂ allowance trading price is given by:

$$T_y^{\text{CO}_2} = \frac{-C_y^{\text{CO}_2, \text{marg}}}{D_{\text{Cost}, y}^{\text{OM}}} \quad \forall y \in \mathbb{Y} \quad (10)$$

3.4.4. Policy cost

Some scenarios in this study include fiscal intervention by the government: in particular, CO₂ taxes represent a cost to the energy system (and a revenue to the government), whilst hydrogen FITs are a revenue for the energy system (but a cost to the government). The total financial values of these interventions, in (discounted) present day terms, have already been defined in Equation 3 (CO₂ tax) and Equation 6 (hydrogen FITs), and give an indication of the scale of government intervention in a scenario.

Although the financial values of these interventions are included in the optimisation objective function, they are removed from the overall system costs that are presented in the results in this study. This means that scenarios can be compared without financial interventions affecting the overall system cost: any differences in costs are caused by differing decarbonisation pathways and investment decisions that arise from the policies, rather than the policies themselves. This effectively assumes that the policy is revenue-neutral, in that any costs or revenues imposed on the energy system by the government would be balanced by other policies elsewhere.

3.4.5. Consumer costs

To assess the consumer impact of different decarbonisation pathways, two 2050 consumer heating bills were estimated from the value chain optimisation results: one assuming electrification and the other hydrogen.

Although the optimisation minimises net present (i.e. discounted) costs, the typical consumer’s energy bill was post-calculated using un-discounted costs, as this what the consumer would actually pay.

The value chain optimisation results include the numbers of technologies installed in each decade, their operating regimes, and the total costs of installing and operating the technologies. Therefore the average unit cost (£/MWh) for producing a given resource, such as hydrogen, electricity or heat, can be calculated, although assumptions are required when technologies and infrastructures are shared between multiple value chains.

The electrification of heating scenario was calculated from the “steady” CO₂ budgets case, in which the majority of heating is electrified by 2050, and represents an approximate annual heating bill for a typical domestic consumer using an electric heat pump. The unit cost of electricity production was calculated from the sum of all of the electricity production technologies in the scenario results, including wind power, solar PV, nuclear power and natural gas power plants. The unit costs for electricity transmission and distribution were each based on the associated technologies within the VWM, and assumed to be divided equally between each MWh of electricity flowing through the networks. Annual electricity consumption was taken from the average consumption of a domestic electric heat pump in the final decade of the scenario.

Other fixed costs that would usually be included in a consumer energy bill, such as supplier overheads, are not included in the VWM, so were assumed to be the same, per MWh of electricity, as in present-day electricity bills. These data were taken from Ofgem [84]. Finally, the annualised cost to the consumer of installing the heat pump and any other necessary in-home upgrades was calculated, assuming that the initial capital investment would be annualised over the lifetime of the heat pump. Although these costs would not typically be included in an energy bill, they still represent a consumer cost, therefore it is important consider them when comparing heating scenarios.

The hydrogen heating scenario was calculated from the “high” hydrogen injection obligations case, where there is a required minimum injection of hydrogen into the gas grids of 300 TWh/yr in 2050-2060. The annual heating bill was calculated in a similar manner to the electrification bill: unit costs were calculated for hydrogen production, transmission, storage and distribution. The hydrogen production cost was calculated from the costs of the hydrogen production technologies in the scenario results, including the cost of CCS, which was assumed to be shared between all users, including SMR plants and other natural gas users. The costs of hydrogen transmission and storage infrastructure from the scenario results were assumed to be shared between domestic, commercial and industrial consumers of hydrogen. Likewise, hydrogen distribution costs, including conversion of existing gas grids to hydrogen, were assumed to be shared between all users of distributed hydrogen, based on their energy consumption. Other fixed costs were assumed to be the same as in present-day natural gas bills [85]. Finally, annualised costs of a new hydrogen boiler and any necessary in-home safety checks for conversion from natural gas to hydrogen were included.

For comparison, a benchmark present-day bill for a consumer using natural gas for heating was also estimated from Ofgem [85] and BEIS [86] data. For equivalence with the other scenarios, annualised costs for a new natural gas boiler were also included.

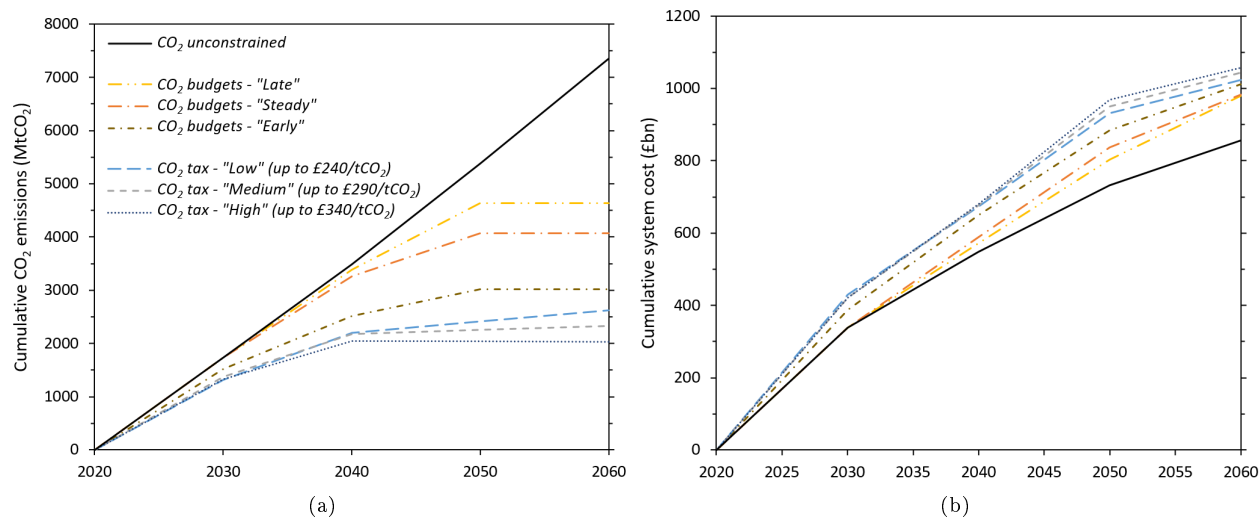


Figure 4: Cumulative CO₂ emissions (a) and costs (b) in a selection of scenarios. Costs are overall system costs, discounted to 2020.

4. Results and discussion

Results from the optimisation scenarios are presented and discussed in this section. The results from the scenarios with policies for penalising existing technologies, to achieve system decarbonisation, are discussed first. Then, the uptake of hydrogen in the scenarios is considered, including scenarios with and without additional policies to support hydrogen technologies. Finally, the scenario results are used to consider the impact on consumer costs of different decarbonisation pathways, in particular electrification vs. conversion of gas grids to hydrogen.

4.1. Policies for decarbonisation

Figure 4 shows the cumulative costs and CO₂ emissions for a selection of scenarios. The “CO₂ unconstrained” scenario has the lowest overall cost but the highest emissions, with annual emissions increasing by the final decade, due to rising energy demands and a continued high contribution of natural gas to the energy supply. The scenarios with CO₂ budgets and CO₂ taxes all have lower CO₂ emissions, but with different decarbonisation trajectories and costs.

4.1.1. CO₂ budgets

The emissions limits in the CO₂ budgets scenarios are strictly controlled, so all achieve net-zero emissions in the final decade (indicated by zero slope in the final decade of Figure 4(a)). However, the different budget trajectories in each case result in different overall levels of emissions and net-present (discounted) system costs. As Figure 4(a) shows, cases with more stringent budgets in the early decades result in significantly lower emissions overall. For example, the total CO₂ emitted over four decades in the “early” decarbonisation case is more than 1.6 GtCO₂ lower than in the “late” decarbonisation case.

Despite the differences in total CO₂ emitted, the range in costs of the different CO₂ budget scenarios is small: for example, the “early” decarbonisation case is only 3% more expensive than the “late” decarbonisation case. As Figure 4(b) shows, the cases with more stringent CO₂ budgets in the earlier decades incur greater costs in these decades, but by the final decade costs converge. This suggests that the overall costs of decarbonisation arise predominantly from shifting the system to net-zero, and the timescales over which this transition is achieved is not as significant.

As a result, if the objective is to minimise the total CO₂ emitted into the atmosphere, earlier decarbonisation is more cost-effective (per unit of prevented CO₂ emissions). Comparing the CO₂ budgets scenarios to the CO₂ unconstrained scenario, the “late” decarbonisation case saves a total of 2.7 GtCO₂, whilst the “steady” and “early” cases save 3.3 GtCO₂ and 4.3 GtCO₂ respectively. Since each case has similar overall costs, this means that the “late” case has a higher average cost of CO₂ saved: £45/tCO₂ compared to the unconstrained case, whilst the “steady” and “early” cases have average CO₂ costs of £38/tCO₂ and £36/tCO₂ respectively.

If the CO₂ budgets were to represent a CO₂ cap and trade scheme, the approximate CO₂ allowance trading price can be calculated from Equation 10. For net-zero emissions in 2050-2060, the trading price would be approximately £1720/tCO₂ in the “late” decarbonisation case, £600/tCO₂ in the “steady” case, and £460/tCO₂ in the “early” case. Although these potential CO₂ trading prices are very high, it is important to note that they reflect the cost of removing the final tonne of CO₂ of emissions from the system, and the majority of emissions can be removed at lower cost.

The wide range in CO₂ allowance trading prices between the cases is also significant. The very high trading price, in excess of £1700/tCO₂, occurs in the “late” case, which has no decarbonisation action until the final decade; the final trading prices are much lower in the cases that have more stringent CO₂ budgets in the preceding decades. This shows that with more decarbonisation early on, a more gradual transition to net-zero can be achieved, and the costs are shared over multiple decades. As a result, the final costs of achieving net-zero are lower, and the resulting CO₂ trading price is more stable.

4.1.2. Carbon tax

Results from the CO₂ tax scenarios can also be seen in Figure 4. Only the “high” taxation case achieves net-zero by 2050-2060, suggesting that a CO₂ tax rate greater than £300/tCO₂ is necessary to incentivise the system to achieve net-zero emissions in 2050.

As Figure 4(a) shows, the CO₂ tax scenarios typically deliver greater levels of decarbonisation in the early decades than the CO₂ budget scenarios (since the cumulative emissions are lower). Clearly this result depends on the modelled CO₂ tax trajectory, with higher taxes leading to greater emissions reductions. The CO₂ tax trajectories that were modelled in this study were linear between the first and last decades. This result shows that lower CO₂ taxes can incentivise initial emissions reductions, when the cost of doing so is lower, but an increasing tax rate is necessary as the net-zero target is approached. This emphasises that stronger policy intervention earlier can be more effective for reducing the total amount of CO₂ emitted.

As was discussed in Section 4.1.1, greater levels of decarbonisation early on result in a lower final marginal cost for achieving net-zero emissions. This explains why the required CO₂ tax rate for achieving net-zero

(more than £300/tCO₂) is lower than the CO₂ trading prices estimated from the CO₂ budgets scenarios (£460/tCO₂ or more). With lower CO₂ tax rates in the early decades, a higher final CO₂ tax is likely to be required to achieve net-zero.

Figure 4(b) shows that the CO₂ tax scenarios are more expensive than the CO₂ budget scenarios. These results do not include the cost of the CO₂ tax itself: it is assumed that the government would re-invest this tax revenue into the energy system. Therefore for reaching a net-zero energy system by 2050, CO₂ taxes appear to be more expensive overall, with an extra cost of £78bn in the “high” CO₂ tax case compared to the “late” CO₂ budget case. Nonetheless, given the lower cumulative level of emissions in the CO₂ tax cases, the average costs per tonne of CO₂ averted are similar for the CO₂ tax cases and the CO₂ budget cases, with a range of £35–38/tCO₂ for the CO₂ tax cases, compared to £36–45/tCO₂ for the CO₂ budget cases. The total system cost (or government revenue) of the CO₂ tax over all decades (Equation 3) ranges from £125bn in the “high” tax case to £156bn in the “low” tax case.

4.1.3. Effect of discount rate

All the scenarios described so far were modelled with a discount rate of 3.5%. However, a sensitivity study was also performed in which the same scenarios were modelled with discount rates of 0.1% and 8%. Detailed results from these scenarios are provided in the supplementary material and are summarised here. The discount rate determines the importance of future costs relative to present day costs. With a discount rate of 0.1%, future costs have almost equal weighting to present-day costs in the optimisation objective function, whilst with higher discount rates the importance of future costs falls.

In the case of CO₂ budgets, this means that with higher discount rates, investment in decarbonisation is delayed until it is essential, as the associated costs are seen to reduce. The level of voluntary early decarbonisation, i.e. the reduction in CO₂ emissions in a given decade beyond what is required by the CO₂ budget, is notably higher in the cases with a discount rate of 0.1% than the cases with higher discount rates. Examples of this voluntary early decarbonisation include earlier investment in renewable electricity generation and long-life infrastructure such as electricity distribution networks. As a result, the cases with a discount rate of 0.1% have lower total CO₂ emissions than the cases with a discount rate of 3.5%: 21% lower in the “late” CO₂ budget case and 11% lower in the “steady” case.

The discount rate also reduces the importance of the costs arising from future CO₂ taxes in the optimisation objective function, thus reducing the impact of future CO₂ taxes. This can be seen in the sensitivity study results: with a discount rate of 3.5%, a CO₂ tax of £340/tCO₂ was required in 2050-2060 to achieve net-zero emissions, but this was achieved with a CO₂ tax of £290/tCO₂ when a discount rate of 0.1% was used.

Finally, given that most decarbonisation spending occurs in later decades, the effect of the discount rate in all scenarios is to reduce the apparent costs of this decarbonisation. This can be seen in the average costs of CO₂ reductions compared to the respective reference cases (with no decarbonisation policies). From all of the CO₂ tax and CO₂ budget cases, the average cost of CO₂ is £80–103/tCO₂ for a discount rate of 0.1%; £35–45/tCO₂ for a discount rate of 3.5%; and £9–12/tCO₂ for a discount rate of 8%.

These results show the importance of the discount rate when considering investment decisions over long time periods. Whilst it is difficult to know what the most appropriate discount rate is for a given assessment, it is essential that the discount rate is taken into consideration when interpreting scenario results.

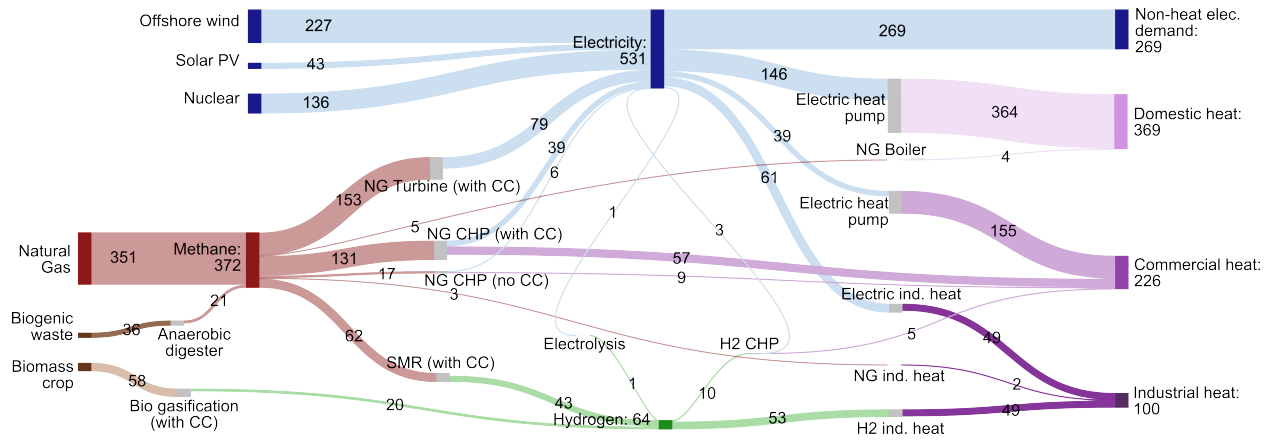


Figure 5: Sankey diagram of annual energy flows in a net-zero energy system in 2050-2060. The results shown are from the “steady” CO₂ budgets scenario. The numbers denote energy flows in TWh/yr, and flows smaller than 1 TWh/yr are not shown.

4.2. Policies for incentivising hydrogen

The scenarios for supporting hydrogen technologies are studied in more detail in this section, including the resulting energy system design and the role of hydrogen. First, the uptake of hydrogen in a scenario without any specific hydrogen policies is considered. This is then compared to further scenarios with different policies supporting hydrogen technologies.

4.2.1. Net-zero system without hydrogen incentives

To compare the effectiveness of policies supporting hydrogen technologies, first a scenario is considered in which no specific hydrogen policies were included. The “steady” CO₂ budgets scenario is used for this purpose, as this represents the most probable decarbonisation pathway, reaching net-zero emissions by 2050 with equal reductions in each decade. In any case, the details of the final energy system in the other CO₂-budgets scenarios are similar. Figure 5 shows a Sankey diagram of the annual energy flows in the final decade of the “steady” CO₂ budgets scenario.

The optimised net-zero energy system includes a balanced mix of electricity supply. Offshore wind and nuclear power are the main contributors, supplying 43% and 25% of annual supply respectively. Natural gas with CO₂ capture makes up 22% of annual supply (all captured CO₂ is sequestered offshore). A small amount of electricity balancing is provided at peak times by natural gas without CO₂ capture and hydrogen combined heat and power (CHP): each contributes around 1% to annual electricity supply. The heat from the hydrogen CHP is used for commercial heating applications.

The optimal decarbonised heat supply is less diverse, with 87% of domestic and commercial heat demands being satisfied by electric heat pumps. As found in previous work, electric heat pumps appear in the optimal heat supply chain because the heat pump COP results in a high heat supply chain efficiency compared to the alternatives [5]. Given the prevalence of electric heat pumps in the scenario results, a sensitivity study was performed in which lower heat pump COPs were assumed. This had some impact on electric heat pump uptake but they were still the preferred technology, satisfying 73% of domestic and commercial heat demands in 2050-2060; further details and discussion can be found in the supplementary material. Other than electric

heat pumps, the other main contribution to commercial heating is from natural gas CHP with CO₂ capture. Industrial heating is shared between electricity (54%) and hydrogen (44%).

The role of hydrogen in the optimised net-zero system is fairly limited, with an annual supply of only 64 TWh/yr. The main role for hydrogen is for industrial heat, although some is used in CHP, mostly at peak times. Hydrogen supply is predominantly from SMR with CO₂ capture (67%). Bioenergy also makes up 31% of the hydrogen supply, which utilises almost all of the primary biomass available. The bioenergy-to-hydrogen value chain is responsible for 2% of final energy demands and delivers a total of 12 MtCO₂/yr of negative emissions. Electrolysers are used to convert excess renewable electricity to hydrogen. However, with large electricity demands for heating, there is limited low-cost electricity available. Therefore, hydrogen production from power-to-gas contributes only 1% of the annual total. Although this contribution of hydrogen is relatively small, it arises without any specific policy support.

4.2.2. Effect of hydrogen incentives

Various scenarios with incentives for hydrogen have been modelled, including: obligations for a minimum level of hydrogen injection into the gas grid, FITs for each MWh of hydrogen injected into the gas grid, and capital grants for hydrogen boilers. Each of these scenarios also included CO₂ budgets, matching the budgets in the “steady” CO₂ budgets case, to ensure that the system reaches net-zero emissions by 2050.

Figure 6 shows details of total hydrogen production and consumption in each decade of each scenario. The “steady” CO₂ budgets case is also included, representing the comparative scenario in which no hydrogen incentives are included.

As was described in Section 4.2.1, there is some hydrogen usage in the “steady” CO₂-budgets case, without any specific hydrogen incentives. This is focussed on the industrial sector and only arises in the final decade, when the net-zero CO₂ budget is in place.

The hydrogen injection obligations scenarios, where a minimum level of injection is enforced, have a greater uptake of hydrogen. In these scenarios, most hydrogen is produced from SMR with CCS and is used for domestic and commercial heating, supplied through natural gas distribution grids that have been converted to hydrogen. Total hydrogen usage rises with the gas grid injection obligation in each decade. Further details of the “high” hydrogen injection obligations case are shown in Figure 7 to give an indication of the hydrogen value chains used.

Figure 7 shows that hydrogen technologies are installed in most zones in 2050-2060, with most hydrogen production (via SMR with CCS) focussed in Central and Northern England. Consequently, there is greater use of hydrogen for heating in these zones, via converted natural gas distribution grids. Further from the centre of the country, hydrogen uptake is lower, and electrification of heating is preferred. However, many zones still have power-to-gas installations, with a total installed capacity of 11 GW. The power-to-gas absorbs excess electricity at off-peak times and either feeds hydrogen into the gas grid or uses it in industrial or CHP plants.

A total storage capacity of over 3 TWh of underground hydrogen storage is installed in the system, which helps to compensate for the large seasonal variations in demand for hydrogen for heating. Although hydrogen

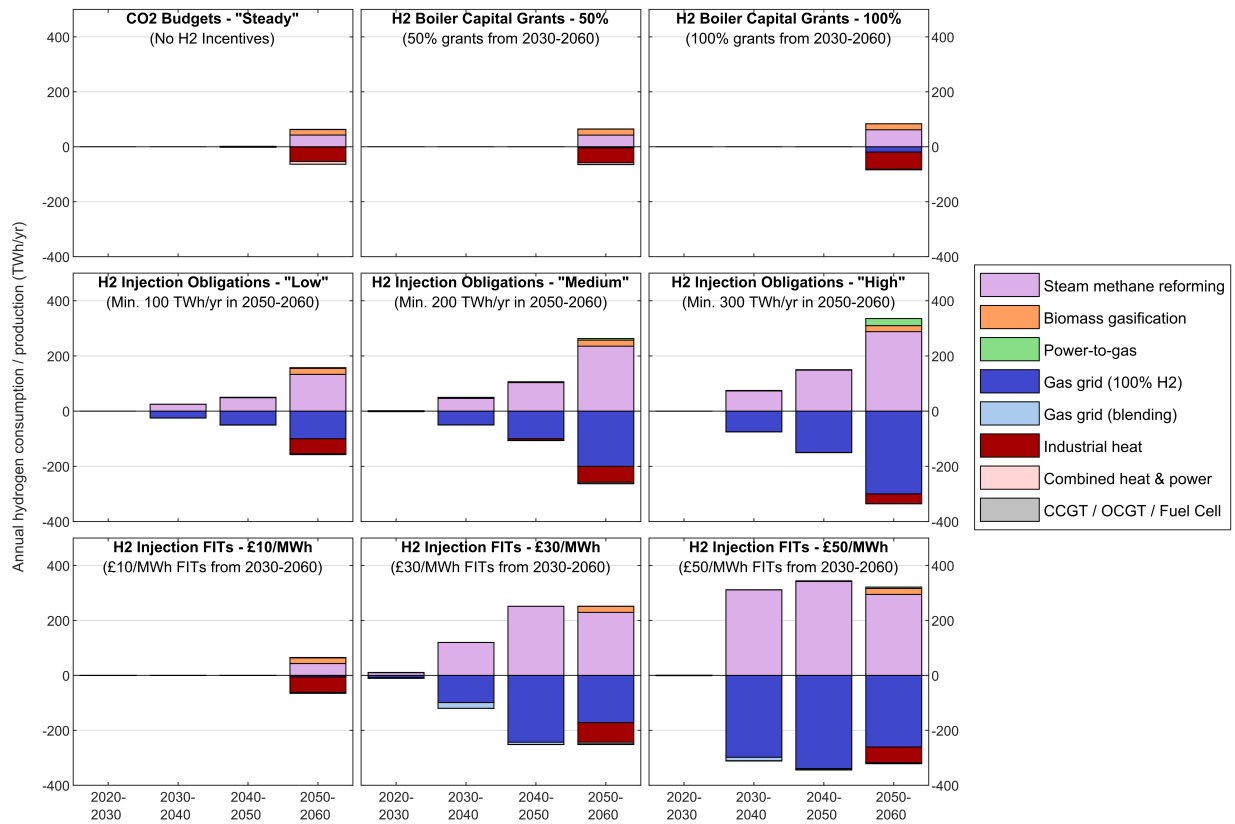


Figure 6: Hydrogen production and consumption by technology or application in each decade, for each scenario. Positive values denote hydrogen production, negative denote consumption.

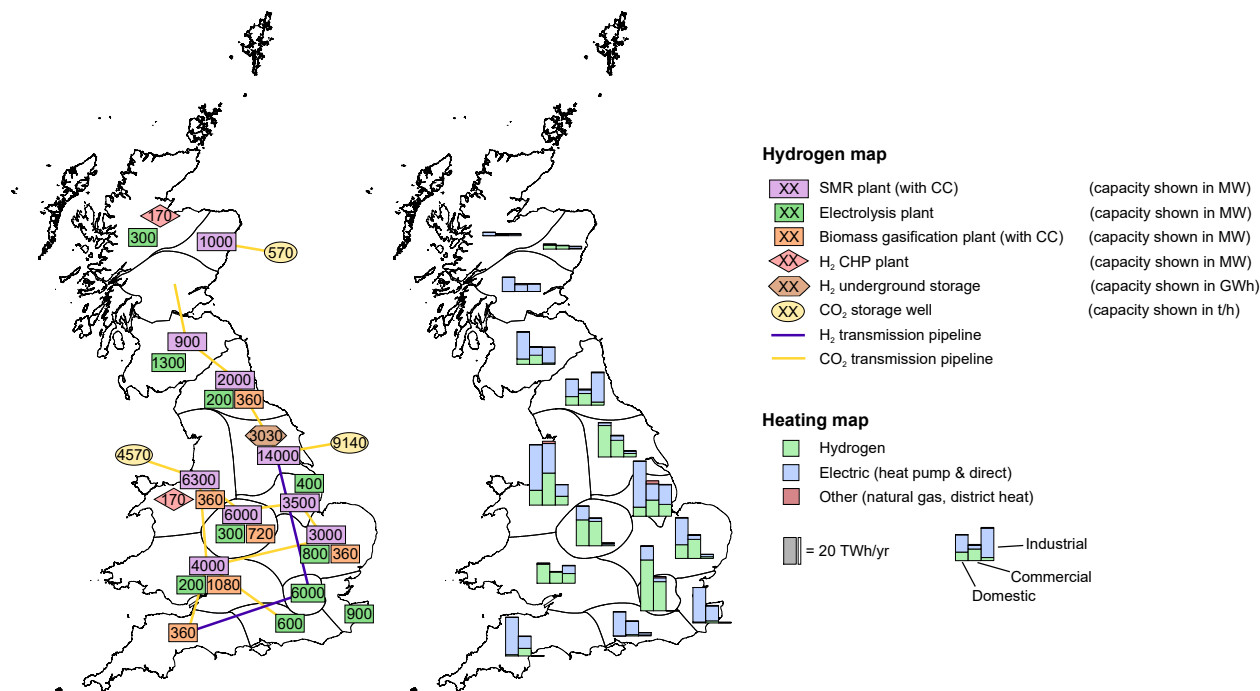


Figure 7: Details of the energy system in the scenario with a minimum of 300 TWh/yr of hydrogen injection in 2050-2060 (“high” hydrogen injection obligations case). Left: map of installed capacities of hydrogen and related technologies in each spatial zone in 2050-2060; some technologies are not shown, including the natural gas transmission system, electricity generating technologies and hydrogen pressure vessel storage. Right: map of annual heat provision in each spatial zone in 2050-2060; the columns in each zone represent domestic, commercial and industrial heating respectively from left to right.

pressure vessel storage is not shown in Figure 7, it is installed in almost all zones, with a total storage capacity of 260 GWh. This is used to balance within-day imbalances in hydrogen supply and demand. There is an increased need for within-day storage for hydrogen compared to an equivalent natural gas system, because a natural gas system can utilise the linepack flexibility of its transmission and distribution pipelines to a greater extent. Due to the lower energy density of hydrogen, the linepack flexibility (storage capacity) of a pipeline may be 70-83% lower with hydrogen than with natural gas under the same operating conditions [5].

As Figure 6 shows, hydrogen injection FITs are also effective for incentivising increased hydrogen usage. A FIT of £10/MWh is insufficient to incentivise any further hydrogen usage but FITs of £30/MWh and £50/MWh result in a significant increase. In these cases, FITs are available from 2030 onwards, causing a greater uptake of hydrogen from this date onwards. In the final decade of the £50/MWh case, 261 TWh/yr of hydrogen is used in converted gas grids, 57 TWh/yr is used in industry, and 4 TWh/yr is used in either hydrogen turbines or CHP plants.

Partial injection of hydrogen into gas grids is also rewarded by the FIT, and has greatest uptake in the early decades. For example in the £50/MWh case, 12 TWh/yr of hydrogen is blended into the natural gas distribution network in 2030-2040, representing an average injection of 19 vol.% over the entire year. However, due to the more stringent CO₂ budgets in later decades, natural gas usage is reduced, so there is little opportunity for partial hydrogen injection. Capital grants for hydrogen boilers are less effective for incentivising hydrogen. With 100% capital grants in place, 19 TWh/yr of hydrogen is used in gas grids, 62 TWh/yr is used in industry, and 2 TWh/yr is used in CHP plants. Capital grants of 50% have a negligible impact on hydrogen usage.

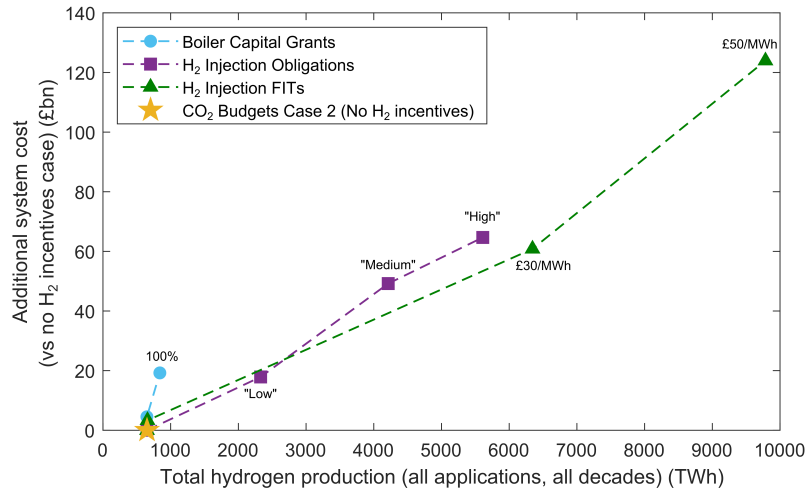


Figure 8: Total hydrogen production and overall system cost in scenarios with different hydrogen incentives. Total hydrogen production is for all applications, including industrial, commercial, and domestic demands. Overall system cost is the net present (discounted) value and is measured relative to the case with no hydrogen incentives (CO₂ Budgets Case 2).

There is little variation between scenarios regarding how hydrogen is produced or used. All scenarios have a similar level of hydrogen usage in industry in the final decade, of around 60 TWh/yr (which also exists when no hydrogen-specific incentives are included). Otherwise, hydrogen usage is focussed on the gas grid (unsurprising, given that this is the focus of the policy incentives). Although SMR with CCS is preferred for most hydrogen production, biomass gasification consistently provides around 21 TWh/yr of hydrogen.

The biomass to hydrogen value chain is valuable in all of the scenarios due to the negative CO₂ emissions that it provides, and therefore in most scenarios the total biomass utilisation is close to its maximum availability in the final decade. Other biomass value chains, such as for electricity and heat, were beyond the scope of this hydrogen-focussed study but may be more favourable than the biomass-to-hydrogen value chain considered here.

A lower COP of 2 for both domestic and commercial electric heat pumps had a limited effect on the results in Figure 6. More details and discussion can be found in the supplementary material.

The cost effectiveness of the different policies can also be compared. Figure 8 shows the total hydrogen production across all decades for each scenario, plotted against the overall system cost. The overall system cost is measured relative to the “steady” CO₂ budgets case, thus showing the additional cost to the system of the hydrogen intervention. These cost results assume that policies are revenue-neutral: for example, the payments made by the government for FITs or capital grants would be recouped elsewhere, e.g. through taxation. Therefore increases in system cost are not affected by the financial value of the policy intervention but only by its influence on the overall system behaviour.

As Figure 8 shows, hydrogen injection obligations and FITs both show a similar relationship between the increase in overall hydrogen usage and the impact on overall system costs. However, this policy cost-effectiveness, as defined in Equation 9, shows some variation depending on policy type and magnitude.

Capital grants are clearly the least cost-effective incentive. The 50% capital grant has a negligible impact on hydrogen usage, whilst increasing system costs by £4.5bn compared to the case with no hydrogen incentives.

The 100% capital grant is marginally more effective, but the hydrogen policy cost-effectiveness is over £100/MWh.

Figure 8 shows that the hydrogen policy cost-effectiveness is quite consistent for the hydrogen injection obligations. In the “low” obligation case, with a minimum injection of 100 TWh/yr in 2050-2060, the increase in system cost is equal to £11 for each additional MWh of hydrogen production; this value rises to £14/MWh in Case 3 (with 300 TWh/yr of injection in 2050-2060). With a lower overall level of hydrogen in the system, the most cost-effective applications are used first (for example, only gas grids local to hydrogen production plants are converted); as the overall hydrogen injection requirement rises, more of the gas grid will be converted to hydrogen, but potentially in regions where the cost difference between hydrogen and the alternative (e.g. electrification) is greater.

As was shown in Figure 6, FITs of £10/MWh have a negligible effect on hydrogen uptake. However, FITs of £30/MWh are quite cost-effective, increasing overall hydrogen uptake at a system cost of £11/MWh. In the £50/MWh case, the cost-effectiveness falls to £14/MWh, as larger FITs incentivise hydrogen injection in locations with a greater cost difference to the alternative. The total magnitude of FIT payments in the final decade is £5bn/yr in the £30/MWh case and £13bn/yr in the £50/MWh case (un-discounted values).

Each of the scenarios in this section was constrained by the same CO₂ budgets and therefore has the same pathway of CO₂ emissions throughout its time horizon. Therefore the average CO₂ costs in these scenarios are driven by the additional overall system costs shown in Figure 8. The scenarios with lower levels of intervention, such as the “low” injection obligations case, have an average CO₂ cost of around £44/tCO₂; the scenarios with moderate intervention, including the “medium” and “high” injection obligations cases and the £30/MWh FIT case, have average CO₂ costs of £54–58/tCO₂; finally the £50/MWh case has an average CO₂ cost of £76/tCO₂.

4.3. Consumer costs

Overall system costs are useful for comparing the relative costs of different decarbonisation pathways but in reality, it is likely that any energy policy costs will be borne by the consumer. Therefore, it is also valuable to calculate and compare consumer costs. Figure 9 presents estimates for annual consumer heating bills for three different heating scenarios. Details on how these bills were calculated are given in Section 3.4.5.

As can be seen from Figure 9, electrification results in lower overall consumer heating bills than hydrogen. The annual electrification bill is £715/yr, which is 10% greater than a typical present-day natural gas bill (£708/yr, based on 15 MWh/yr); meanwhile the hydrogen bill is £1070/yr, which is 51% higher than the natural gas benchmark.

In the electrification scenario, the energy costs are relatively low, at only £18 per MWh of heat consumed. There are two reasons for this. First, the cost of electricity production in the final decade of the optimised electrification scenario is relatively low, at approximately £43/MWh. This is the average cost for the entire energy mix (as shown in Figure 5), including the natural gas and hydrogen peaking plants. Second, heat pumps require much less energy input to produce 1 MWh of heat than using a hydrogen boiler. The annual electricity consumption for this bill was 5.1 MWh/yr, which is the average consumption for a household with a heat pump in the scenario results.

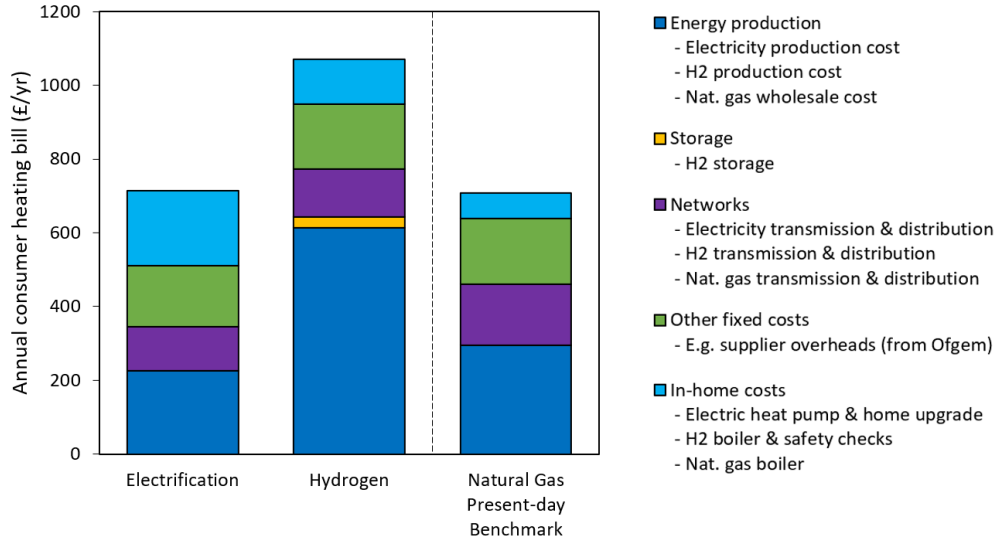


Figure 9: Annual consumer heating costs for three different heating scenarios. The electrification scenario is based on a domestic electric heat pump and is calculated from the results of the “steady” CO₂ budgets case. The hydrogen scenario is based on conversion of gas grids to hydrogen and is taken from the “high” hydrogen injection obligations case. Finally, a typical present-day natural gas bill for a UK consumer is presented for comparison (based on data from Ofgem [85] and BEIS [86]).

Infrastructure costs (including transmission and distribution) are also relatively low in the electrification scenario, despite the fact that electricity infrastructure is relatively expensive on a per-capacity basis [73]. This is also partly due to the heat pump coefficient of performance: for each 1 MWh of heat delivered, only 0.4 MWh of electricity must be distributed. Furthermore, in the electrification scenario, electricity infrastructure is used to deliver both heat and non-heat electricity demands. This has two benefits: the infrastructure costs are shared across a larger total energy demand; and the non-heat demands are less variable, so the overall utilisation factor for the electricity infrastructure is higher, resulting in a lower infrastructure cost per MWh of capacity.

Finally, the in-home costs associated with electrification, including installation of a heat pump and any further home upgrades, such as installing new radiators, are a significant contributor to the annual cost to the consumer. Although these are larger than in the other cases, they are offset by the other cost components being cheaper. The equivalent consumer heating bill was also calculated for the heat pump sensitivity case, with a COP of 2, and the annual bill was found to be £863/yr: 21% greater than the electrification scenario with a COP of 2.5, but still 19% lower than the hydrogen scenario.

As Figure 9 shows, the annual heating bill in the hydrogen scenario is dominated by the energy costs of the hydrogen itself. The cost of the hydrogen production was based on SMR with CCS, with an average cost of £44/MWh, driven primarily by a natural gas price of £24/MWh and the costs of the SMR + CCS installations. SMR with CCS contributes 81% of hydrogen production in the scenario results: the costs of hydrogen from bioenergy and power-to-gas were not included, as these value chains have wider system interactions that are harder to account for. For example, the average bioenergy hydrogen cost in the scenario is around £126/MWh, but this does not account for the negative emissions benefits of this value chain. Meanwhile power-to-gas primarily uses excess electricity with an uncertain price: assuming that the electricity is zero-cost, the average power-to-gas hydrogen cost is around £19/MWh.

Compared to the electrification scenario, the hydrogen scenario does not benefit from an apparent efficiency of more than 1, so the final contribution of hydrogen costs to the heating bill is £48 per MWh of heat (compared with £18/MWh for the electricity scenario). The annual hydrogen consumption for this bill was 13.9 MWh/yr, which is the average consumption for a household with a hydrogen boiler in the scenario results. This value is lower than the benchmark present-day natural gas consumption of 15 MWh/yr, mainly due to projected improvements in household thermal performance between now and 2050.

The costs of the distribution infrastructure in the hydrogen case are very similar to the costs in the present-day natural gas bill and are driven by the fixed operating costs of the networks. The investment costs arising from converting natural gas grids to hydrogen, assumed to be £3500 per MW of grid capacity [73], contribute only £1.60 to the annual consumer heating bill.

Therefore, despite the relatively high costs of installing an electric heat pump, the electrification scenario is cheaper than the hydrogen scenario overall. Between the three options shown in Figure 9, most cost components are very similar. However, the high energy costs for hydrogen result in a significantly higher annual cost in this scenario. These results also highlight the limited effectiveness of capital grants, for either the conversion of distribution grids to hydrogen or the installation of hydrogen boilers in homes, as neither of these is sufficient to reduce the consumer cost to less than the equivalent cost of electrification.

It may be possible for hydrogen to be produced more cheaply, for example through power-to-gas with low-cost electricity. However, the results presented in Figure 9 represent the optimal supply chain identified in this study for delivering 300 TWh/yr of hydrogen to the gas grid. At this scale, SMR is the lowest-cost option. The results in this study suggest that the capacity for low-cost power-to-gas is limited, due to a limited availability of low-cost electricity, and competing electricity demands. For example, in all of the scenarios with various hydrogen incentives presented in Figure 6, the largest contribution of power-to-gas is 25 TWh/yr.

5. Conclusions

This study examined energy and decarbonisation policies and evaluated their applicability to hydrogen. The Value Web Model, an energy value chain optimisation model, was developed and applied to a representative national energy system to quantify the effects of different policies on the pathway to a net-zero energy system and the role of hydrogen within the system. This is the first study to use spatio-temporal value chain optimisation to evaluate the effectiveness of energy policies.

The optimisation results showed that both CO₂ budgets and CO₂ taxation can achieve net-zero emissions but result in different system costs and decarbonisation trajectories. Policies that promote earlier reductions in CO₂ emissions are slightly more expensive overall but result in significantly lower total emissions, hence lower costs per tonne of CO₂ saved. For carbon cap-and-trade schemes, earlier decarbonisation allows costs to be spread over a longer time period, with a lower final CO₂ trading price. CO₂ prices depend on pricing policy, e.g. taxation or trading, and may need to be in excess of £300/tCO₂ in 2050 to achieve net-zero emissions. These results suggest that the overall policy choice is less important than ensuring that the scheme is well-designed. Ensuring that the policy is robust and incentivises early emissions reductions can lead to both lower overall emissions and less sharply rising costs as the net-zero deadline approaches.

Without direct policy support, hydrogen could have a significant role in industry in a net-zero system but limited penetration potential elsewhere. Considering the costs of conversion of gas grids to hydrogen, for example, consumer heating bills may be 50% higher when using hydrogen for heating than when using electric heat pumps. This cost difference is driven by energy costs; infrastructure costs for the two heating value chains were found to be similar.

Obligations and feed-in tariffs for injection of hydrogen into gas grids were found to be similarly effective for incentivising hydrogen technologies, with overall system costs increased at a rate of £11–14 per additional MWh of hydrogen used. Capital grants for hydrogen boilers, however, were not found to influence the optimal decarbonisation pathway.

Steam methane reforming (with CO₂ capture and storage) was found to be the preferred hydrogen production method in all scenarios with a significant level of hydrogen uptake. Both power-to-gas and biomass gasification were found to make only modest contributions, though they are valuable for providing system flexibility and negative CO₂ emissions, respectively, due to limited availability of low-cost electricity and sustainable biomass sources.

The results highlight that policymakers should be cautious in designing policies to support specific energy technologies and should carefully consider the impact on consumers. Different technology pathways (e.g. hydrogen for heating versus electrification) may have similar overall system costs but consumer costs could be significantly different.

Future work includes modelling with higher spatio-temporal resolutions for more insight into the flexibility-provision of the technologies considered, although computational tractability is a challenge. Value chain optimisation is a valuable tool for exploring the implications of net-zero energy systems and negative-emissions technologies (NETs), and this study has begun to do this. It is expected that NETs will start to play a role in decarbonisation when the marginal system cost of reducing CO₂ emissions exceeds the unit NET costs; thus, the NETs would be used to decarbonise the last few percent of emissions. Further work in this area would be valuable in determining the optimal levels of NET investment required and to examine the wider impacts of NETs such as biomass energy with CO₂ capture and storage (BECCS).

Although this study provides insights into the optimal pathways to reach net-zero and the potential effects of different policy interventions, challenges exist in converting optimisation results into real-life policy actions. For instance, CO₂ budgets were found to be the most efficient way of achieving a net-zero system by 2050. However, this assumes that all emissions across the system can be tracked and controlled, which would be challenging to implement. Carbon cap-and-trade and similar schemes can assist with this, but work is required to design sector-specific regulations that will likely be needed. A further case is where technologies provide valuable services that are not rewarded by conventional energy markets. Hydrogen was found to have a valuable role in providing system flexibility, with underground and pressure vessel hydrogen storage being used in net-zero energy systems. Through optimisation, it is clear that these technologies can reduce overall system costs. Future work can explore how these flexibility services should be valued, e.g. through specific support of the technologies or creation of flexibility markets.

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References

- [1] Sheila Samsatli and Nouri J. Samsatli. A multi-objective MILP model for the design and operation of future integrated multi-vector energy networks capturing detailed spatio-temporal dependencies. *Applied Energy*, 220:893 – 920, 2018.
- [2] J. Rogelj, D. Shindell, K. Jiang, S. Fifita, P. Forster, V. Ginzburg, C. Handa, H. Khesghi, S. Kobayashi, E. Kriegler, L. Mundaca, R. S  ferian, and M. V. Vilari  o. Mitigation pathways compatible with 1.5  c in the context of sustainable development. In V. Masson-Delmotte, P. Zhai, H. O. P  rtner, D. Roberts, J. Skea, P.R. Shukla, A. Pirani, W. Moufouma-Okia, C. P  an, R. Pidcock, S. Connors, J. B. R. Matthews, Y. Chen, X. Zhou, M. I. Gomis, E. Lonnoy, T. Maycock, M. Tignor, and T. Waterfield, editors, *Global warming of 1.5  C. An IPCC Special Report on the impacts of global warming of 1.5  C above pre-industrial levels and related global greenhouse gas emission pathways, in the context of strengthening the global response to the threat of climate change, sustainable development, and efforts to eradicate poverty*, chapter 2. 2018.
- [3] Iain Staffell, Daniel Scamman, Anthony Velazquez Abad, Paul Balcombe, Paul E. Dodds, Paul Ekins, Nilay Shah, and Kate R. Ward. The role of hydrogen and fuel cells in the global energy system. *Energy Environ. Sci.*, 12:463–491, 2019.
- [4] International Energy Agency. The future of hydrogen: Seizing today’s opportunities. Report, 2019. Available online at www.iea.org/reports/the-future-of-hydrogen.
- [5] Christopher J. Quarton and Sheila Samsatli. Should we inject hydrogen into gas grids? Practicalities and whole-system value chain optimisation. *Applied Energy*, 275:115172, 2020.
- [6] Christopher J. Quarton, Olfa Tlili, Lara Welder, Christine Mansilla, Herib Blanco, Heidi Heinrichs, Jonathan Leaver, Nouri J. Samsatli, Paul Lucchese, Martin Robinius, and Sheila Samsatli. The curious case of the conflicting roles of hydrogen in global energy scenarios. *Sustainable Energy and Fuels*, 4: 80–95, 2020.
- [7] Qimin Chai and Xiliang Zhang. Technologies and policies for the transition to a sustainable energy system in China. *Energy*, 35(10):3995 – 4002, 2010.
- [8] Thomas Martinsen. Global technology learning and national policy - an incentive scheme for governments to assume the high cost of early deployment exemplified by norway. *Energy Policy*, 38(8):4163 – 4172, 2010.
- [9] International Energy Agency. World Energy Outlook 2019. Report, 2019. More information at www.iea.org/weo2019/.
- [10] Michael Ball and Marcel Weeda. The hydrogen economy - vision or reality? *International Journal of Hydrogen Energy*, 40(25):7903–7919, 2015.
- [11] Hydrogen Council. Path to hydrogen competitiveness: A cost perspective. Report, 2020. Available online at https://hydrogencouncil.com/wp-content/uploads/2020/01/Path-to-Hydrogen-Competitiveness_Full-Study-1.pdf.

- [12] Evangelos Panos, Tom Kober, and Alexander Wokaun. Long term evaluation of electric storage technologies vs alternative flexibility options for the Swiss energy system. *Applied Energy*, 252:113470, 2019.
- [13] Herib Blanco, Wouter Nijs, Johannes Ruf, and André Faaij. Potential for hydrogen and Power-to-Liquid in a low-carbon EU energy system using cost optimization. *Applied Energy*, 232:617 – 639, 2018.
- [14] Madeleine McPherson, Nils Johnson, and Manfred Strubegger. The role of electricity storage and hydrogen technologies in enabling global low-carbon energy transitions. *Applied Energy*, 216:649 – 661, 2018.
- [15] S. Cerniauskas, T. Grube, A. Praktijnjo, D. Stolten, and M. Robinius. Future hydrogen markets for transportation and industry: The impact of CO2 taxes. *Energies*, 12(24), 2019.
- [16] D. Thomas, D. Mertens, M. Meeus, W. Van der Laak, and I. Francois. Power-to-gas roadmap for Flanders. Report, Hydrogenics, Colruyt, Sustesco and WaterstofNet, 2016. Available online at www.power-to-gas.be/sites/default/files/P2G%20Roadmap%20for%20Flanders%20-%20Final%20report.pdf.
- [17] Steven J. Davis, Nathan S. Lewis, Matthew Shaner, Sonia Aggarwal, Doug Arent, Inês L. Azevedo, Sally M. Benson, Thomas Bradley, Jack Brouwer, Yet-Ming Chiang, Christopher T. M. Clack, Armond Cohen, Stephen Doig, Jae Edmonds, Paul Fennell, Christopher B. Field, Bryan Hannegan, Bri-Mathias Hodge, Martin I. Hoffert, Eric Ingersoll, Paulina Jaramillo, Klaus S. Lackner, Katharine J. Mach, Michael Mastrandrea, Joan Ogden, Per F. Peterson, Daniel L. Sanchez, Daniel Sperling, Joseph Stagner, Jessika E. Trancik, Chi-Jen Yang, and Ken Caldeira. Net-zero emissions energy systems. *Science*, 360(6396):1419, 2018.
- [18] D. Scamman, K. Hyde, M. Newborough, and G. Cooley. Power-to-gas: A UK feasibility study. Report, ITM Power plc, 2013.
- [19] Christoph Budny, Reinhard Madlener, and Christoph Hilgers. Economic feasibility of pipe storage and underground reservoir storage options for power-to-gas load balancing. *Energy Conversion and Management*, 102(Supplement C):258 – 266, 2015.
- [20] Vicki Norberg-Bohm. Creating Incentives for Environmentally Enhancing Technological Change: Lessons From 30 Years of U.S. Energy Technology Policy. *Technological Forecasting and Social Change*, 65(2):125 – 148, 2000.
- [21] Brian Murray and Nicholas Rivers. British Columbia’s revenue-neutral carbon tax: A review of the latest "grand experiment" in environmental policy. *Energy Policy*, 86:674 – 683, 2015.
- [22] Easwaran Narassimhan, Kelly S. Gallagher, Stefan Koester, and Julio Rivera Alejo. Carbon pricing in practice: a review of existing emissions trading systems. *Climate Policy*, 18(8):967–991, 2018.
- [23] T. Johnson and A. Joshi. Review of vehicle engine efficiency and emissions. *SAE International Journal of Engines*, 11(6):1307–1330, 2018.

- [24] Isabella Burch and Jock Gilchrist. Survey of global activity to phase out internal combustion engine vehicles. Report, The Climate Center, 2020. Available online at <https://theclimatecenter.org/wp-content/uploads/2020/03/Survey-on-Global-Activities-to-Phase-Out-ICE-Vehicles-update-3.18.20-1.pdf>.
- [25] Department for Environment, Food and Rural Affairs. Government takes action to cut pollution from household burning. Press release, 2020. Available online at www.gov.uk/government/news/government-takes-action-to-cut-pollution-from-household-burning.
- [26] Jenny Sumner, Lori Bird, and Hillary Dobos. Carbon taxes: a review of experience and policy design considerations. *Climate Policy*, 11(2):922–943, 2011.
- [27] Lawrence H Goulder and Andrew R Schein. Carbon taxes versus cap and trade: A critical review. *Climate Change Economics*, 4(3):1 – 28, 2013.
- [28] Xiaoling Zhang and Yue Wang. How to reduce household carbon emissions: A review of experience and policy design considerations. *Energy Policy*, 102:116 – 124, 2017.
- [29] David Hirst. Carbon price floor (CPF) and the price support mechanism. Report, House of Commons Library, 2018. Available online at <https://commonslibrary.parliament.uk/research-briefings/sn05927/>.
- [30] US Department of Energy. Website: Hydrogen & fuel cells program. Available at www.hydrogen.energy.gov/, 2019. Accessed 14/11/2019.
- [31] Shigeki Iida and Ko Sakata. Hydrogen technologies and developments in Japan. *Clean Energy*, 3(2): 105–113, 05 2019.
- [32] Fuel Cells and Hydrogen Joint Undertaking. Website: Fuel Cells and Hydrogen Joint Undertaking. Available at www.fch.europa.eu/, 2019. Accessed 14/11/2019.
- [33] Zeineb Abdmouleh, Rashid A.M. Alammari, and Adel Gastli. Review of policies encouraging renewable energy integration & best practices. *Renewable and Sustainable Energy Reviews*, 45:249 – 262, 2015.
- [34] Ricardo. Website: Hydrogen for Transport Programme. Available online at <https://ee.ricardo.com/htpgrants>, 2020. Accessed: 17/04/2020.
- [35] Green Car Congress. Website: California Energy Commission selects 16 hydrogen station projects for up to \$33.4M in funding. Available online at www.greencarcongress.com/2017/02/20170221-cec.html, 2017. Published: 21/02/2017.
- [36] Lucy Butler and Karsten Neuhoff. Comparison of feed-in tariff, quota and auction mechanisms to support wind power development. *Renewable Energy*, 33(8):1854 – 1867, 2008.
- [37] Department for Business, Energy and Industrial Strategy. Electricity market reform: Contracts for difference. Available online at www.gov.uk/government/collections/electricity-market-reform-contracts-for-difference, 2017.
- [38] Richard Lowes, Bridget Woodman, and Oscar Fitch-Roy. Policy change, power and the development of Great Britain’s Renewable Heat Incentive. *Energy Policy*, 131:410 – 421, 2019.

- [39] Reinhard Haas, Gustav Resch, Christian Panzer, Sebastian Busch, Mario Ragwitz, and Anne Held. Efficiency and effectiveness of promotion systems for electricity generation from renewable energy sources - Lessons from EU countries. *Energy*, 36(4):2186 – 2193, 2011.
- [40] Department for Transport. Website: Renewable Transport Fuel Obligation. Available at www.gov.uk/guidance/renewable-transport-fuels-obligation, 2012. Accessed 8/11/19.
- [41] California Air Resources Board. Low Carbon Fuel Standard. Notes, California Air Resources Board, 2019. Available online at ww3.arb.ca.gov/fuels/lcfs/background/basics-notes.pdf.
- [42] ENTSOE. Electricity Balancing in Europe: An overview of the European balancing market and electricity balancing guideline. Report, European Network of Transmission System Operators for Electricity, 2018.
- [43] International Energy Agency. Website: Energy Technology RD&D - Tracking trends in spending on research, development and demonstration. Available at www.iea.org/statistics/rdd/, 2019. Accessed: 13/11/19.
- [44] Sandia National Laboratories. DOE Global Energy Storage Database. Database, 2019. Available online at www.energystorageexchange.org. Accessed: 13/08/2019.
- [45] US Department of Energy. Website: H2@ Scale. Available at <https://www.energy.gov/eere/fuelcells/h2-scale>, 2018. Accessed 02/08/2018.
- [46] Pavlos Nikolaidis and Andreas Poullikkas. A comparative overview of hydrogen production processes. *Renewable and Sustainable Energy Reviews*, 67:597 – 611, 2017.
- [47] GWEC and IRENA. 30 years of policies for wind energy: Lessons from 12 wind energy markets. Report, 2013. Available online at www.irena.org/publications/2013/Jan/30-Years-of-Policies-for-Wind-Energy-Lessons-from-12-Wind-Energy-Markets.
- [48] Osamu Kimura and Tatsujiro Suzuki. 30 years of solar energy development in Japan: co-evolution process of technology, policies, and the market. In *2006 Berlin Conference on the Human Dimensions of Global Environmental Change*, 2006.
- [49] H2 Mobility. Website: H2 Mobility. Available online at <https://h2.live/en/h2mobility>, 2020. Accessed: 17/04/2020.
- [50] UK Government. Website: Low-emission vehicles eligible for a plug-in grant. Available at www.gov.uk/plug-in-car-van-grants, 2019. Accessed 07/11/19.
- [51] Federal Ministry of Transport and Digital Infrastructure. Website: The future of mobility is electric. Available at www.bmvi.de/SharedDocs/EN/Dossier/Electric-Mobility-Sector/top-04-fuel-cell-technology.html, 2019. Accessed 07/11/19.
- [52] California Air Resources Board. Website: California Vehicle Rebate Program (CVRP). Available at ww3.arb.ca.gov/msprog/lct/cvrp.htm, 2019. Accessed 07/11/19.

- [53] National Public Radio. Website: Japan Is Betting Big On The Future Of Hydrogen Cars. Available at www.npr.org/2019/03/18/700877189/japan-is-betting-big-on-the-future-of-hydrogen-cars?t=1573134149947, 2019. Accessed 07/11/19.
- [54] Electrive.com. Website: South Korea announces new EV subsidies for 2020. Available at www.electrive.com/2019/09/02/south-korea-announces-ev-subsidies/, 2019. Accessed 07/11/19.
- [55] Greentech Media. Website: China to Eliminate Subsidies for Hydrogen Fuel-Cell Cars: Report. Available at www.greentechmedia.com/articles/read/china-to-eliminate-subsidies-for-fuel-cell-cars, 2019. Accessed 07/11/19.
- [56] Manuel Frondel, Nolan Ritter, Christoph M. Schmidt, and Colin Vance. Economic impacts from the promotion of renewable energy technologies: The German experience. *Energy Policy*, 38(8):4048 – 4056, 2010.
- [57] Ofgem. Non-Domestic RHI tariff table (Q2 - 2019/20). Dataset, available online at www.ofgem.gov.uk/publications-and-updates/non-domestic-rhi-tariff-table, 2019.
- [58] L. Maggioni and C. Pieroni. Deliverable d5.2: Report on the biomethane injection into national gas grid. Report, Increasing Social Awareness and Acceptance of Biogas and Biomethane, 2016. Available online at www.isaac-project.it/wp-content/uploads/2017/07/D5.2-Report-on-the-biomethane-injection-into-national-gas-grid.pdf.
- [59] Paulo Henrique de Mello Santana. Cost-effectiveness as energy policy mechanisms: The paradox of technology-neutral and technology-specific policies in the short and long term. *Renewable and Sustainable Energy Reviews*, 58:1216 – 1222, 2016.
- [60] Greentech Media. Website: Leaked Document Lifts Lid on EU’s Green Deal ‘Recovery’ Package. Available at www.greentechmedia.com/articles/read/a-green-hydrogen-cfd-and-eu-wide-renewables-tenders-leak-lifts-lid-on-eus-green-deal, 2020. Accessed 28/05/2020.
- [61] Sean M. Jarvis and Sheila Samsatli. Technologies and infrastructures underpinning future CO₂ value chains: A comprehensive review and comparative analysis. *Renewable and Sustainable Energy Reviews*, 85:46 – 68, 2018.
- [62] Yaping Hua, Monica Oliphant, and Eric Jing Hu. Development of renewable energy in Australia and China: A comparison of policies and status. *Renewable Energy*, 85:1044 – 1051, 2016.
- [63] Union of Concerned Scientists. Website: What is ZEV? Available at www.ucsusa.org/resources/what-zev, 2019. Accessed 07/11/19.
- [64] Malcolm Keay. UK energy policy - Stuck in ideological limbo? *Energy Policy*, 94:247 – 252, 2016.
- [65] José Villar, Ricardo Bessa, and Manuel Matos. Flexibility products and markets: Literature review. *Electric Power Systems Research*, 154:329 – 340, 2018.
- [66] National Grid ESO. ESO Balancing Services: A guide to contracting, tendering and providing response and reserve services. Slides, 2019. Available online at www.nationalgrideso.com/document/142161/download.

- [67] Simone Minniti, Niyam Haque, Phuong Nguyen, and Guus Pemen. Local markets for flexibility trading: Key stages and enablers. *Energies*, 11(11), 2018.
- [68] Andreas Abdon, Xiaojin Zhang, David Parra, Martin K. Patel, Christian Bauer, and Jörg Worlitschek. Techno-economic and environmental assessment of stationary electricity storage technologies for different time scales. *Energy*, 139:1173 – 1187, 2017.
- [69] Feras Alshehri, Víctor García Suárez, José L. Rueda Torres, Arcadio Perilla, and M.A.M.M. van der Meijden. Modelling and evaluation of PEM hydrogen technologies for frequency ancillary services in future multi-energy sustainable power systems. *Heliyon*, 5(4):e01396, 2019.
- [70] Sheila Samsatli and Nouri J. Samsatli. The role of renewable hydrogen and inter-seasonal storage in decarbonising heat - comprehensive optimisation of future renewable energy value chains. *Applied Energy*, 233-234:854–893, 2019.
- [71] Sheila Samsatli and Nouri J. Samsatli. A general mixed integer linear programming model for the design and operation of integrated urban energy systems. *Journal of Cleaner Production*, 191:458 – 479, 2018.
- [72] Christopher J. Quarton and Sheila Samsatli. The value of hydrogen and carbon capture, storage and utilisation in decarbonising energy: Insights from integrated value chain optimisation. *Applied Energy*, 257:113936, 2020.
- [73] Christopher J. Quarton and Sheila Samsatli. Resource and technology data for spatio-temporal value chain modelling of the Great Britain energy system. *Data in Brief*, 31:105886, 2020.
- [74] Felix Creutzig, N H Ravindranath, Göran Berndes, Simon Bolwig, Ryan Bright, Francesco Cherubini, Helena Chum, Esteve Corbera, Mark Delucchi, Andre Faaij, Joseph Fargione, Helmut Haberl, Garvin Heath, Oswaldo Lucon, Richard Plevin, Alexander Popp, Carmenza Robledo-Abad, Steven Rose, Pete Smith, and Anders Stromman. Bioenergy and climate change mitigation: an assessment. *Global change biology*, 7(5):916–944, 2015.
- [75] National Grid. Review of balancing mechanism reporting service (BMRS) zones. Report, 2011. Available online at www.elexon.co.uk/wp-content/uploads/2012/02/181_08_Review_of_BMRS_zones.pdf.
- [76] HM Revenue & Customs. HMRC yearly average and spot rates. Available online at www.gov.uk/government/publications/exchange-rates-for-customs-and-vat-yearly, 2019.
- [77] Committee on Climate Change. Reducing UK emissions - 2018 Progress Report to Parliament. Report, 2018. Available online at www.theccc.org.uk/publication/reducing-uk-emissions-2018-progress-report-to-parliament/.
- [78] National Grid. Future Energy Scenarios. Report, 2019. Available online at www.fes.nationalgrid.com/fes-document/.
- [79] National Grid. Website: National Grid Data Item Explorer. Available at <http://mip-prod-web.azurewebsites.net/DataItemExplorer>, 2020. Accessed: 20/04/2020.
- [80] Johannes Emmerling, Laurent Drouet, Kaj-Ivar van der Wijst, Detlef van Vuuren, Valentina Bosetti, and Massimo Tavoni. The role of the discount rate for emission pathways and negative emissions. *Environmental Research Letters*, 14(10):104008, 2019.

- [81] N. H. Stern. *The economics of climate change: The Stern review*, volume 9780521877251. Cambridge University Press, Cambridge, 2007. ISBN 0521700809 (pbk.).
- [82] HM Treasury. The Green Book: Central Government Guidance on Appraisal and Evaluation. Guidance document, UK Government, 2018. Available online at www.gov.uk/government/publications/the-green-book-appraisal-and-evaluation-in-central-government.
- [83] Marcel Roelofs and Johannes Bisschop. AIMMS - The Language Reference. User guide, AIMMS B.V., 2020. Available online at www.aimms.com/english/developers/resources/manuals/.
- [84] Ofgem. Website: Breakdown of an electricity bill. Available at www.ofgem.gov.uk/data-portal/breakdown-electricity-bill, 2019. Updated August 2019.
- [85] Ofgem. Website: Breakdown of a gas bill. Available at www.ofgem.gov.uk/data-portal/breakdown-gas-bill, 2019. Updated August 2019.
- [86] Department for Business, Energy and Industrial Strategy. Annual domestic energy bills. Dataset, 2019. Available online at www.gov.uk/government/statistical-data-sets/annual-domestic-energy-price-statistics#targetText=Annual%20domestic%20energy%20bills,on%20household%20expenditure%20on%20fuel.

Supplementary Material:

How to incentivise hydrogen energy technologies for net zero: Whole-system value chain optimisation of policy scenarios

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1. Model input data

The VWM input data used in the study, including spatio-temporal resource data (availabilities and demands) and technology data (costs, capacities and operational characteristics), are based on the dataset presented in [1]. The following subsections provide details of any input data used in this study that are not detailed in [1].

1.1. Bioenergy value chains

Two bioenergy value chains were modelled in this study: conversion of biogenic waste to biomethane and gasification of a biomass crop to produce hydrogen.

A representative conversion technology was modelled for conversion of biogenic waste to biomethane, representing a biogas plant that carries out anaerobic digestion of waste to biogas and upgrading of biogas to biomethane. The produced biomethane is indistinguishable from natural gas (which is predominantly methane) in the model. Key data for the anaerobic digestion & biogas upgrading plant are taken from [2] and are shown in Table 1.

A total availability of biogenic waste of 36.5 Mt/yr was assumed, allowing for biomethane production of up to 21 TWh/yr, as in [3]. This waste availability is shared amongst all 16 spatial zones, with the availability assumed to be proportional to total electricity demand in the zone (i.e. electricity demand and waste generation are both dependent on the population in the same way). Utilisation of the waste receives a gate-fee revenue of £25/t. The entire waste-to-biomethane value chain, including end use of the biomethane, was modelled with a CO₂ impact of zero, in accordance with UK government guidance for CO₂ accounting of biogas [4].

The other bioenergy value chain modelled in this study represents conversion of “non-waste” biomass to hydrogen. A generic biomass energy crop was modelled, using data representative of a miscanthus-type crop. The crop can be converted to hydrogen through a gasification plant that includes CO₂ capture at a rate of 91%.

The biomass crop is assumed to have a yield of 35 MWh/ha/yr, which includes energy requirements for processing into pellets. The cost of biomass pellets was assumed to be £24/MWh [5, 6], which includes all costs upstream of the gasification plant, i.e. biomass cultivation, processing and transportation. Available land for growing crops was taken from [7], where it was assumed that the crop would be grown on grassland and a GIS analysis of GB was used to find available land.

For the first decade (2020-2030), it was assumed that only 18% of the total suitable land could be used for bioenergy, giving rise to a primary energy availability of 20 TWh/yr. This constraint is relaxed in each decade, reaching a limit of 58% of suitable land in the final decade (2050-2060), giving rise to a primary energy availability of 64 TWh/yr. This availability is in line with Committee on Climate Change estimates [3, 6].

The biomass gasification to hydrogen is based on data for the integrated gasification combined cycle (IGCC) with CO₂ capture (excluding the power island) in [5]. Key data for this technology are shown in Table 1.

Assessing the value chain impacts of bioenergy crops is complex, as biomass cultivation can have far-reaching impacts, including on greenhouse gas emissions, water usage, food security and soil erosion [8]. Furthermore, the magnitudes of these impacts will vary depending on which of the various crops and land types are used.

Estimates for the CO₂ impacts of bioenergy crops vary widely. Typically, it is assumed that the CO₂ released when biomass is converted to another energy form (e.g. through combustion or gasification) is balanced by the CO₂ consumed by the crop during growth. Hence, if CO₂ capture is used at the energy conversion stage, it may be possible to achieve net negative emissions. This is the reason for the strong interest in Bioenergy with CCS (BECCS) for future energy systems [9].

However, bioenergy value chains have other CO₂ impacts, arising from the crop cultivation, processing and transportation for example. Depending on the crop used and processing and transport required, estimates

Table 1: Model input data for bioenergy conversion technologies.

	Anaerobic digester + upgrade to biomethane	Gasification to hydrogen
Input resource	Biogenic waste	Biomass pellet
Output resource	Methane	Hydrogen
Conversion efficiency	0.57 MWh _{CH₄} /t _{waste}	0.34 MWh _{H₂} /MWh _{pellet}
CO ₂ capture rate	<i>See Note 1</i>	0.10 tCO ₂ /MWh _{H₂}
CO ₂ emission rate	<i>See Note 1</i>	1.00 tCO ₂ /MWh _{H₂}
Maximum operating rate (MW output)	8.4	358.0
Minimum operating rate (MW output)	4.2	179.0
Plant capex (£M)	18.5	556
Plant fixed opex (£M/yr)	4.7	27.8
Plant lifetime (yr)	20	25
Reference	[2]	[5]

Note 1 - Anaerobic digester plant emissions are modelled as zero, as it is assumed that any CO₂ emitted along the biogas value chain is biogenic [4].

for the CO₂ impacts of these stages range between 20 and 240 kgCO₂ per MWh of biomass [9]. Moreover, further CO₂ impacts may arise from converting land to grow energy crops (land use change emissions). These emissions depend heavily on the land type, with estimates of 0-0.07 tCO₂/ha for marginal land, 75-200 tCO₂/ha for grassland, 350-720 tCO₂/ha for forest, and in excess of 1,000 tCO₂/ha for wetland [9]. Further emissions may also arise from land-use change elsewhere as a consequence of the primary land use changes, known as “indirect” land use change emissions.

Clearly, bioenergy value chains are complex and it is important that they are designed carefully to ensure that their overall system impact is positive. However, optimisation of bioenergy value chains was not the focus of this study. Instead, the reason for including bioenergy in this study is to explore the implications of bioenergy value chains with the potential for net-negative emissions on the role of hydrogen in the energy system.

In this study, the CO₂ impact of producing the biomass pellets, including cultivation, processing and transportation, but excluding CO₂ consumed by the crop during growth, was assumed to be 130 kgCO₂ per MWh of biomass. Assuming that the CO₂ consumed by the crop during growth is equal to the CO₂ emitted during gasification (before CO₂ capture), and with the conversion technology details in Table 1, this results in a net CO₂ impact for the hydrogen produced from biomass of -610 kgCO₂ per MWh of hydrogen.

1.2. Hydrogen fuel cells

Hydrogen fuel cells are an interesting option for generation of electricity and heat from hydrogen, as they have the potential to achieve high efficiencies with flexible operation. Worldwide there are relatively few large-scale fuel cell installations, although there are several in South Korea, including a 59 MW plant (the world’s largest) [10].

The data for hydrogen fuel cell plants in the VWM were updated in this study, based on a state-of-the-art commercially-available fuel cell system [11]. Two sizes of fuel cell plant are modelled, with maximum electricity outputs of 10 MW and 100 MW. Each plant requires 1.67 MWh of hydrogen per MWh of electricity produced and also produces 0.2 MWh of heat, that for example can be used for district heating [11]. The fuel cells have a lifetime of 10 years and can be operated flexibly. Plant costs have been estimated from [12]: the 10 MW plant has a modelled capex of £35m in 2020, falling to £21m in 2050; the 100 MW plant has a capex of £320m in 2020, falling to £192m in 2050. The plant fixed opex is assumed to be 4% of the capex.

1.3. Other data alterations

Two other alterations were made to the previous model dataset ([1]):

- The fixed operating costs for natural gas (and hydrogen) distribution grids were reduced from 3% of capex to 1% of capex, giving a new operating cost for each MW of grid capacity of £13,400 per year. This results in a more representative figure for the average operating costs per customer [13].

- As four decades were modelled in this study, estimates for the future cost of producing or importing natural gas were included, based on the base case in the National Grid Future Energy Scenarios [14]. The cost in the first decade (2020-2030) is £18.10/MWh, rising to £23.90/MWh by the final decade (2050-2060).

2. Sensitivity studies

In addition to the 15 scenarios that were described in detail in the main text, a further 23 scenarios were modelled to explore sensitivities for two critical input data: the discount rate, and the heat pump coefficient of performance.

2.1. Discount rate

2.1.1. Sensitivity scenarios

In the main scenarios that were modelled in this study, a discount rate of 3.5% was used, following UK government guidance [15]. However, as discussed in the main text, the choice of discount rate can significantly influence results when considering decarbonisation decisions over long time periods. Therefore additional sensitivity scenarios with different discount rates were modelled in order to assess the impact of the discount rate on the scenario results. Scenarios with discount rates of 0.1% and 8% were modelled. All of the scenarios with policies focussing on decarbonisation, detailed in Table 3 of the main text, were repeated with these alternative discount rates. Consequently, 14 additional scenarios were modelled.

2.1.2. Results

The results for the sensitivity runs with a discount rate of 0.1% are shown in Figure 1; equivalent results for a discount rate of 8% are shown in Figure 2. Finally, Figure 3 provides overall (discounted) cost and CO₂ results, and the average cost of CO₂ savings, for each scenario.

The discount rate determines the importance of future costs relative to present day costs. With a discount rate of 0.1%, future costs have almost equal weighting to present-day costs in the optimisation objective function, whilst with higher discount rates the importance of future costs falls.

In the case of CO₂ budgets, this effect means that with higher discount rates, investment in decarbonisation is delayed until it is essential, as the associated costs are seen to reduce. The level of “voluntary” early decarbonisation, i.e. the reduction in CO₂ emissions in a given decade beyond what is required by the CO₂ budget, is notably higher in the cases with lower discount rates. With a discount rate of 0.1% for example, as Figure 1 shows, CO₂ emissions in the “late” CO₂ budgets scenario follow a very close trajectory to the “steady” scenario, despite having not being required to by the CO₂ budgets. Examples of this voluntary early decarbonisation include earlier investment in renewable electricity generation and long-life infrastructure such as electricity distribution networks. As can be seen in Figure 3(b), the result of this earlier decarbonisation is a lower overall level of CO₂ emissions. For example, in the “late” CO₂ budgets cases, overall emissions are 21% lower with a discount rate of 0.1% than with a discount rate of 3.5%, and 27% lower than with a discount rate of 8%.

The discount rate has a less significant effect on the scenarios with CO₂ taxes, however a lower discount rate does appear to increase the potency of a tax. For example, with a discount rate of 0.1%, a CO₂ tax of £290/tCO₂ is sufficient to achieve net-zero emissions by 2050-2060, whilst in the scenarios with higher discount rates, a tax rate of £340/tCO₂ is necessary.

Finally, given that the majority of spending on decarbonisation occurs in later decades, the effect of the discount rate in all scenarios is to reduce the apparent costs of this decarbonisation. Figure 3(c) shows the average costs of CO₂ reductions for each scenario (as defined in Equation 6 of the main text). For each discount rate, this cost is calculated with respect to the “CO₂ unconstrained” scenario with the same discount rate. As Figure 3(c) shows, the average CO₂ costs range widely, from a maximum of £12/tCO₂ in the cases with a discount rate of 8% to a maximum of £103/tCO₂ in the cases with a discount rate of 0.1%.

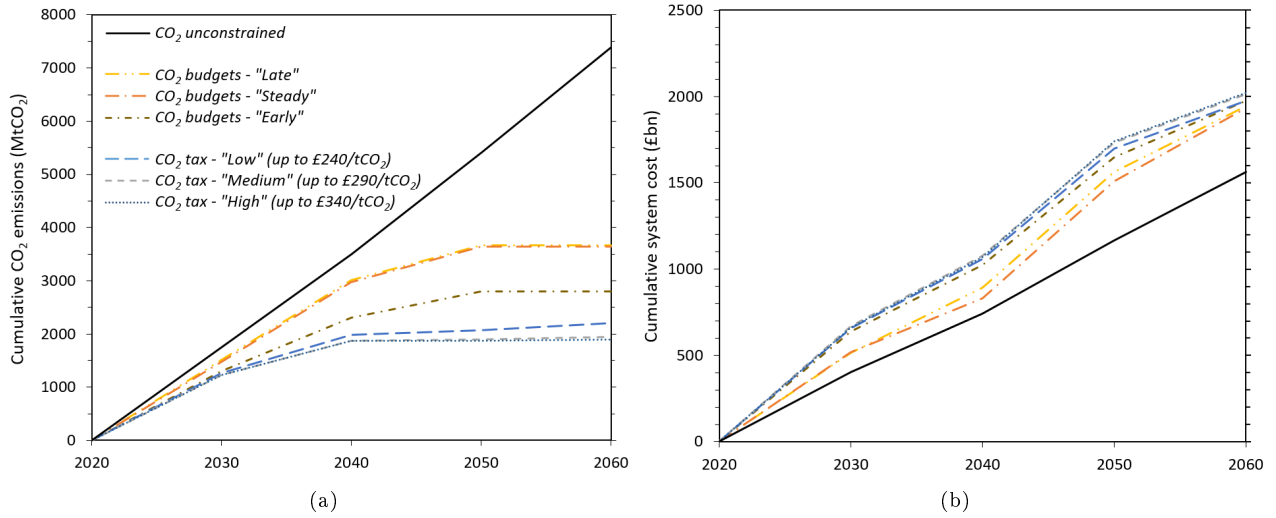


Figure 1: Cumulative CO₂ emissions (a) and costs (b) in scenarios with decarbonisation policies and a discount rate of 0.1%. Costs are overall system costs, discounted to 2020.

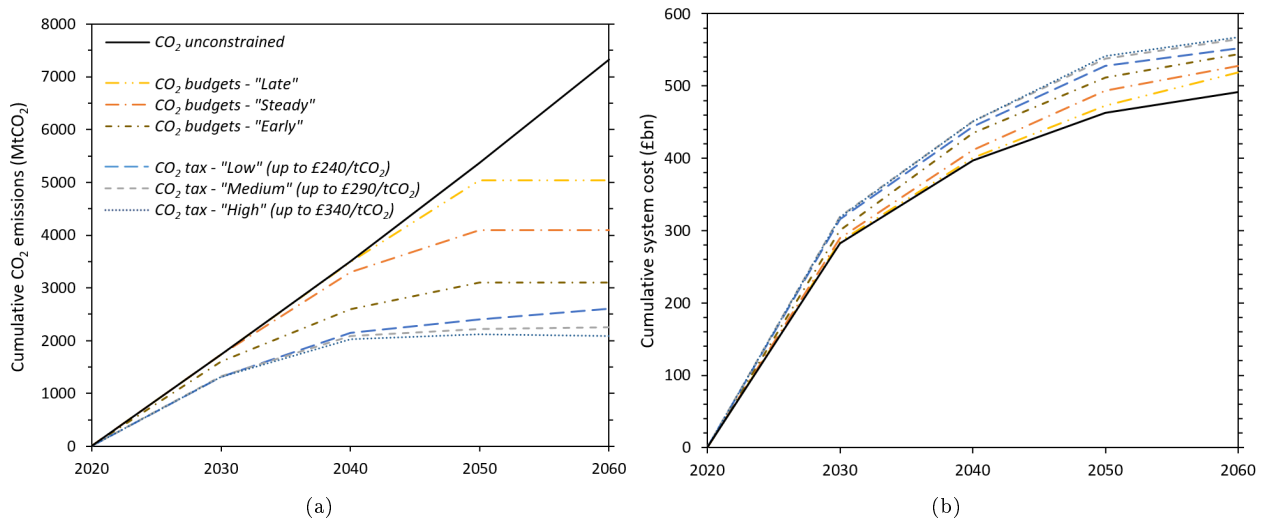
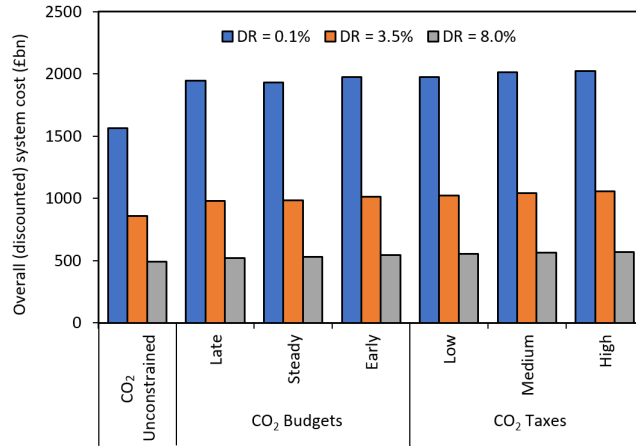
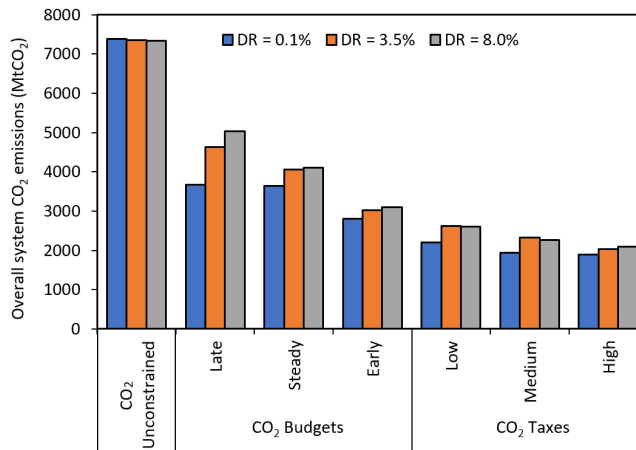


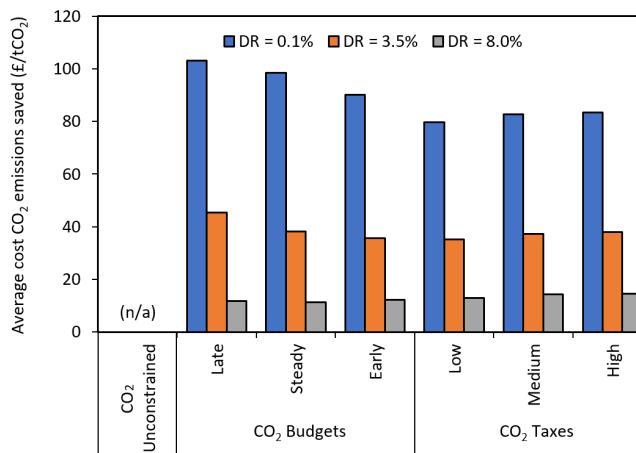
Figure 2: Cumulative CO₂ emissions (a) and costs (b) in scenarios with decarbonisation policies and a discount rate of 8%. Costs are overall system costs, discounted to 2020.



(a)



(b)



(c)

Figure 3: Cost and CO₂ results for scenarios with decarbonisation policies and of discount rates of 0.1%, 3.5% and 8%: (a) Overall (discounted) system cost; (b) Overall system CO₂ emissions; (c) Average cost of CO₂ savings

2.1.3. Conclusion

These results show the importance of the discount rate when considering investment decisions over long time periods. Whilst it is difficult to know what the most appropriate discount rate is for a given assessment, it is essential that the discount rate is taken into consideration when interpreting scenario results.

2.2. Electric heat pump coefficient of performance

2.2.1. Sensitivity scenarios

In the scenario results presented in the main article, electric heat pumps were found to have a high contribution to the decarbonised energy system. In the “steady” CO₂ budgets case, for example, 87% of domestic and commercial heat demands in 2050-2060 were satisfied by electric heat pumps. In the context of heat provision, electric heat pumps are an alternative to hydrogen, and therefore the uptake of hydrogen is likely to be adversely affected by their uptake. Therefore, the modelling assumptions behind electric heat pumps should be considered carefully.

The coefficient of performance (COP) represents the amount of heat energy delivered per unit of electrical energy input. Since heat pumps can have COPs in excess of two, this means they have an apparent efficiency of greater than 100% (whereas alternative technologies all have efficiencies lower than 100%) and thus the value of the COP is a key assumption for modelling heat pumps. In the main scenarios that were modelled in this study, the COP was assumed to be 2.5 for domestic electric heat pumps and 4 for commercial electricity heat pumps, based on values in the literature [3, 16]. As a sensitivity study, further scenarios were modelled in which the COP was set to 2 for both domestic and commercial heat pumps. The “steady” CO₂ budgets case and all of the scenarios with specific policies for incentivising hydrogen were included in this sensitivity study, in order to explore the effect of the COP assumption on hydrogen uptake.

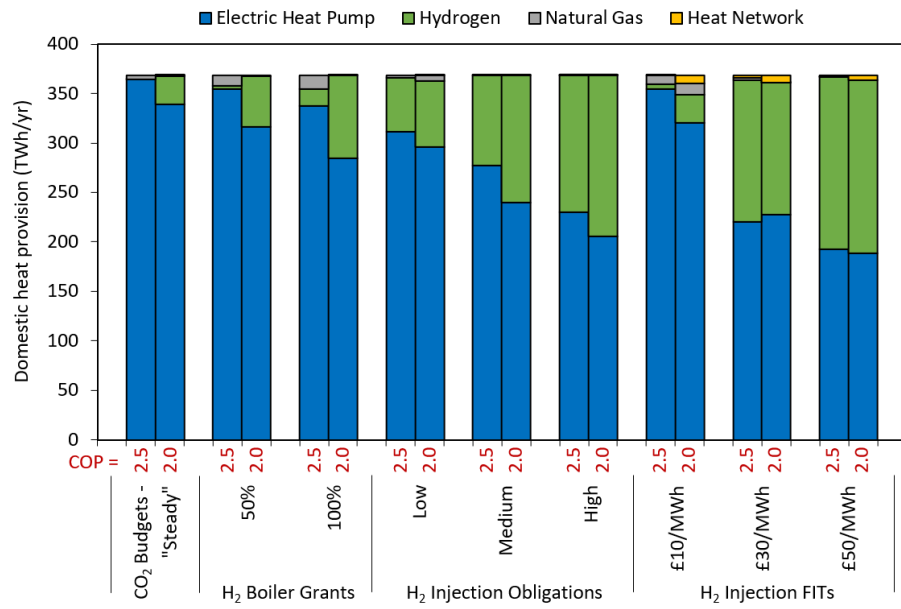
2.2.2. Effect on heat pump and hydrogen uptake

The results from these sensitivity scenarios are shown below. Figure 4 shows the overall provision of domestic and commercial heat in 2050-2060 in each of the scenarios, for both the original scenarios and the sensitivity scenarios with reduced heat pump COPs. Figure 5 shows results for hydrogen uptake in the sensitivity scenarios (the equivalent results for the original scenarios are shown in Figure 6 of the main text). Figures 4 and 5 suggest that the heat pump COP does have an impact on hydrogen uptake, but that it is relatively small.

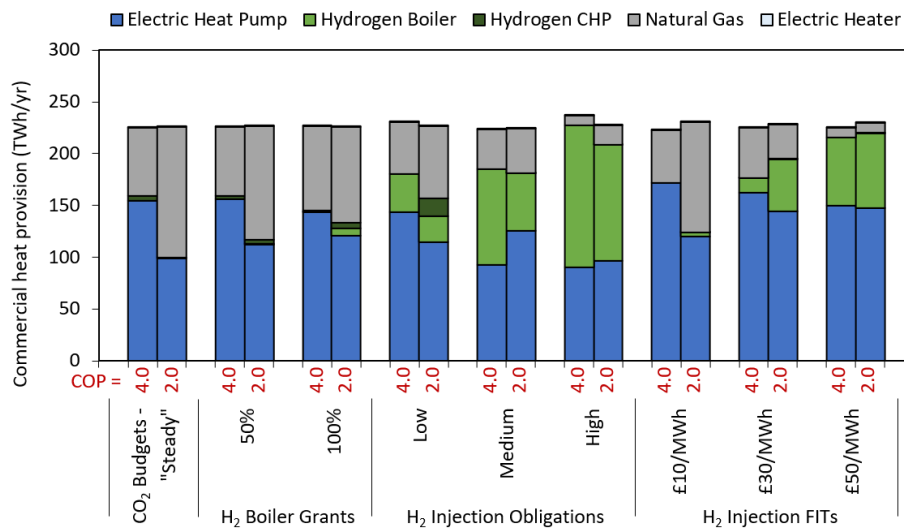
The impact of the reduced heat pump COP is most significant in the domestic sector and in the cases with less hydrogen uptake overall. In the “steady” CO₂ budgets cases, for example, use of hydrogen for domestic heat is 28 TWh/yr in 2050-2060 in the case with a reduced electric heat pump COP, compared to 0.3 TWh/yr in the original scenario. Interestingly, although capital grants for hydrogen boilers were found to be relatively ineffective for incentivising hydrogen in the original runs, with a lower COP assumption their effectiveness increases. This can be seen by comparing provision of heat by hydrogen between the case with 100% capital grants and the equivalent case without this policy in place (the “steady” CO₂ budgets case): with the original heat pump COP assumptions, 100% capital grants increase hydrogen usage in domestic heat by 17 TWh/yr in 2050-2060; with reduced COP assumptions, the increase is 56 TWh/yr.

Meanwhile, as Figure 4(a) shows, the effect of heat pump COP on hydrogen uptake is smaller in the cases that already have higher hydrogen uptake. This suggests that in these scenarios the hydrogen incentives have been effective and have already helped to overcome the cost difference between electric heat pumps and hydrogen; therefore, the reduced COP has little impact. In the cases with less support for hydrogen, the cost difference between heat pumps and hydrogen still exists in the original runs, but reducing the heat pump COP increases the competitiveness of hydrogen.

Finally, as shown in Figure 4(b), heat pump COP also has less influence on hydrogen uptake in the commercial sector. This is partly because in the commercial sector, natural gas is also a competitive low-carbon heat source, due to the availability of natural gas combined heat and power (CHP) plants with CO₂ capture. Therefore, the reduced competitiveness of electric heat pumps tends to lead to increased natural gas usage, rather than hydrogen. In fact, in cases with obligations for hydrogen injection, hydrogen usage in the commercial sector reduces with a lower heat pump COP. This is because total hydrogen injection into the



(a)



(b)

Figure 4: Heating provision in (a) the domestic sector and (b) the commercial sector in 2050-2060 for a range of scenarios, comparing the original COPs with the sensitivity scenarios with COP = 2.

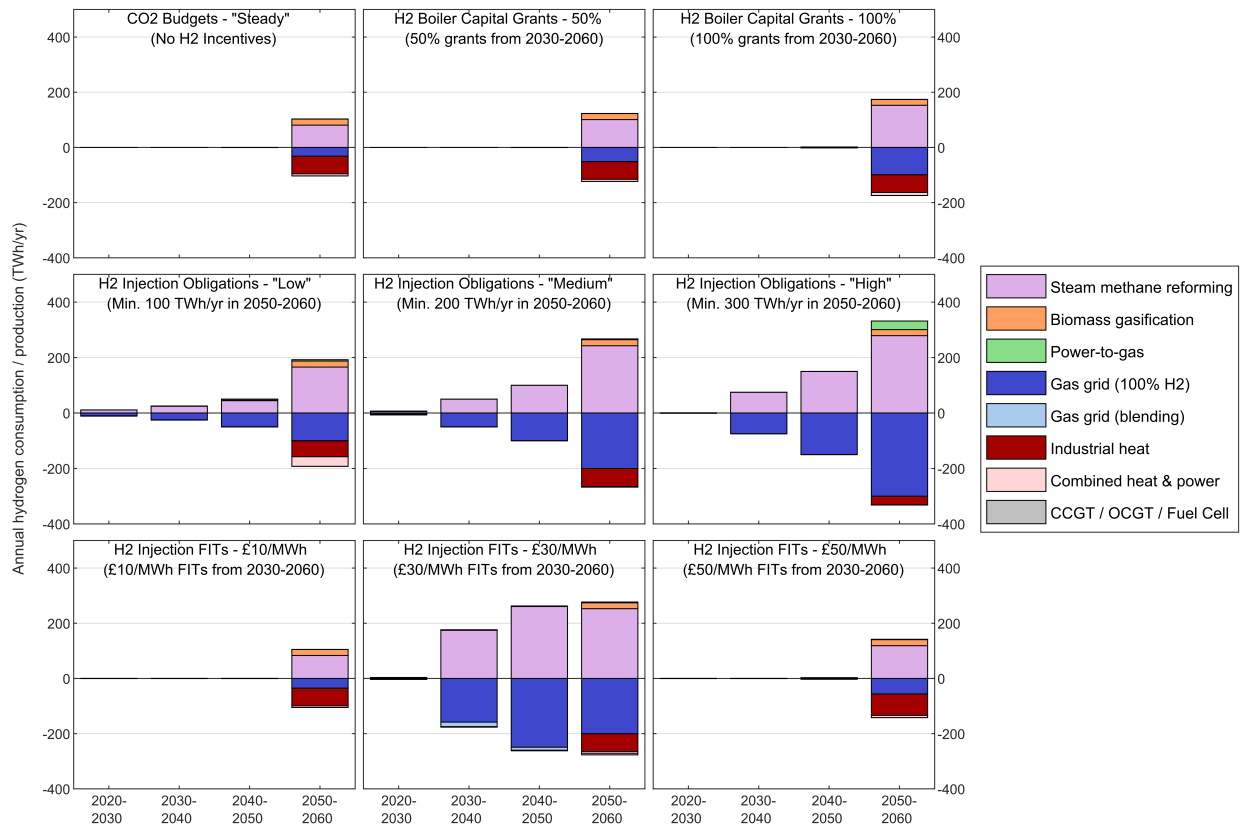


Figure 5: Hydrogen production and consumption by technology or application in each decade, for a range of scenarios (with a heat pump coefficient of performance of 2). Positive values denote hydrogen production, negative denote consumption.

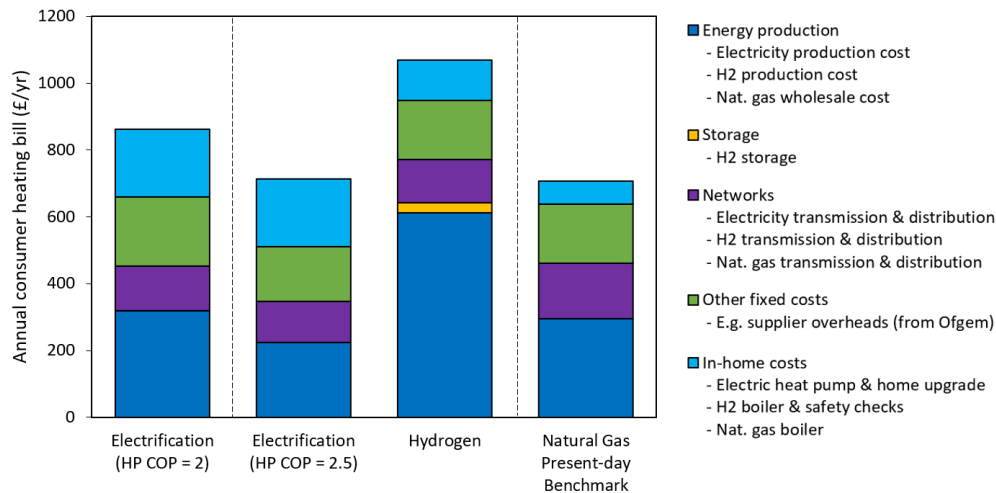


Figure 6: Annual consumer heating costs for a range of different heating scenarios. “Electrification (HP COP = 2)” was calculated from the “steady” CO₂ budgets scenario in the sensitivity study; the remaining cases are replicated from Figure 9 in the main text.

gas grid remains constant (at the level specified by the obligation) and domestic hydrogen usage becomes more favourable when the COPs are reduced; therefore, domestic usage increases and commercial usage reduces.

These results show that, to some extent, the competitiveness of heat pumps is affected by their COP. Furthermore, lower COPs for heat pumps do lead to an increase in competitiveness for hydrogen. However, in the sensitivity study performed here, the impact is relatively small. In particular, in all scenarios the overall mix of heating provision and the preferred heating technology remains unchanged when the heat pump COP is reduced.

2.2.3. Effect on consumer heating bill

Finally, a typical annual domestic heat bill was calculated from the “steady” CO₂ budgets case, with a heat pump COP of 2. This can be compared to the annual heating bills presented in Section 4.3 of the main text, including the annual heating bill for a heat pump with a COP of 2.5. The new heating bill for a domestic electric heat pump with a COP of 2 is shown in Figure 6, with the original heating bills that were presented in the main text.

The new annual electric heat pump heating bill, with a reduced COP of 2, is 21% higher than the original electric heat pump bill, at £863/yr. This is due primarily to increased electricity demand, which is reflected in increased costs from electricity production and from the fixed costs arising from the supply of electricity (although these are “fixed” costs, it is assumed they would be shared amongst electricity users based on their electricity consumption; therefore, domestic users would pay an increased proportion of these costs if their electricity demand increased).

The new annual heating bill is now closer to, but still lower than, the annual bill that was calculated for hydrogen, which was calculated to be £1070/yr. This helps to explain the previously-discussed result, that the “smaller” hydrogen incentives become more effective when the electric heat pump COP is reduced. In the original scenarios, the difference between the electrification heating bill and the hydrogen heating bill was £355/yr; this is reduced to £207/yr with the electrification bill based on a heat pump COP of 2. This difference is easier to overcome for hydrogen incentives.

2.2.4. Conclusion

In conclusion, the reduced heat pump coefficient of performance modelled in this sensitivity study increases the consumer costs of heating using a heat pump by around 19% and, as a result, hydrogen becomes more competitive as a decarbonised heating option. This leads to greater uptake of hydrogen, in particular in cases

with small but previously ineffective hydrogen incentives. However, despite the reduction in heat pump cost-effectiveness, they remain the lowest cost decarbonised heating option in the majority of cases. Therefore, the reduced heat pump COP does not lead to a significant change in hydrogen uptake in the scenario results.

3. Value Web Model formulation

The complete mathematical formulation of the Value Web Model (VWM), including the nomenclature, is explained in this section. The VWM was developed by Samsatli and Samsatli [7, 17], and more details on the model can be found in those publications.

3.1. Model Nomenclature

As the majority of the resources that were modelled are energy vectors, the most convenient unit for quantities of these resources is MWh and for flows of these resources is MW (MWh/h). However, these units may not be appropriate for all resources in a value web. For example, in this thesis, the units used for CO₂ are t and t/h (tonnes and tonnes per hour). In the following nomenclature section, the units for each resource are indicated by the unit ‘‘UoR’’, for ‘‘unit of resource’’, which stands for the relevant unit for that resource: e.g. MWh for most energy resources, t for CO₂, and so on. The rates of operation of conversion technologies are all in MW, since most are concerned with the production of energy vectors. The units of the conversion factors convert from operation in MW to production of each resource in its own units: thus the units of the conversion factors are (UoR/h)/MW.

Indices and sets

$b \in \mathbb{B}$	Transport infrastructures c
$c \in \mathbb{C} \subset \mathbb{R}$	Biomass resources (‘‘crops’’)
$d \in \mathbb{D}$	Daily interval types (e.g. weekday, weekend)
$\mathbb{E} \subset \mathbb{R}$	End vectors
$f \in \mathbb{F}$	Transportation direction of flow
$i \in \mathbb{I}$	System impacts (e.g. costs, CO ₂ emissions)
$h \in \mathbb{H}$	Hourly intervals
$l \in \mathbb{L}$	Linepack technologies
$m \in \mathbb{M}$	Transport technologies
$p \in \mathbb{P}$	Conversion technologies
$\mathbb{P}^D \subseteq \mathbb{P}$	Domestic conversion technologies
$\mathbb{P}^C \subseteq \mathbb{P}$	Commercial/industrial conversion technologies
$\mathbb{P}^{\text{HIGG}} \subseteq \mathbb{P}^C$	Conversion technologies relating to partial hydrogen injection
$\mathbb{P}^{\text{Dist}} \subseteq \mathbb{P}^C$	Gas distribution conversion technologies (including natural gas and hydrogen)
$r \in \mathbb{R}$	Resources
$s \in \mathbb{S}$	Storage facilities
$\mathbb{S}^{\text{Dist}} \subseteq \mathbb{S}$	Gas distribution storage technologies (representing gas grid linepack)
$sl \in \mathbb{SL}$	Solar PV installation types (e.g. solar farm and rooftop)
$t \in \mathbb{T}$	Seasonal time intervals
$w \in \mathbb{W}$	Wind turbine type (e.g. onshore and offshore)
$y \in \mathbb{Y}$	Long term planning time intervals (e.g. decadal)
$\tilde{y} \in \tilde{\mathbb{Y}}$	Yearly intervals used for discounting costs
$z \in \mathbb{Z}$	Spatial zones

Parameters

$A_{wzy}^{W,\max}$	Total area of land available for wind turbine type w in zone z in planning period y [m ²]
$A_{slzy}^{S,\max}$	Total area of land available for solar PV installation type sl in zone z in planning period y [m ²]
$A_{zy}^{\text{Bio},\max}$	Total area of land available for growing biomass in zone z in planning period y [ha]
a_{lz}	Binary value determining whether there is availability to build a connection (pipeline) to linepack system l in zone z ($a_{lz} = 1$ if a connection may be built, 0 otherwise)
a_{sz}	Binary value determining whether there is availability for a storage facility s in zone z ($a_{sz} = 1$ if a facility may be built, 0 otherwise)
BR_{py}	Total allowable number of conversion technologies p that may be built in planning period y (build rate)
b_b^{\max}	Maximum flow rate of transport infrastructure b [UoR/h]
C_{biy}^B	System impact of the capital investment in a length of transport infrastructure b in planning period y [£/(connection-km) or tCO ₂ /(connection-km)]
C_{piy}^P	System impact of the capital investment in a conversion technology p in planning period y [£ or tCO ₂]
C_{sly}^S	System impact of the capital investment in a storage facility s in planning period y [£ or tCO ₂]
C_{liy}^L	System impact of the capital investment in a connection to linepack system l in planning period y [£ or tCO ₂]
C_{wiy}^W	System impact of the capital investment in wind turbine type w in planning period y [£ or tCO ₂]
C_{sliy}^S	System impact of the capital investment in solar PV installation type sl in planning period y [£ or tCO ₂]
c_{ctiy}^{Bio}	System impact of producing a unit of biomass crop c in season t of planning period y [£/UoR or tCO ₂ /UoR] (impacts of planting, cultivating and harvesting the crop)
c_{rihdy}^M	System impact of importing a unit of resource r during hour h , day type d , season t and planning period y [£/UoR or tCO ₂ /UoR]
c_{rihdy}^U	System impact of producing a unit of resource r during hour h , day type d , season t and planning period y (e.g. domestic natural gas production) [£/UoR or tCO ₂ /UoR]
c_{rihdy}^X	System impact of exporting a unit of resource r during hour h , day type d , season t and planning period y [£/UoR or tCO ₂ /UoR]
D_{*iy}^C	Factor for discounting capital investments made in planning period y back to the beginning of the time horizon (i.e. the start of the first planning period). \star represents transport infrastructures b , conversion technologies p , storage technologies s or linepack technologies l .
D_{iy}^{OM}	Factor for discounting O&M impacts incurred in planning period y back to the beginning of the time horizon
D_{wiy}^C	Factor for discounting capital investments in new wind turbines made in planning period y back to the beginning of the time horizon
D_{sliy}^C	Factor for discounting capital investments in new solar PV installations made in planning period y back to the beginning of the time horizon
D_{rzhdy}^{act}	Demand for resource r in zone z during hour h , day type d , season t and planning period y [UoR/h]
D_{rzhdy}^{comp}	Compulsory demand (that must always be satisfied) for resource r in zone z during hour h , day type d , season t and planning period y [UoR/h]
D_{rzhdy}^{opt}	Optional demand (that may be satisfied if there are system benefits, e.g. revenues) for resource r in zone z during hour h , day type d , season t and yearly period y [UoR/h]
$d_{zz'}$	Distance between the centres (demand-weighted) of spatial zones z and z' [km]

f_{zy}^{loc}	Maximum allowable fraction of suitable biomass growing area in zone z that may be used in planning period y
f_y^{nat}	Maximum allowable fraction of suitable biomass growing area across the entire country that may be used in planning period y
$l_l^{\text{get,max}}$	Maximum withdrawal rate from a linepack system l via a single connection (pipeline) [UoR/h]
$l_l^{\text{put,max}}$	Maximum injection rate into a linepack system l via a single connection (pipeline) [UoR/h]
$l_l^{\text{hold,max}}$	Maximum storage inventory represented by each single connection (pipeline) of linepack system l [UoR]
$l_l^{\text{hold,min}}$	Minimum storage inventory represented by each single connection (pipeline) of linepack system l [UoR]
MB_{lb}	Binary value that determines whether transport technology l can use infrastructure b , (= 1 if it can, 0 otherwise)
m_{rzhdy}^{max}	Maximum allowable import rate of resource r in zone z during hour h , day type d , season t and planning period y [UoR/h]
n_h^{hd}	Duration of hourly interval h [h]
n_d^{dw}	Number of occurrences of day type d in a week (e.g. 5 for a weekday, 2 for a weekend)
n_t^{wt}	Number of repeated weeks in season t
n_y^{yy}	Number of repeated years in planning period y
N_{slzy}^{ES}	Number of pre-existing solar PV installations of type sl in zone z in planning period y (accounts for estimated retirement dates)
N_{wzy}^{EW}	Number of pre-existing wind turbines of type w in zone z in planning period y (accounts for estimated retirement dates)
N_{pz}^{EPC}	Number of pre-existing commercial conversion technologies of type p in zone z
NR_{pzy}^{EPC}	Number of pre-existing commercial conversion technologies of type p in zone z that retire at the beginning of planning period y
N_{sz}^{ES}	Number of pre-existing storage technologies of type s in zone z
NR_{szy}^{ES}	Number of pre-existing storage technologies of type s in zone z that retire at the beginning of planning period y
$N_{bzz'}^{\text{EB}}$	Number of pre-existing transport infrastructure connections of type b between zones z and z'
N_{lz}^{EL}	Number of pre-existing linepack connections (pipelines) of type l in zone z
NR_{lzy}^{EL}	Number of pre-existing linepack connections (pipelines) of type l in zone z that retire at the beginning of planning period y
N_{zy}^{house}	Number of households in zone z in planning period y
p_p^{max}	Maximum operating rate of technology p [MW]
p_p^{min}	Minimum operating rate of technology p [MW]
\mathcal{P}_{sl}^S	Maximum operating rate of solar PV installation sl [MW]
q_m^{max}	Maximum operating rate of transport technology l [MW]
R_w^{EW}	Rotor radius of pre-existing wind turbines of type w [m]
R_w^{W}	Rotor radius of new wind turbines of type w [m]
$RT_{py'y}^{\text{P}}$	Binary value determining whether conversion technology p , invested in at the beginning of planning period y' , retires at the beginning of planning period y (1 if it does retire, 0 otherwise)
$RT_{sy'y}^{\text{S}}$	Binary value determining whether storage facility s , invested in at the beginning of planning period y' , retires at the beginning of planning period y (1 if it does retire, 0 otherwise)

$RT_{ly'y}^L$	Binary value determining whether a connection of linepack system l , invested in at the beginning of planning period y' , retires at the beginning of planning period y (1 if it does retire, 0 otherwise)
$RT_{wy'y}^W$	Binary value determining whether wind turbine type w , invested in at the beginning of planning period y' , retires at the beginning of planning period y (1 if it does retire, 0 otherwise)
$s_s^{\text{get,max}}$	Maximum withdrawal rate from storage facility s [UoR/h]
$s_s^{\text{hold,max}}$	Maximum storage capacity of a single storage facility s [UoR]
$s_s^{\text{put,max}}$	Maximum injection rate into storage facility s [UoR/h]
$v_w^{\text{cut-in}}$	Minimum operational wind speed for wind turbine [m/s]
$v_w^{\text{cut-out}}$	Maximum operational wind speed for wind turbine [m/s]
v_w^{rated}	Wind speed at which wind turbine produces maximum power (rated power) [m/s]
V_{riy}	Value (e.g. price) of a unit of resource r in planning period y [£/UoR or tCO ₂ /UoR]
$V_y^{CO_2}$	The cost impact of 1 tonne of CO ₂ emissions (i.e. the CO ₂ price) in planning period y [£]
v_{wzhdty}	Wind speed for turbine type w in zone z during hour h of day type d in season t of planning period y [m/s]
x_z	x-coordinate of the centre of demand of spatial zone z
y_z	y-coordinate of the centre of demand of spatial zone z
Y_{czt}^{Bio}	Biomass yield potential for crop c in zone z for season t of planning period y [UoR/ha/season]
α_{rpy}	Conversion factor of resource r in technology p in planning period y
β_b	Directionality parameter for transport infrastructures b : = -1 if one-way unidirectional (can only be built and operated in one direction); = 0 if two-way unidirectional (unidirectional infrastructure but can be built in both directions); = 1 if bidirectional (only one infrastructure needed that can be operated in either direction)
ϵ	Weighting factor for including total energy production in objective function
γ	Finance rate
η_w	Wind turbine efficiency for wind turbine type w
ι	Discount rate
λ_{\star}	Economic lifetime of technologies [year] ($\star \in \{b, p, s\}$ for transport infrastructures, conversion technologies and storage technologies, respectively)
$\lambda_{lrfy}^{\text{get}}$	Conversion factor for performing “get” task with linepack technology l on resource r in planning period y
$\lambda_{lrfy}^{\text{hold}}$	Conversion factor for performing “hold” task with linepack technology l on resource r in planning period y
$\lambda_{lrfy}^{\text{put}}$	Conversion factor for performing “put” task with linepack technology l on resource r in planning period y
$\nu_{zz'}$	Binary parameter, 1 if zone z is adjacent to zone z'
ρ^{air}	Air density [kg/m ³]
$\sigma_{srfy}^{\text{get}}$	Conversion factor for performing “get” task with storage technology s on resource r in planning period y
$\sigma_{srfy}^{\text{hold}}$	Conversion factor for performing “hold” task with storage technology s on resource r in planning period y
$\sigma_{srfy}^{\text{put}}$	Conversion factor for performing “put” task with storage technology s on resource r in planning period y
ς	Scaling factor for impacts in the objective function. Multiplies by 10 ⁻⁶ to improve scaling in the optimisation (£ to £M and t to Mt)

$\bar{\tau}_{mrfy}$	Conversion factor for transport technology l transporting resource r in planning period y (distance-independent)
$\hat{\tau}_{mrfy}$	Conversion factor for transport technology l transporting resource r in planning period y (distance-dependent)
ϕ_{biy}^B	Annual O&M impact of transport infrastructure b in planning period y [(£ or tCO ₂)/(connection-km-yr)]
ϕ_{piy}^P	Annual O&M (fixed) impact of conversion technology p in planning period y [£/yr or tCO ₂ /yr]
ϕ_{siy}^S	Annual O&M (fixed) impact of storage facility s in planning period y [£/yr or tCO ₂ /yr]
ϕ_{sly}^L	Annual O&M (fixed) impact of a connection to linepack system l in planning period y [£/yr or tCO ₂ /yr]
ϕ_{wiy}^W	Annual O&M (fixed) impact of wind turbines in planning period y [£/yr or tCO ₂ /yr]
ϕ_{sly}^S	Annual O&M (fixed) impact of solar PV installations in planning period y [£/yr or tCO ₂ /yr]
φ_{piy}^P	Variable operating impact of conversion technology p in planning period y [£/UoR or tCO ₂ /UoR]
$\hat{\varphi}_{miy}^Q$	Distance-dependent variable operating impact of transport process l in planning period y [£/km/UoR or tCO ₂ /km/UoR]
$\bar{\varphi}_{miy}^Q$	Distance-independent variable operating impact of transport process l in planning period y [£/UoR or tCO ₂ /UoR] (e.g. flat rate freight charges)
φ_{siy}^{SG}	Variable operating impact of “get” task for storage facility s in planning period y [£/UoR or tCO ₂ /UoR]
φ_{siy}^{SH}	Unit variable operating impact of “hold” task for storage facility s in planning period y [£/UoR or tCO ₂ /UoR]
φ_{siy}^{SP}	Unit variable operating impact of “put” task for storage facility s in planning period y [£/UoR or tCO ₂ /UoR]
φ_{liy}^{LG}	Variable operating impact of “get” task for connection to linepack system l in planning period y [£/UoR or tCO ₂ /UoR]
φ_{liy}^{LH}	Unit variable operating impact of “hold” task for connection to linepack system l in planning period y [£/UoR or tCO ₂ /UoR]
φ_{liy}^{LP}	Unit variable operating impact of “put” task for connection to linepack system l in planning period y [£/UoR or tCO ₂ /UoR]
χ_{rzhdy}^{\max}	Maximum export rate of resource r in zone z in planning period y [UoR/h]
ω_i	Weighting factor for including key performance indicator i in objective function

Positive variables

A_{czy}^{Bio}	Area allocated to production of biomass (crop) c in zone z during planning period y [ha]
A_{sl}^S	Total area occupied by solar PV installations of type sl in zone z during planning period y [m ²]
$\mathcal{C}_{zhdy}^{\text{IET}}$	Amount of “capturable” CO ₂ emitted in zone z during hour h of day type d in season t of planning period y [tCO ₂]
$\mathcal{C}_{zhdy}^{\text{US}}$	Amount of CO ₂ utilised or stored in zone z during hour h of day type d in season t of planning period y [tCO ₂]
D_{rzhdy}^{sat}	Optional demands satisfied in zone z during hour h of day type d in season t of planning period y [UoR/h]
E_{rzhdy}	Excess production of resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]
f_{piy}^{heat}	Fraction of heat satisfied by domestic heating technology p in zone z in planning period y

I_{szhdt}	Inventory in storage facility s in zone z during hour h of day type d in season t of planning period y [UoR]
$I_{szdt}^{0,act}$	Inventory in storage facility s in zone z at the start of day type d of season t in planning period y [UoR]
$I_{szdt}^{0,sim}$	Inventory in storage facility s in zone z at the start of the simulated cycle for day type d of season t in planning period y [UoR]
\mathcal{I}_{iy}^{total}	Total net present impact of all resources and technologies in planning period y [£M or MtCO ₂]
$\mathcal{I}_{iy}^{CO_2price}$	Total net present impact of the CO ₂ price in planning period y [£M]
\mathcal{I}_{iy}^P	Total net present impact of building new conversion technologies in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^S	Total net present impact of building new storage technologies in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^Q	Total net present impact of building new transport infrastructures in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^L	Total net present impact of building new linepack connections in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^W	Total net present capital impact of building new wind turbines in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^{SL}	Total net present capital impact of building new solar PV installations in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^m	Total net present impact of importing resources in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^{fp}	Total net present fixed O&M impact of conversion technologies in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^{fq}	Total net present fixed O&M impact of transport infrastructures in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^{fs}	Total net present fixed O&M impact of storage technologies in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^{fl}	Total net present fixed O&M impact of linepack connections in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^w	Total net present O&M impact of wind turbines in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^{sl}	Total net present O&M impact of solar PV installations in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^{Rev}	Total net present revenue from the sales of energy services for satisfying demands in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^U	Total impact of utilising natural resources in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^C	Total impact of resource curtailment in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^{VP}	Total net present variable operating impact of production facilities in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^{vs}	Total net present variable operating impact of storage facilities in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^{vq}	Total net present variable operating impact of transport technologies in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^{vl}	Total net present variable operating impact of linepack connections in planning period y [£M or MtCO ₂]
\mathcal{I}_{iy}^x	Total net present impact of exporting resources in planning period y [£M or MtCO ₂]
J_{lhdt}	Inventory in linepack system l during hour h of day type d in season t of planning period y [UoR]
$J_{ldt}^{0,act}$	Inventory in linepack system l at the start of day type d of season t in planning period y [UoR]

$J_{ldty}^{0,sim}$	Inventory in linepack system l at the start of the simulated cycle for day type d of season t in planning period y [UoR]
M_{rzhdty}	Import rate of resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]
N_{pzy}^{PD}	Millions of domestic conversion technology $p \in \mathbb{P}^D$ in zone z in planning period y
U_{rzhdty}	Utilisation of natural resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]
u_{rzhdty}^{max}	Maximum availability of natural resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]
X_{rzhdty}	Export rate of resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]
\mathcal{P}_{pzhdy}^h	Total rate of operation of hourly variable conversion technology p in zone z during hour h of day type d in season t of planning period y [MW]
\mathcal{P}_{pzdty}^d	Total rate of operation of daily variable conversion technology p in zone z during day type d in season t of planning period y [MW]
$\mathcal{Q}_{mzz'hdty}$	Operation rate of transport technology l from zone z to zone z' during hour h of day type d in season t of planning period y [UoR/h]
$\mathcal{S}_{szhdty}^{get}$	Operation rate of “get” task by storage s in zone z during hour h of day type d in season t of planning period y [UoR/h]
$\mathcal{S}_{szhdty}^{hold}$	Operation rate of “hold” task by storage s in zone z during hour h of day type d in season t of planning period y [UoR/h]
$\mathcal{S}_{szhdty}^{put}$	Operation rate of “put” task by storage s in zone z during hour h of day type d in season t of planning period y [UoR/h]
$\mathcal{L}_{lzhdy}^{get}$	Operation rate of “get” task by linepack system l in zone z during hour h of day type d in season t of planning period y [UoR/h]
$\mathcal{L}_{lhdy}^{hold}$	Operation rate of “hold” task by linepack system l in zone z during hour h of day type d in season t of planning period y [UoR/h]
$\mathcal{L}_{lzhdy}^{put}$	Operation rate of “put” task by linepack system l in zone z during hour h of day type d in season t of planning period y [UoR/h]

Free variables

L_{zlhdy}	Net rate of transfer of resource r into zone z from the linepack transmission system during hour h of day type d in season t of planning period y [UoR/h]
P_{rzhdy}^h	Net rate of production by hourly variable technologies of resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]
P_{rzdty}^d	Net rate of production by daily variable technologies of resource r in zone z during day type d in season t of planning period y [UoR/h]
P_y^{P,CO_2}	Total (net) production of CO ₂ by conversion technologies in planning period y
Q_{rzhdy}	Net transport rate of resource r into zone z from all other zones during hour h of day type d in season t of planning period y [UoR/h]
S_{rzhdy}	Net production of resource r in zone z due to the operation of storage technologies during hour h of day type d in season t of planning period y [UoR/h]
Z	Objective function
δ_{szdy}^d	Net surplus put into storage s in zone z over one day in day type d in season t of planning period y [UoR]
δ_{spty}^t	Net surplus put into storage s in zone z over one week in season t of planning period y [UoR]
δ_{szy}^y	Net surplus put into storage s in zone z over one year in planning period y [UoR]
Δ_{ldty}^d	Net surplus put into linepack system l over one day in day type d in season t of planning period y [UoR]

$\Delta_{lt_y}^t$	Net surplus put into linepack system l over one week in season t of planning period y [UoR]
Δ_{ly}^y	Net surplus put into linepack system l over one year in planning period y [UoR]

Integer variables

$N_{bzz'y}^B$	Number of transport infrastructure b installed between zones z and z' during planning period y
N_{pzy}^{PC}	Total number of commercial conversion technology $p \in \mathbb{P}^C$ in zone z during planning period y
N_{szy}^S	Total number of storage technology s in zone z during planning period y
N_{lzy}^L	Total number of connections of linepack system l in zone z during planning period y
N_{wzy}^W	Total number of wind turbines of type w in zone z during planning period y
N_{slzy}^S	Total number of solar PV installations of type sl in zone z during planning period y
$NI_{bzz'y}^B$	Number of new transport infrastructure b invested in at the beginning of planning period y between zones z and z'
NI_{pzy}^{PC}	Number of new commercial conversion technology $p \in \mathbb{P}^C$ invested in at the beginning of planning period y in zone z
NI_{szy}^S	Number of new storage facility s invested in at the beginning of planning period y in zone z
NI_{lzy}^L	Number of new connections of linepack system l invested in at the beginning of planning period y in zone z
NI_{wzy}^W	Number of new wind turbines of type w invested in at the beginning of planning period y in zone z
NI_{slzy}^S	Number of new solar PV installations of type sl invested in at the beginning of planning period y in zone z
NR_{pzy}^{PC}	Number of commercial conversion technology $p \in \mathbb{P}^C$ retired in zone z at the beginning of planning period y
NR_{szy}^S	Number of storage facility s retired in zone z at the beginning of planning period y
NR_{lzy}^L	Number of connections of linepack system l retired in zone z at the beginning of planning period y
NR_{wzy}^W	Number of wind turbines of type w retired in zone z at the beginning of planning period y
NR_{slzy}^S	Number of solar PV installations of type sl retired in zone z at the beginning of planning period y

3.2. Objective function

The objective function in the Value Web Model is a weighted sum of “impacts” in the overall energy system, and is defined as follows:

$$Z = \sum_{iy} \omega_i \mathcal{I}_{iy}^{total} \quad (1)$$

Most impacts are included in the variable \mathcal{I}_{iy}^{total} , which is the sum of all resource and technology impacts, for each performance indicator i in the model in decadal interval y . The range of possible performance indicators is defined by the set \mathbb{I} , which for this study is:

$$\mathbb{I} \equiv \{\text{Cost}, \text{CO}_2\}$$

The parameter ω_i in the objective function is a weighting factor that determines the weighting of the CO₂ and cost impacts in the model: for example, a cost minimisation optimisation would have $\omega_{Cost} = 1$ and $\omega_{CO_2} = 0$; a CO₂ minimisation optimisation would be vice versa.

The sum of all impacts \mathcal{J}_{iy}^{total} includes all of the cost and CO₂ impacts arising from the resources and technologies in the VWM. It is defined as follows:

$$\begin{aligned} \mathcal{J}_{iy}^{total} = & \mathcal{J}_{iy}^W + \mathcal{J}_{iy}^{SL} + \mathcal{J}_{iy}^P + \mathcal{J}_{iy}^S + \mathcal{J}_{iy}^Q + \mathcal{J}_{iy}^L + \mathcal{J}_{iy}^w + \mathcal{J}_{iy}^{sl} + \mathcal{J}_{iy}^{fp} + \mathcal{J}_{iy}^{fs} + \mathcal{J}_{iy}^{fq} + \mathcal{J}_{iy}^{fl} \\ & + \mathcal{J}_{iy}^{vp} + \mathcal{J}_{iy}^{vs} + \mathcal{J}_{iy}^{vq} + \mathcal{J}_{iy}^{vl} + \mathcal{J}_{iy}^m + \mathcal{J}_{iy}^x + \mathcal{J}_{iy}^U + \mathcal{J}_{iy}^C - \mathcal{J}_{iy}^{Rev} + \mathcal{J}_{iy}^{CO_2} + \mathcal{J}_{iy}^{CO_2price} \end{aligned} \quad (2)$$

Each of the terms in this equation represents the impact of a different activity in the model, and is defined in detail in the relevant subsection below. Briefly, the first six impacts shown are the investment impacts (i.e. capex) of the technologies in the model: wind turbines (\mathcal{J}_{iy}^W), solar PV (\mathcal{J}_{iy}^{SL}), conversion technologies (\mathcal{J}_{iy}^P), storage technologies (\mathcal{J}_{iy}^S), transportation technologies (\mathcal{J}_{iy}^Q) and linepack technologies (\mathcal{J}_{iy}^L). The following six impacts represent the fixed operating impacts for the same technologies. The impacts \mathcal{J}_{iy}^{fp} , \mathcal{J}_{iy}^{fs} , \mathcal{J}_{iy}^{fq} and \mathcal{J}_{iy}^{fl} are the variable operating impacts of conversion technologies, storage technologies, transport technologies and linepack technologies respectively. The next five impacts relate to the impacts of resources in the model: \mathcal{J}_{iy}^m and \mathcal{J}_{iy}^x are the impacts of importing and exporting resources respectively; \mathcal{J}_{iy}^U is the impact of utilising primary resources (e.g. biomass); \mathcal{J}_{iy}^C is the impact of any resource curtailment, for example if a penalty is imposed for curtailed wind energy; and \mathcal{J}_{iy}^{Rev} is the revenue that can be received if demands (either compulsory or optional) are satisfied in return for a price. Finally, $\mathcal{J}_{iy}^{CO_2}$ is the CO₂ impact of any uncaptured CO₂ that is produced by conversion technology, whilst $\mathcal{J}_{iy}^{CO_2price}$ is the cost impact of a CO₂ price.

3.2.1. Discounting

The objective function considers the “net present value” of all impacts. Hence, for $i = \text{Cost}$, discount factors are used to calculate the net present value (at the beginning of the modelling horizon) of costs incurred in later time periods. Discount factors for capital and operational costs are included in the definitions of the impacts \mathcal{J}_{iy} .

The discount factor for capital costs is defined as follows:

$$D_{*iy}^C = \begin{cases} \left[\frac{\gamma(1+\gamma)^{\lambda_*}}{(1+\gamma)^{\lambda_*} - 1} \right] \left[\sum_{\tilde{y}=1}^{\lambda_*} (1+\iota)^{-\tilde{y}} \right] \left[(1+\iota)^{-n_{iy}^{yy}(y-1)} \right] & \forall i = \text{Cost}, y \in \mathbb{Y} \\ 1 & \forall i \neq \text{Cost}, y \in \mathbb{Y} \end{cases} \quad (3)$$

This cost discount factor is the product of three terms. The first term calculates the annual repayments that must be made for the capital investment, assuming that the investment is financed over the economic lifetime of the technology, given by λ_* . The annual repayments are calculated based on a finance rate of γ ; the first repayment occurs one year after the release of the funds. The second term calculates the factor to apply to each annual repayment to discount it back to the beginning of the given period y , using a discount rate of ι . Finally, the third term calculates the factor to apply to discount these values back to the beginning of the first period in the model, the time for which the net present value is calculated, also using discount rate ι .

Given that different technologies may have different economic lifetimes, λ_* , they may also have different discount factors, D_{*iy}^C . This is why the \star subscript is used, replacing p , s or b depending on whether production technologies, storage technologies or transport technologies are being considered.

For key performance indicators other than cost, there is no change in the “value” of the impact over time, so the discount factor is equal to one.

It is assumed that operating and maintenance costs are paid at the beginning of each year in each planning period y . The net present value of these costs are calculated with a similar discount factor to the capital cost discount factor, except that in this case a term for the calculation of annual repayments is not required:

$$D_{iy}^{\text{OM}} = \begin{cases} \left[\sum_{\bar{y}=1}^{n_y^{yy}} (1+\iota)^{1-\bar{y}} \right] \left[(1+\iota)^{-n_y^{yy}(y-1)} \right] & \forall i = \text{Cost}, y \in \mathbb{Y} \\ n_y^{yy} & \forall i \neq \text{Cost}, y \in \mathbb{Y} \end{cases} \quad (4)$$

Operating impacts for performance indicators other than cost occur each year, but do not require discounting, so the discount factor is equal to the number of years in the planning period, n_y^{yy} .

3.2.2. CO₂ pricing

Depending on the design of the CO₂ pricing system that is being used, it may be represented differently within the model. In this study, the CO₂ pricing system covers all emissions across the entire energy system. Therefore the total cost impact of the CO₂ price can be easily calculated from the total level of CO₂ emissions, which is given by $\mathcal{S}_{i=CO_2,y}^{\text{Total}}$ (Equation 2 for $i = CO_2$). Thus the overall impact of the CO₂ price is given by:

$$\mathcal{S}_{iy}^{\text{CO}_2\text{price}} = \begin{cases} \mathcal{S}_{i=CO_2,y}^{\text{Total}} V_y^{\text{CO}_2} \frac{D_{i=\text{Cost},y}^{\text{OM}}}{D_{i=CO_2,y}^{\text{OM}}} & \forall i = \text{Cost}, y \in \mathbb{Y} \\ 0 & \forall i \neq \text{Cost}, y \in \mathbb{Y} \end{cases} \quad (5)$$

Here, $V_y^{\text{CO}_2}$ is the CO₂ price, which has a pre-defined value for each decadal interval y . The final expression in Equation 5 relates to discounting of costs and CO₂. As was shown in section 3.2.1, cost impacts and CO₂ impacts have different discount factors included within their definitions; therefore an expression must be included to convert from a CO₂ impact to a cost impact.

3.3. Resource balance

The resource balance is essentially an energy balance that applies to all resources, r , in all zones, z , and at all times: every hourly interval, h , of every day type, d , of each week in every season, t , and yearly planning interval, y . The flows of resource into each zone must be equal to the flows out as follows:

$$\begin{aligned} U_{rzhdt y} + M_{rzhdt y} + P_{rzhdt y}^h + P_{rzdty}^d + S_{rzhdt y} + Q_{rzhdt y} + L_{zlhdt y} \\ = D_{rzhdt y}^{\text{comp}} + D_{rzhdt y}^{\text{sat}} + X_{rzhdt y} + E_{rzhdt y} \\ \forall r \in \mathbb{R}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \end{aligned} \quad (6)$$

Here, $U_{rzhdt y}$ is the rate of utilisation of naturally available resource r in zone z during hour h , day type d , season t and planning period y . Examples of naturally available resources include natural gas, biomass and wind. The utilisation rates for each of these resources are defined in section 3.4.

$P_{rzhdt y}^h$ and P_{rzdty}^d are the net rates of production of resource r by conversion technologies, and are defined in section 3.5.

$S_{rzhdt y}$ is the net flow of resource r into zone z due to the operation of storage technologies, and is defined in section 3.6.

$Q_{rzhdt y}$ is the net rate of transport of resource r into into zone z from all other zones, and is defined in section 3.7.

$L_{zlhdt y}$ is the net flow of resource r into zone z due to the operation of linepack technologies, and is defined in section 3.8.

$M_{rzhdt y}$ and $X_{rzhdt y}$ are the rates of import and export of resource r , and are defined in section 3.4.5.

$D_{rzhdt y}^{\text{comp}}$ and $D_{rzhdt y}^{\text{sat}}$ are the demands for resource r , and are defined in section 3.9.

Finally, $E_{rzhdt y}$ is the excess production of resource r . The excess production variable allows the production of a resource in any zone to exceed the total demands on it (actual demands plus any consumption in conversion technologies, transport out of the zone or injection into storage). This can sometimes occur because many conversion technologies have minimum operating rates and there may be occasions where some energy production needs to be curtailed. Depending on the resource, and the scenario being considered, the excess production variables can be strictly set to zero or can be constrained using a suitable upper bound and/or using impacts in the objective function (e.g. disposal costs or curtailment costs) to penalise overproduction.

3.4. Natural resources

Some naturally-occurring resources may be utilised without requiring conversion technologies. The utilisation rate of a resource r cannot exceed its natural availability:

$$U_{rzhdt y} \leq u_{rzhdt y}^{\max} \quad \forall r \in \mathbb{R} - \mathbb{C}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (7)$$

The availabilities of the different natural resources are defined differently: this is described in the following sections.

3.4.1. Natural gas

The zonal, hourly availability of natural gas, $u_{\text{NG},zhdt y}^{\max}$, is defined as an input parameter.

3.4.2. Electricity

Renewable electricity sources are included as natural resources. The hourly availability of renewable electricity is defined as follows, including both wind and solar power:

$$u_{\text{Elec},zhdt y}^{\max} = u_{\text{Elec},zhdt y}^{\text{wind},\max} + u_{\text{Elec},zhdt y}^{\text{solar},\max} \quad \forall z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (8)$$

The definitions of the wind availability and solar availability are given in the following subsections. Electricity can also be generated from other resources, such as natural gas, but this is represented using conversion technologies (described in section 3.5).

3.4.2.1. Wind. The maximum available wind power is dependent on the amount of power in the wind (based on the wind speed) and the number, size and performance characteristics of the wind turbines (both newly installed, and pre-existing) available to capture it. The index w is used to represent the different types of wind turbine that can be installed (onshore and offshore).

$$u_{\text{Elec},zhdt y}^{\text{wind},\max} = \sum_w \left(0.5 \times 10^{-6} \rho^{\text{air}} \left[N_{wzy}^{\text{W}} \pi (R_w^{\text{W}})^2 \eta_w + N_{wzy}^{\text{EW}} \pi (R_w^{\text{EW}})^2 \eta_w^{\text{EW}} \right] \tilde{v}_{wzhdt y}^3 \right) \quad \forall z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (9)$$

Here, $\tilde{v}_{wzhdt y}$ is the effective wind speed, based on the wind turbine power curve, defined by Eq. 10:

$$\tilde{v}_{wzhdt y} = \begin{cases} v_w^{\text{rated}} & \text{if } v_w^{\text{rated}} \leq v_{wzhdt y} \leq v_w^{\text{cut-out}} \\ v_{wzhdt y} & \text{if } v_w^{\text{cut-in}} \leq v_{wzhdt y} \leq v_w^{\text{rated}} \\ 0 & \text{otherwise.} \end{cases} \quad (10)$$

For wind power, a technology (wind turbine) is required to extract the wind resource. Pre-existing wind turbines that were installed before the beginning of the model time horizon may be included. New wind turbines may also be installed in each planning period, and likewise some wind turbines may retire. Hence, the number of wind turbines in existence in a planning period (excluding pre-existing wind turbines – the parameters N_{wzy}^{EW} are inputs to the model and already account for the retirement of existing wind turbines) is tracked based on investments NI_{wzy}^{W} and retirements NR_{wzy}^{W} :

$$N_{wzy}^{\text{W}} = N_{z,y-1}^{\text{W}} + NI_{wzy}^{\text{W}} - NR_{wzy}^{\text{W}} \quad \forall z \in \mathbb{Z}, y \in \mathbb{Y}, w \in \mathbb{W} \quad (11)$$

The number of wind turbines retired at the beginning of a given planning period is determined using a matrix $RT_{wy'y}^{\text{W}}$, that specifies for a wind turbine installed in planning period y' , the planning period y in which it will retire (based on the technical life of the turbine). An example of this matrix is shown in Table 7, for a generic technology with a technical lifetime of 20 years (assuming that y is a 10-year planning interval).

$$NR_{wzy}^{\text{W}} = \sum_{y'} RT_{wy'y}^{\text{W}} NI_{zy'}^{\text{WT}} \quad \forall z \in \mathbb{Z}, y \in \mathbb{Y}, w \in \mathbb{W} \quad (12)$$

Table 7: **Retirement factors for a technology with a lifetime of 20 years.**

Investment period, y'	Retirement period, y			
	2020-2030	2030-2040	2040-2050	2050-2060
2020-2030	0	0	1	0
2030-2040	0	0	0	1
2040-2050	0	0	0	0
2050-2060	0	0	0	0

A land (or seabed) area constraint is included to ensure that the area occupied by new wind turbines does not exceed the maximum available suitable area:

$$\pi (5R_w^W)^2 N_{wzy}^W \leq A_{wzy}^{W,\max} \quad \forall z \in \mathbb{Z}, y \in \mathbb{Y}, w \in \mathbb{W} \quad (13)$$

The maximum suitable area for wind turbines, $A_{wzy}^{W,\max}$, is a model input parameter. The area already occupied by pre-existing wind turbines was excluded from $A_{wzy}^{W,\max}$.

Finally, wind turbines have impacts associated with their capital investment and operation.

The total net present capital impact for new wind turbines is dependent on the number of turbines installed, NI_{wzy}^W , and their capital cost, C_{wiy}^W :

$$\mathcal{J}_{iy}^W = \varsigma D_{wiy}^C \sum_{zw} C_{wiy}^W NI_{wzy}^W \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (14)$$

The total net present O&M impact for wind turbines depends on the number of new (N_{wzy}^W) and pre-existing (NU_{wzy}^{EW}) turbines in operation, and the operating costs of those turbines, ϕ_{wiy}^W :

$$\mathcal{J}_{iy}^w = \varsigma D_y^{OM} \sum_{zw} \phi_{wiy}^W (N_{wzy}^W + NU_{wzy}^{EW}) \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (15)$$

3.4.2.2. Solar. The availability of solar power is represented in a similar way to wind power, and it depends on the availability of the solar resource (irradiance) and the solar PV panels installed:

$$u_{Elec,zhdt}^{solar,max} = \sum_{sl} \left((N_{slzy}^S + N_{slzy}^{ES}) \mathcal{P}_{sl}^S \varepsilon_{sl}^S \eta_{sl}^S I_{slzhd}^S \right) \quad \forall z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (16)$$

where the index sl represents the different types of solar PV installation (solar farm and rooftop solar); N_{slzy}^S and N_{slzy}^{ES} are the number of new and pre-existing solar PV units installed respectively; I_{slzhd}^S represents the solar irradiance (expressed as a fraction of the maximum possible irradiance); \mathcal{P}_{sl}^S is the maximum electrical capacity of single PV unit; ε_{sl}^S is reduction factor representing imperfect panel siting; and η_{sl}^S is the auxiliary system efficiency.

The number of pre-existing solar units already installed at the beginning of the time horizon, N_{slzy}^{ES} , is a pre-defined input to the model, and accounts for retirements of these units throughout the time horizon. However the number of new solar units installed in each time interval is a variable that is subject to optimisation by the VWM. The number of solar units installed in a given time interval, N_{slzy}^S , is tracked based on retirements, NR_{slzy}^S and new investments, NI_{slzy}^S :

$$N_{slzy}^S = N_{z,y-1}^S + NI_{slzy}^S - NR_{slzy}^S \quad \forall sl \in \mathbb{SL} z \in \mathbb{Z}, y \in \mathbb{Y} \quad (17)$$

The number of solar units retired at the beginning of each planning period is calculated based on the number of units installed in previous planning periods and the technological lifetime of the solar unit.

A land area constraint is included to ensure that the area occupied by new solar units does not exceed the maximum available suitable area:

$$N_{slzy}^S A_{sl}^S \leq A_{slzy}^{S,\max} \quad \forall sl \in \mathbb{SL} \ z \in \mathbb{Z}, y \in \mathbb{Y} \quad (18)$$

Finally, solar units have impacts associated with their capital investment and operation.

The total net present capital impact for new solar units is dependent on the number of units installed, NI_{slzy}^S , and their capital cost, C_{sliy}^S :

$$\mathcal{I}_{iy}^{SL} = \varsigma D_{iy}^C \sum_z C_{sliy}^S NI_{slzy}^S \quad \forall sl \in \mathbb{SL} \ i \in \mathbb{I}, y \in \mathbb{Y} \quad (19)$$

The total net present O&M impact for solar units depends on the number of new (N_{slzy}^S) and pre-existing (N_{slzy}^{ES}) units in operation and the operating costs of those units, ϕ_{sliy}^S :

$$\mathcal{I}_{iy}^{sl} = \varsigma D_y^{OM} \sum_{zw} \phi_{sliy}^S (N_{slzy}^S + N_{slzy}^{ES}) \quad \forall sl \in \mathbb{SL} \ i \in \mathbb{I}, y \in \mathbb{Y} \quad (20)$$

3.4.3. Biomass

Unlike other natural resources, such as wind and natural gas, biomass can only be harvested at certain times of the year. The model assumes that once the biomass is harvested, it can be stored and utilised as required within the same season. Longer-term storage would require dedicated storage facilities to be installed (also supported in the model). The total utilisation of biomass over a season is thus constrained by the availability of the biomass in each season, which depends on the yield potential of the crop in that season (which may be zero in some seasons) and the land area allocated to its production:

$$\sum_{hd} U_{czhdy} n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} \leq A_{czy}^{\text{Bio}} Y_{czy}^{\text{Bio}} \quad \forall c \in \mathbb{C} \subseteq \mathbb{R}, z \in \mathbb{Z}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (21)$$

The total fraction of area occupied by a biomass crop can be constrained per-zone (Eq. 22), and/or across the whole system (Eq. 23):

$$\sum_c A_{czy}^{\text{Bio}} \leq f_{zy}^{\text{loc}} A_{zy}^{\text{Bio},\max} \quad \forall z \in \mathbb{Z}, y \in \mathbb{Y} \quad (22)$$

$$\sum_{cz} A_{czy}^{\text{Bio}} \leq f_y^{\text{nat}} \sum_z A_{zy}^{\text{Bio},\max} \quad \forall y \in \mathbb{Y} \quad (23)$$

The maximum suitable land area for biomass, $A_{zy}^{\text{Bio},\max}$, was determined by performing land suitability analysis using GIS software.

3.4.4. Resource utilisation impacts

Resource utilisation can incur an ‘‘impact’’, such as a cost or CO₂ emissions, which is included in the objective function. This impact \mathcal{I}_{iy}^U is calculated from the impact of one unit of resource (c_{rihdy}^U , or c_{city}^{Bio} for biomass) multiplied by the resource utilisation and summed over all time intervals:

$$\mathcal{I}_{iy}^U = \varsigma D_{iy}^{OM} \left(\sum_{r \in \mathbb{R} - \mathbb{C}} \sum_{zhdt} c_{rihdy}^U U_{rzhdy} n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} + \sum_{czt} c_{city}^{\text{Bio}} U_{czhdy} n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} \right) \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (24)$$

Note that the unit impacts for biomass production, c_{city}^{Bio} , include the costs associated with the storage of harvested crop while it is being utilised throughout the season.

3.4.5. Imports and exports

The maximum import and export rates of resource r in and out of zone z can be constrained based on specified limits. The constraints are as follows:

$$M_{rzhdty} \leq m_{rzhdty}^{\max} \quad \forall r \in \mathbb{R}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (25)$$

$$X_{rzhdty} \leq \chi_{rzhdty}^{\max} \quad \forall r \in \mathbb{R}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (26)$$

Imports and exports are included in the objective function and may have financial and environmental impacts (e.g. the emissions due to the import of electricity that is generated from fossil fuels). The net present impact of imports is:

$$\mathcal{I}_{iy}^m = \varsigma D_{iy}^{\text{OM}} \sum_{rzhdty} c_{rihdy}^M M_{rzhdty} n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (27)$$

Similarly, the net present impact of exports is:

$$\mathcal{I}_{iy}^x = \varsigma D_{iy}^{\text{OM}} \sum_{rzhdty} c_{rihdy}^X X_{rzhdty} n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (28)$$

3.5. Resource conversion

3.5.1. General conversion technology constraints

Conversion technologies take certain resources as inputs, and produce other resources as outputs. Constraints are required to manage both the flow of resources between conversion technologies, and the numbers and impacts of conversion technologies in existence.

Resource conversion technologies are defined as “hourly”, if they are able to vary output on an hourly basis, or “daily”, if they are less flexible and can only vary output on a daily basis. The net rate of production (or consumption) of resource r by hourly and daily technologies is given by equations 29 and 30 respectively:

$$P_{rzhdty}^h = \sum_{p \in \mathbb{P}^D} \mathcal{P}_{pzhdty}^h \alpha_{rpy} \quad \forall r \in \mathbb{R}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (29)$$

$$P_{rzdty}^d = \sum_{p \in \mathbb{P}^C} \mathcal{P}_{pzdty}^d \alpha_{rpy} \quad \forall r \in \mathbb{R}, z \in \mathbb{Z}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (30)$$

Note that the units for both of these constraints is UoR/h.

Constraints are included for the maximum and minimum operating rates of conversion technologies. The overall operating rate of the technology type p depends on the number of technologies installed, N_{pzy}^{PC} , and the physical maximum and minimum (part-load) operating rates of the technology:

$$N_{pzy}^{\text{PC}} P_p^{\min} \leq \mathcal{P}_{pzhdty}^h \leq N_{pzy}^{\text{PC}} P_p^{\max} \quad \forall p \in \mathbb{P}^D, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (31)$$

$$N_{pzy}^{\text{PC}} P_p^{\min} \leq \mathcal{P}_{pzdty}^d \leq N_{pzy}^{\text{PC}} P_p^{\max} \quad \forall p \in \mathbb{P}^C, z \in \mathbb{Z}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (32)$$

The total number of technologies installed in a given zone z in a given planning period y is tracked based on the number of pre-existing technologies, N_{pz}^{EPC} , the number of new technologies installed, NI_{pzy}^{PC} , and the number of new technologies and pre-existing technologies retired (NR_{pzy}^{PC} and NR_{pzy}^{EPC}):

$$N_{pzy}^{\text{PC}} = \begin{cases} N_{pz}^{\text{EPC}} + NI_{pzy}^{\text{PC}} - NR_{pzy}^{\text{PC}} & \forall p \in \mathbb{P}^C, z \in \mathbb{Z}, y = 1 \\ N_{pz,y-1}^{\text{PC}} + NI_{pzy}^{\text{PC}} - NR_{pzy}^{\text{PC}} - NR_{pzy}^{\text{EPC}} & \forall p \in \mathbb{P}^C, z \in \mathbb{Z}, y > 1 \end{cases} \quad (33)$$

The number of technologies retired is determined using a matrix $RF_{py'y}^P$, in the same manner as for wind turbines (see Table 7 for an example matrix):

$$NR_{pzy}^{PC} = \sum_{y'} RF_{py'y}^P NI_{pzy'}^P \quad \forall p \in \mathbb{P}^C, z \in \mathbb{Z}, y \in \mathbb{Y} \quad (34)$$

The maximum total number of commercial technologies that can be built in planning period y (i.e. the build rate) is also constrained:

$$\sum_z NI_{pzy}^{PC} \leq BR_{py} \quad \forall p \in \mathbb{P}^C, y \in \mathbb{Y} \quad (35)$$

3.5.1.1. Domestic conversion technologies. Given that domestic conversion technologies are likely to be installed in very large number, they are counted with a continuous variable, N_{pzy}^{PD} , rather than an integer variable. The total production rate of all domestic technologies $p \in \mathbb{P}^D$ in zone z is therefore:

$$\mathcal{P}_{pzhdt y}^h \leq 10^6 N_{pzy}^{PD} p_p^{\max} \quad \forall p \in \mathbb{P}^D, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (36)$$

Domestic heating technologies are also constrained so that the fraction of overall heat provided by a given technology in a zone in any time interval is fixed across the whole year. This is to prevent, for example, heat pumps being used at maximum capacity throughout the year, and gas boilers being used for “peak” heat demands during the winter (this is not realistic as it does not represent one-technology-per-home). The quantity of heat provided by each domestic technology in each time interval is constrained to equal a given amount based on an annual fraction of the overall heat demand in that zone.

$$P_{rzhdt y}^h \alpha_{rpy} = D_{rzhdt y}^{\text{comp}} f_{piy}^{\text{heat}} \quad \forall r = \text{“heat” } z \in \mathbb{Z} h \in \mathbb{H} d \in \mathbb{D} t \in \mathbb{T} y \in \mathbb{Y} p \in \mathbb{P}^D \quad (37)$$

Finally, a constraint is also included to ensure that at least one domestic heating technology is installed in every home.

$$\sum_{p \in \mathbb{P}^D} N_{pzy}^{PD} \geq N_{zy}^{\text{house}} \quad \forall z \in \mathbb{Z}, y \in \mathbb{Y} \quad (38)$$

3.5.1.2. Distribution technologies. Constraints are included to manage the relationships between existing natural gas grids and the technologies that represent partial hydrogen injection and complete conversion to hydrogen.

“Complete conversion” of natural gas distribution grids to hydrogen is represented by the installation of a new conversion technology that converts “centralised” hydrogen to “distributed” hydrogen. Each “complete conversion” technology has equivalent operating parameters to a single natural gas distribution technology (although accounting for the differing behaviour of hydrogen and natural gas). The number of “complete conversion” technologies that can be installed cannot exceed the existing number of natural gas distribution grids available for conversion:

$$N_{HIGG-ComCon,zy}^{PC} \leq N_{NGDistGrid,zy}^{PC} \quad \forall z \in \mathbb{Z} y \in \mathbb{Y} \quad (39)$$

Otherwise, “complete conversion” technologies are governed by the same constraints as any other conversion technology.

Partial hydrogen injection is modelled with a new technology, with a capacity equivalent to a single existing gas distribution technology, that converts hydrogen and natural gas in a fixed ratio (e.g. 0.07 H₂ : 0.93 NG) to the “distributed” gas. In any given time interval, either the existing gas grid technology can operate (i.e. no hydrogen injection), the new injection technology can operate (i.e. maximum hydrogen injection), or a combination of both can operate (for partial hydrogen injection below the maximum limit). Because the new injection technology does not increase the capacity of the grid, a constraint is included to ensure that the

maximum operation of the gas grid in a given spatial zone, with hydrogen injection technologies installed, is no more than the upper bound on the gas grid capacity:

$$\sum_{p \in \mathbb{P}^{\text{HIGG}}} \mathcal{P}_{pzhdty}^h \leq (N_{NG \text{ DistGrid}, zy}^{PC} - N_{HIGG-ComCon, zy}^{PC}) P_{NG \text{ DistGrid}}^{\max} \quad \forall z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (40)$$

The subset \mathbb{P}^{HIGG} includes the natural gas distribution technology and the partial injection technology. The total operating rate of all of these technologies in a spatial zone cannot exceed the maximum operating rate of a single natural gas distribution technology ($P_{NG \text{ DistGrid}}^{\max}$), multiplied by the number of available natural gas distribution technologies (excluding distribution technologies that have been converted completely to hydrogen).

3.5.2. Conversion technology impacts

Conversion technologies are included in the objective function, as they incur impacts from their investment and operation.

The total net present capital impact for building new conversion technologies depends on the number invested in and the capital cost:

$$\mathcal{I}_{iy}^P = \varsigma \sum_z \left(\sum_{p \in \mathbb{P}^{\text{D}}} D_{piy}^C C_{piy}^P N_{pzy}^{PC} \beta_{piz} \kappa_{piy} + \sum_{p \in \mathbb{P}^{\text{C}}} 10^6 D_{piy}^C C_{piy}^P N_{pzy}^{\text{PD}} \beta_{piz} \kappa_{piy} \right) \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (41)$$

The total net present O&M impact for conversion technologies depends on the number in operation and the O&M impact of the technology:

$$\mathcal{I}_{iy}^{\text{fP}} = \varsigma \sum_z \left(\sum_{p \in \mathbb{P}^{\text{D}}} D_{iy}^{\text{OM}} \phi_{piy}^P N_{pzy}^{PC} \beta_{piz} \kappa_{piy} + \sum_{p \in \mathbb{P}^{\text{C}}} 10^6 D_{iy}^{\text{OM}} \phi_{piy}^P N_{pzy}^{\text{PD}} \beta_{piz} \kappa_{piy} \right) \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (42)$$

The total net present variable operating impact of conversion technologies depends on the operating rates and the variable operating impacts of the given technology:

$$\mathcal{I}_{iy}^{\text{vP}} = \varsigma D_{iy}^{\text{OM}} \left(\sum_{p \in \mathbb{P}^{\text{D}}} \sum_{zhd} \varphi_{piy}^P \mathcal{P}_{pzhdty}^h n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} + \sum_{p \in \mathbb{P}^{\text{C}}} \sum_{zdt} \varphi_{piy}^P \mathcal{P}_{pzdtty}^d n_d^{\text{dw}} n_t^{\text{wt}} \right) \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (43)$$

Impacts are calculated on a overall system basis, rather than “per plant”. For example, the operating impact for a particular technology does not directly include the impact of any raw materials consumed. The resource balance ensures that consumption of a resource must be balanced by: import, transport from another zone, production by other technologies, utilisation of available resource (e.g. wind, biomass) or utilisation of stored resource. Each of these options for providing the resource have their own impacts associated with them, such as the costs of import, or CO₂ emissions from the production process. Hence, the “life-cycle” impacts for a given plant are not specifically calculated, but the overall system impacts are accounted for correctly.

3.5.2.1. CO₂ emissions associated with conversion technologies. The impacts described in section 3.5.2 are used to represent indirect emissions associated with conversion technologies (e.g. the CO₂ emitted in the construction of the technology). However, CO₂ is also modelled as a resource in the model, and many conversion technologies produce CO₂, which may be captured and utilised or stored. Therefore, a separate impact must be used to keep track of any CO₂ resource that is produced by conversion technologies but not captured. First, the net production of CO₂ by conversion technologies is calculated:

$$P_y^{P,CO_2} = \sum_{pzhdty} (\alpha_{rpy} (P_{rzhdt_y}^h + P_{rzdty}^d) n_h^{hd} n_d^{dw} n_t^{wt}) \quad \forall r = CO_2, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (44)$$

This annual quantity of CO₂ emissions is then converted to a system impact:

$$\mathcal{I}_{iy}^{CO_2} = \begin{cases} \varsigma D_{iy}^{OM} P_y^{P,CO_2} & \forall y \in \mathbb{Y}, i = CO_2 \\ 0 & otherwise \end{cases} \quad (45)$$

3.6. Storage

3.6.1. General storage technology constraints

In any given time interval, resources can be loaded into storage (put), held in storage (hold), or extracted from storage (get). The flows of resources into and out of storage are tracked as follows:

$$S_{rzhdt_y} = \sum_s \left(\mathcal{I}_{szhdty}^{put} \sigma_{sr,src,y}^{put} + \mathcal{I}_{szhdty}^{hold} \sigma_{sr,dst,y}^{hold} + \mathcal{I}_{szhdty}^{get} \sigma_{sr,dst,y}^{get} \right) \quad (46)$$

$$\forall r \in \mathbb{R}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y}$$

S_{rzhdt_y} is the net flow of resource from a storage technology into a zone. For the resource being stored, it is negative if the storage is being filled (the zone has to produce resource in order to store it) or it is positive if the storage is being emptied (the zone gains resource to use by taking it out of storage). Other resources can be produced in or required of the zone, such as emissions and energy required to power the storage activities. Each storage task has a conversion factor, σ_{srfy}^* ($\star \in \{\text{put, hold, get}\}$), associated with it, which when multiplied by the rate of operation of the tasks ($\mathcal{I}_{szhdty}^{put}$, $\mathcal{I}_{szhdty}^{hold}$ and $\mathcal{I}_{szhdty}^{get}$) gives the flow of each resource into and out of storage (the index f describes the source or destination of the storage task).

The overall maximum rates at which resources can be loaded into storage (put), or withdrawn from storage (get), are constrained based on the number of storage facilities installed and the physical limitations of those facilities:

$$\mathcal{I}_{szhdty}^{put} \leq N_{szy}^S s_s^{put,max} a_{sz} \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (47)$$

$$\mathcal{I}_{szhdty}^{get} \leq N_{szy}^S s_s^{get,max} a_{sz} \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (48)$$

where $s_s^{put,max}$ and $s_s^{get,max}$ are the maximum rates that a resource can be loaded into storage and withdrawn from storage for a single storage facility of type s ; a_{sz} is a parameter that can be set to 0 or 1 to specify where certain storage facilities may be placed.

As well as tracking the resource flows into and out of storage, the overall inventory of a given storage technology s is also tracked (note the value of the index f is the opposite of that in Eq. (46) – whatever goes into storage has to be provided by the zone, and whatever comes out of storage is made available to the zone):

$$I_{szhdty} = n_h^{hd} \sum_r \left(\mathcal{I}_{szhdty}^{put} \sigma_{sr,dst,y}^{put} + \mathcal{I}_{szhdty}^{hold} \sigma_{sr,src,y}^{hold} + \mathcal{I}_{szhdty}^{get} \sigma_{sr,src,y}^{get} \right) \quad (49)$$

$$\forall s \in \mathbb{S}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y}$$

The rate of operation of the “hold” task is defined as the current inventory level divided by the length of the time interval:

$$\mathcal{I}_{sz,1,dt y}^{\text{hold}} = I_{szdt y}^{0,\text{sim}} / n_1^{\text{hd}} \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (50)$$

$$\mathcal{I}_{szhdt y}^{\text{hold}} = I_{sz,h-1,dt y} / n_h^{\text{hd}} \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, h > 1 \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (51)$$

The daily storage “surplus” is the change in inventory level between the first and last hourly intervals of the given day type d :

$$\delta_{szdt y}^{\text{d}} = I_{sz,|\mathbb{H}|,dt y} - I_{szdt y}^{0,\text{sim}} \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (52)$$

The surplus for a week in season t is then calculated from the sum of the daily surpluses of each day type d in the given week, accounting for the number of repeated day types n_d^{dw} :

$$\delta_{szty}^{\text{t}} = \sum_d \delta_{szdt y}^{\text{d}} n_d^{\text{dw}} \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (53)$$

The surplus for a season is the weekly surplus in that season multiplied by the number of weeks in that season. Finally, the surplus over year y is the sum of all seasonal surpluses:

$$\delta_{szy}^{\text{y}} = \sum_t \delta_{szty}^{\text{t}} n_t^{\text{wt}} \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (54)$$

If it is necessary to keep the storage inventory over one year stationary, i.e. no yearly storage surplus (or deficit), then an optional constraint can be included:

$$\delta_{szy}^{\text{y}} = 0 \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, y \in \mathbb{Y} \quad (55)$$

The inventory levels over the entire time horizon need to be evaluated in order to ensure that the storage capacity of all installed storage technologies is not exceeded and to calculate the total impacts of holding inventory. Due to the repeated days in a week and repeated seasons in each year, the full inventory profile can be obtained from only the $I_{szhdt y}$, $\delta_{szdt y}^{\text{d}}$, δ_{szty}^{t} and δ_{szy}^{y} variables. Therefore the total impacts and resource requirements are easily calculated, but these can equivalently be calculated by using an inventory profile averaged over all of the individual days, weeks and years in each day type, season and yearly period. Thus, it can be shown that if the initial inventory at the beginning of the first day in day type d , first week in season t and first year in yearly period y is $I_{szdt y}^{0,\text{act}}$, then the inventory profile given by equations 49, 50 and 51 will give the correct average impacts and resource requirements if:

$$I_{szdt y}^{0,\text{sim}} = I_{szdt y}^{0,\text{act}} + [(n_d^{\text{dw}} - 1) \delta_{szdt y}^{\text{d}} + (n_t^{\text{wt}} - 1) \delta_{szty}^{\text{t}} + (n_y^{\text{yy}} - 1) \delta_{szy}^{\text{y}}] / 2 \quad (56)$$

$$\forall s \in \mathbb{S}, z \in \mathbb{Z}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y}$$

and if the $I_{szdt y}^{0,\text{act}}$ variables are linked as follows.

The inventory level at the beginning of a day type is calculated from the inventory at the beginning of the previous day type, plus the storage surplus over all days in the previous day type:

$$I_{szdt y}^{0,\text{act}} = I_{sz,d-1,ty}^{0,\text{act}} + n_{d-1}^{\text{dw}} \delta_{sz,d-1,ty}^{\text{d}} \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, d > 1 \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (57)$$

The same procedure is used to link seasons and years:

$$I_{sz,1,ty}^{0,\text{act}} = I_{sz,1,t-1,y}^{0,\text{act}} + n_{t-1}^{\text{wt}} \delta_{sz,t-1,y}^{\text{t}} \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, t > 1 \in \mathbb{T}, y \in \mathbb{Y} \quad (58)$$

$$I_{sz,1,1,y}^{0,act} = I_{sz,1,1,y-1}^{0,act} + n_{y-1}^{yy} \delta_{sz,y-1}^y \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, y > 1 \in \mathbb{Y} \quad (59)$$

Maximum and minimum storage capacities are defined ($s_s^{\text{hold,max}}$ and $s_s^{\text{hold,min}}$, respectively), and constraints are put in place to ensure the inventory is kept between these limits. Since the daily storage surpluses are identical for each day of a given day type, maximum and minimum inventory levels will occur in the first or last days of the day type. Hence, only these days need to be constrained within the storage capacity limits. The same applies for weeks in a season, and years in the planning period. The combinations of first and last day, first and last week, and first and last year result in a requirement of 8 constraints, which is then doubled to 16 in order to constrain both the minimum and maximum inventories. These 16 constraints are shown in shorthand below, where all eight possible combinations of plus and minus should be taken to give each pair of constraints (minimum and maximum inventory level constraints):

$$s_s^{\text{hold,min}} N_{szy}^S a_{sz} \leq I_{szhdt y} \pm \frac{(n_d^{\text{dw}} - 1) \delta_{szdty}^d \pm (n_t^{\text{wt}} - 1) \delta_{szt y}^t \pm (n_y^{\text{yy}} - 1) \delta_{szy}^y}{2} \leq s_s^{\text{hold,max}} N_{szy}^S a_{sz} \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (60)$$

As with conversion technologies, the total number of storage technologies installed in given zone z in a given planning period y is tracked based on the number of pre-existing technologies, N_{sz}^{ES} , number of technologies installed, NI_{szy}^S , and number of technologies and pre-existing technologies retired (NR_{szy}^S and NR_{szy}^{ES}):

$$N_{szy}^S = \begin{cases} N_{sz}^{\text{ES}} + NI_{szy}^S - NR_{szy}^S & \forall s \in \mathbb{S}, z \in \mathbb{Z}, y = 1 \\ N_{sz,y-1}^S + NI_{szy}^S - NR_{szy}^S - NR_{szy}^{\text{ES}} & \forall s \in \mathbb{S}, z \in \mathbb{Z}, y > 1 \end{cases} \quad (61)$$

Again, the number of technologies retired is determined using a matrix $RF_{sy'y}^S$ (see Table 7 for an example matrix):

$$NR_{szy}^S = \sum_{y'} RF_{sy'y}^S NI_{szy'}^S \quad \forall s \in \mathbb{S}, z \in \mathbb{Z}, y \in \mathbb{Y} \quad (62)$$

Finally, compressors and expanders are included in the model to enable resources such as hydrogen to be converted to and from the high pressures needed for storage. These conversion technologies are sized to exactly match the storage technologies in the model, so to prevent them being installed for other (incorrect) purposes, constraints are included that limit the number of compressors/expanders to no more than the number of corresponding storage technologies. An example of these constraints for the case of a large hydrogen storage tank (CGH₂S – L) is shown below. Note that an inequality is used as it is still possible for the number of storage technologies to exceed the number of compressors/expanders if the storage gas does not require compression/expansion (e.g. if it is obtained from, or subsequently used for, a high-pressure purpose).

$$N_{\text{COMP-L},z}^P \leq N_{\text{CGH2S-L},z}^S \quad \forall z \in \mathbb{Z} \quad (63)$$

$$N_{\text{EXP-L},z}^P \leq N_{\text{CGH2S-L},z}^S \quad \forall z \in \mathbb{Z} \quad (64)$$

3.6.2. Distribution storage (linepack) constraints

The storage (linepack) capacities of natural gas and hydrogen distribution grids (for natural gas and hydrogen) are included in the model by including “dummy” storage technologies, that are coupled to the equivalent distribution grid conversion technologies. These technologies behave in the same way as other storage technologies, but have no impacts associated with them (all impacts are accounted for by the conversion technology), and the number installed is constrained to equal the number of equivalent conversion technologies installed (in this case, each storage technology is directly linked to the corresponding production technology):

$$N_{szy}^S = N_{pzy}^{\text{PC}} \quad \forall s \in \mathbb{S}^{\text{Dist}}, z \in \mathbb{Z}, y \in \mathbb{Y}, p \in \mathbb{P}^{\text{Dist}} \quad (65)$$

3.6.3. Storage technology impacts

The total net present capital impact for building new storage technologies depends on the number invested in and the capital cost:

$$\mathcal{I}_{iy}^S = \varsigma \sum_{sz} D_{sly}^C C_{sly}^S N_{sly}^S \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (66)$$

The total net present O&M impact for storage technologies depends on the number in operation and the O&M impact of the technology:

$$\mathcal{I}_{iy}^{fs} = \varsigma D_{iy}^{OM} \sum_{sz} \phi_{sly}^S N_{sly}^S \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (67)$$

The total net present variable operating impact of storage technologies depends on the operating rates and the variable operating impacts of the given technology:

$$\mathcal{I}_{iy}^{vs} = \varsigma D_{iy}^{OM} \sum_{szhdt} \left(\varphi_{sly}^{SP} \mathcal{I}_{szhdt}^{put} + \varphi_{sly}^{SH} \mathcal{I}_{szhdt}^{hold} + \varphi_{sly}^{SG} \mathcal{I}_{szhdt}^{get} \right) n_h^{hd} n_d^{dw} n_t^{wt} \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (68)$$

3.7. Transport

Transport of resources between zones is allowed through transport technologies, which utilise transport infrastructures. In many cases, the technology and infrastructure may be the same (for example, electricity transmission lines). However in some cases the distinction is useful, for example in road transport, where more than one resource can be transported by road: individual transport technologies represent the transport of each resource and they all require the road itself (the infrastructure) to operate on. Constraints are required to manage the flow of transported resources and the installation and operation of transport technologies and infrastructures.

The distance between spatial zones is used to calculate losses and impacts associated with transport, and is calculated based on the geographical locations of the zones' demand centres:

$$d_{zz'} = \sqrt{(x_z - x_{z'})^2 + (y_z - y_{z'})^2} \quad \forall z, z' \in \mathbb{Z} \quad (69)$$

Resource flows are calculated from the operating rate of the transport technology, $\mathcal{Q}_{mzz'hdt}$, and both distance-independent and distance-dependent conversion factors ($\bar{\tau}_{mrfy}$ and $\hat{\tau}_{mrfy}$, respectively). Similar to the storage tasks, these conversion factors allow for the both the flow of the resource being transported as well as any other resource requirements or losses associated with the transport process. The net flow of resource into a zone due to the operation of transport technologies is:

$$\begin{aligned} Q_{rzhdt} = & \sum_{z' | \nu_{z'} = 1} \sum_{m \in \mathbb{M}} [(\bar{\tau}_{mr, \text{dst}, y} + \hat{\tau}_{mr, \text{dst}, y} d_{z'z}) \mathcal{Q}_{mz'zhdt}] \\ & + \sum_{z' | \nu_{zz'} = 1} \sum_{m \in \mathbb{M}} [(\bar{\tau}_{mr, \text{src}, y} + \hat{\tau}_{mr, \text{src}, y} d_{zz'}) \mathcal{Q}_{mzz'hdt}] \end{aligned} \quad \forall r \in \mathbb{R}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (70)$$

The rate of operation of each transport technology m cannot exceed its maximum operating rate multiplied by the number of infrastructures in place between zones z and z' :

$$\mathcal{Q}_{mzz'hdt} \leq \sum_{b \in \mathbb{B}} q_m^{\max} N_{bzz'y}^B |MB_{tb=1 \wedge \nu_{zz'}=1} \quad \forall m \in \mathbb{M}; z, z' \in \mathbb{Z}; h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (71)$$

where the binary parameter, MB_{lb} , is used to determine which transport technologies use which infrastructures and $\nu_{zz'}$ defines all possible connections between zones (it is 1 if zone z may be connected to zone z').

Where transport infrastructures b differ from the transport technology m , a constraint is included to ensure that the operating rate of all transport technologies does not exceed the capacity of the infrastructure.

$$\sum_{m \in \mathbb{M}} \mathcal{Q}_{mzz'hdt} MB_{lb} \leq b_b^{\max} N_{bzz'y}^{\mathbb{B}} \quad \forall b \in \mathbb{B}; z, z' \in \mathbb{Z}; h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (72)$$

Similar to conversion and storage technologies, the total number of transport infrastructures installed in zone z in a given planning period y is tracked based on the number of pre-existing infrastructures, $N_{bzz'}^{\mathbb{EB}}$, and the number of new infrastructures installed. It is assumed that transport infrastructures have a lifetime longer than the model time horizon, so retirements are not included.

$$N_{bzz'y}^{\mathbb{B}} = \begin{cases} N_{bzz'}^{\mathbb{EB}} + NI_{bzz'y}^{\mathbb{B}} & \forall b \in \mathbb{B}, z, z' \in \mathbb{Z}, y = 1 \\ N_{bzz',y-1}^{\mathbb{B}} + NI_{bzz'y}^{\mathbb{B}} & \forall b \in \mathbb{B}, z, z' \in \mathbb{Z}, y > 1 \end{cases} \quad (73)$$

The model distinguishes between transport infrastructures that may only be operated in one direction (one-way unidirectional, e.g. some pipelines), infrastructures that can be only operated in one direction, but can be built in combination with an identical infrastructure in the opposite direction (two-way unidirectional, e.g. roads), and infrastructures that can be operated in either direction (bidirectional, e.g. electricity transmission lines). Constraints are defined for these configurations used the directionality parameter β_b ($\beta_b = -1$ for one-way unidirectional, $\beta_b = 0$ for two-way unidirectional, and $\beta_b = 1$ for bidirectional):

$$N_{bzz'y}^{\mathbb{B}} = N_{bz'zy}^{\mathbb{B}} \quad \forall b \in \mathbb{B} | \beta_b = 1, z \neq z' \in \mathbb{Z} \quad (74)$$

$$N_{bzz'y}^{\mathbb{B}} + N_{bz'zy}^{\mathbb{B}} \leq 1 \quad \forall b \in \mathbb{B} | \beta_b = -1, z \neq z' \in \mathbb{Z} \quad (75)$$

3.7.1. Transport infrastructure impacts

The total net present capital impact for building new transport infrastructures depends on the number invested in, the infrastructure length and the unit capital impact:

$$\mathcal{I}_{iy}^{\mathbb{Q}} = \varsigma \sum_{bzz'} D_{biy}^{\mathbb{C}} C_{biy}^{\mathbb{B}} NI_{bzz'y}^{\mathbb{B}} d_{zz'} (1 - 0.5|\beta_b=1) \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (76)$$

The total net present O&M impact for transport infrastructures depends on the number in operation, the infrastructure length and the unit O&M impact:

$$\mathcal{I}_{iy}^{\text{fq}} = \varsigma D_{iy}^{\text{OM}} \sum_{bzz'} \phi_{biy}^{\mathbb{B}} NI_{bzz'y}^{\mathbb{B}} d_{zz'} (1 - 0.5|\beta_b=1) \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (77)$$

The total net present variable operating impact of transport technologies depends on the operating rates, the infrastructure length and the unit variable operating impacts:

$$\mathcal{I}_{iy}^{\text{vq}} = \varsigma D_{iy}^{\text{OM}} \sum_{lzz'hdt} \left(\hat{\varphi}_{mly}^{\mathbb{Q}} d_{zz'} + \bar{\varphi}_{mly}^{\mathbb{Q}} \right) \mathcal{Q}_{mzz'hdt} n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (78)$$

Given that bidirectional infrastructures are modelled by effectively building a unidirectional infrastructure in both directions (see Constraint 74), the $0.5|\beta_b=1$ is included in Eqs. 76 and 77 (for bidirectional infrastructures only, $\beta_b = 1$) so that the impact incurred is only representative of building a single infrastructure. For the case where real unidirectional infrastructures are built in both directions, $\beta_b = 0$ and the term disappears.

3.8. Linepack

The formulation for linepack technologies is very similar to storage. The only difference is that whilst storage technologies are built in each zone and kept separate, linepack “connections” are built in each zone, and join up. This means that one overall storage inventory is calculated for all linepack connections, and that resource can be added to the linepack in one zone and withdrawn from another.

Flows of resource into and out of linepack are tracked using “put”, “hold”, and “get” tasks, in the same way as for storage:

$$L_{zlhdt y} = \sum_l \left(\mathcal{L}_{lzhdt y}^{\text{put}} \lambda_{lr,src,y}^{\text{put}} + \mathcal{L}_{lhdt y}^{\text{hold}} \lambda_{lr,dst,y}^{\text{hold}} + \mathcal{L}_{lzhdt y}^{\text{get}} \lambda_{lr,dst,y}^{\text{get}} \right) \quad (79)$$

$$\forall l \in \mathbb{L}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y}$$

$L_{zlhdt y}$ is the net flow of resource from a linepack technology into a zone. The net flow is negative if resource is being added to the linepack system, or it is positive if the linepack is being depleted. Each linepack task has a conversion factor, $\lambda_{lr,f y}^*$ ($\star \in \{\text{put}, \text{hold}, \text{get}\}$), associated with it, which when multiplied by the rate of operation of the tasks ($\mathcal{L}_{lzhdt y}^{\text{put}}$, $\mathcal{L}_{lhdt y}^{\text{hold}}$ and $\mathcal{L}_{lzhdt y}^{\text{get}}$) gives the flow of each resource into and out of linepack (the index f describes the source or destination of the linepack task).

The overall maximum rates at which resources can be loaded into linepack (put), or withdrawn from linepack (get), are constrained based on the number of linepack connections installed in a given zone and the physical limitations of those facilities:

$$\mathcal{L}_{lzhdt y}^{\text{put}} \leq N_{lzy}^{\mathbb{L}} l_l^{\text{put,max}} a_{lz} \quad \forall l \in \mathbb{L}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (80)$$

$$\mathcal{L}_{lzhdt y}^{\text{get}} \leq N_{lzy}^{\mathbb{L}} l_l^{\text{get,max}} a_{lz} \quad \forall l \in \mathbb{L}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (81)$$

where $l_l^{\text{put,max}}$ and $l_l^{\text{get,max}}$ are the maximum rates that a resource can be loaded into linepack and withdrawn from linepack for a given linepack system l ; a_{lz} is a parameter that can be set to 0 or 1 to specify whether a zone may connect to the given linepack system.

The overall inventory of a given linepack system is tracked in the same way as for storage, except that it is also summed over all zones:

$$J_{lhdt y} = n_h^{\text{hd}} \sum_{rz} \left(\mathcal{L}_{lzhdt y}^{\text{put}} \lambda_{lr,dst,y}^{\text{put}} + \mathcal{L}_{lhdt y}^{\text{hold}} \lambda_{lr,src,y}^{\text{hold}} + \mathcal{L}_{lzhdt y}^{\text{get}} \lambda_{lr,src,y}^{\text{get}} \right) \quad (82)$$

$$\forall l \in \mathbb{L}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y}$$

The rate of operation of the “hold” task is defined as the current linepack level divided by the length of the time interval:

$$\mathcal{L}_{l,1,dty}^{\text{hold}} = J_{ldty}^{0,\text{sim}} / n_1^{\text{hd}} \quad \forall l \in \mathbb{L}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (83)$$

$$\mathcal{L}_{lhdt y}^{\text{hold}} = J_{l,h-1,dty} / n_h^{\text{hd}} \quad \forall l \in \mathbb{L}, h > 1 \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (84)$$

The daily linepack “surplus” is the change in linepack between the first and last hourly intervals of the given day type d :

$$\Delta_{ldty}^{\text{d}} = J_{l,|\mathbb{H}|,dty} - J_{ldty}^{0,\text{sim}} \quad \forall l \in \mathbb{L}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (85)$$

The surplus for a week in season t is then calculated from the sum of the daily surpluses of each day type d in the given week, accounting for the number of repeated day types n_d^{dw} :

$$\Delta_{lty}^t = \sum_d \Delta_{lnty}^d n_d^{\text{dw}} \quad \forall l \in \mathbb{L}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (86)$$

The surplus for a season is the weekly surplus in that season multiplied by the number of weeks in that season. Finally, the surplus over year y is the sum of all seasonal surpluses:

$$\Delta_{ly}^y = \sum_t \Delta_{lty}^t n_t^{\text{wt}} \quad \forall l \in \mathbb{L}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (87)$$

If it is necessary to keep the linepack over one year stationary, i.e. no yearly linepack surplus (or deficit), then an optional constraint can be included:

$$\Delta_{ly}^y = 0 \quad \forall l \in \mathbb{L}, y \in \mathbb{Y} \quad (88)$$

The linepack inventory over the entire time horizon need to be evaluated in order to ensure that the linepack capacity of the whole system is not exceeded and to calculate the total impacts of holding linepack. Due to the repeated days in a week and repeated seasons in each year, the full inventory profile can be obtained from only the J_{lhnty} , Δ_{lnty}^d , Δ_{lty}^t and Δ_{ly}^y variables. Therefore the total impacts and resource requirements are easily calculated, but these can equivalently be calculated by using a linepack inventory profile averaged over all of the individual days, weeks and years in each day type, season and yearly period. Thus, it can be shown that if the initial linepack at the beginning of the first day in day type d , first week in season t and first year in yearly period y is $J_{lnty}^{0,\text{act}}$, then the inventory profile given by equations 82, 83 and 84 will give the correct average impacts and resource requirements if:

$$J_{lnty}^{0,\text{sim}} = J_{lnty}^{0,\text{act}} + \left[(n_d^{\text{dw}} - 1) \Delta_{lnty}^d + (n_t^{\text{wt}} - 1) \Delta_{lty}^t + (n_y^{\text{yy}} - 1) \Delta_{ly}^y \right] / 2 \quad (89)$$

$$\forall l \in \mathbb{L}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y}$$

and if the $J_{lnty}^{0,\text{act}}$ variables are linked as follows.

The linepack inventory at the beginning of a day type is calculated from the linepack at the beginning of the previous day type, plus the linepack surplus over all days in the previous day type:

$$J_{lnty}^{0,\text{act}} = J_{l,d-1,ty}^{0,\text{act}} + n_{d-1}^{\text{dw}} \Delta_{l,d-1,ty}^d \quad \forall l \in \mathbb{L}, d > 1 \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (90)$$

The same procedure is used to link seasons and years:

$$J_{l,1,ty}^{0,\text{act}} = J_{l,1,t-1,y}^{0,\text{act}} + n_{t-1}^{\text{wt}} \Delta_{l,t-1,y}^t \quad \forall l \in \mathbb{L}, t > 1 \in \mathbb{T}, y \in \mathbb{Y} \quad (91)$$

$$J_{l,1,1,y}^{0,\text{act}} = J_{l,1,1,y-1}^{0,\text{act}} + n_{y-1}^{\text{yy}} \Delta_{l,y-1}^y \quad \forall l \in \mathbb{L}, y > 1 \in \mathbb{Y} \quad (92)$$

Maximum and minimum linepack capacities are defined ($l_l^{\text{hold,max}}$ and $l_l^{\text{hold,min}}$, respectively), and constraints are put in place to ensure the inventory is kept between these limits. Unlike with storage technologies, one linepack system spans multiple zones, so $l_l^{\text{hold,max}}$ and $l_l^{\text{hold,min}}$ describe the linepack storage capacity of a single linepack “connection”: the overall linepack storage capacity is the sum of all of the linepack connections in all zones. Otherwise, the constraints are set up in the same way as for storage technologies, with only the first and last time intervals being constrained to be within the allowable limits.

The combinations of first and last day, first and last week, and first and last year result in a requirement of 8 constraints, which is then doubled to 16 in order to constrain both the minimum and maximum inventories.

These 16 constraints are shown in shorthand below, where all eight possible combinations of plus and minus should be taken to give each pair of constraints (minimum and maximum linepack inventory constraints):

$$l_i^{\text{hold,min}} \sum_z N_{lzy}^L a_{lz} \leq J_{lhty} \pm G_{lhty} \leq l_i^{\text{hold,max}} \sum_z N_{lzy}^L a_{lz}$$

$$\text{where } G_{lhty} = \frac{(n_d^{\text{dw}} - 1) \Delta_{lhty}^d \pm (n_t^{\text{wt}} - 1) \Delta_{lhty}^t \pm (n_y^{\text{yy}} - 1) \Delta_{lhty}^y}{2} \quad \forall l \in \mathbb{L}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (93)$$

As with conversion technologies, the total number of linepack connections installed in given zone z in a given planning period y is tracked based on the number of pre-existing connections, N_{lz}^{EL} , number of connections installed, NI_{lzy}^L , and number of connections and pre-existing connections retired (NR_{lzy}^L and NR_{lzy}^{EL}):

$$N_{lzy}^L = \begin{cases} N_{lz}^{\text{EL}} + NI_{lzy}^L - NR_{lzy}^L & \forall l \in \mathbb{L}, z \in \mathbb{Z}, y = 1 \\ N_{lz,y-1}^{\text{EL}} + NI_{lzy}^L - NR_{lzy}^L - NR_{lzy}^{\text{EL}} & \forall l \in \mathbb{L}, z \in \mathbb{Z}, y > 1 \end{cases} \quad (94)$$

Again, the number of technologies retired is determined using a matrix $RT_{ly'y}^L$ (see Table 7 for an example matrix):

$$NR_{lzy}^L = \sum_{y'} RT_{ly'y}^L NI_{lzy'}^L \quad \forall l \in \mathbb{L}, z \in \mathbb{Z}, y \in \mathbb{Y} \quad (95)$$

3.8.1. Linepack technology impacts

The total net present capital impact for building new linepack connections depends on the number invested in and the capital cost:

$$\mathcal{I}_{iy}^L = \varsigma \sum_{lz} D_{liy}^C C_{liy}^L NI_{lzy}^L \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (96)$$

The total net present O&M impact for linepack systems depends on the number of linepack connections in operation and the O&M impact of each connection:

$$\mathcal{I}_{iy}^{\text{fl}} = \varsigma D_{iy}^{\text{OM}} \sum_{lz} \phi_{liy}^L NI_{lzy}^L \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (97)$$

The total net present variable operating impact of linepack systems depends on the operating rates and the variable operating impacts of the given technology:

$$\mathcal{I}_{iy}^{\text{vl}} = \varsigma D_{iy}^{\text{OM}} \sum_{lzhdt} \left(\varphi_{liy}^{\text{LP}} \mathcal{L}_{lzhdt}^{\text{put}} + \varphi_{liy}^{\text{LH}} \mathcal{L}_{lzhdt}^{\text{hold}} + \varphi_{liy}^{\text{LG}} \mathcal{L}_{lzhdt}^{\text{get}} \right) n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (98)$$

3.9. Demand satisfaction

For some resources, it is compulsory that demands are satisfied, so these are included in D_{rzhdt}^{comp} . For others, a demand may exist but it is optional whether this demand is satisfied. For example, optional demands can be used for resources that are outside the main scope of the study, but can be sold to provide a revenue. The total level of optional demand (i.e. market size) is defined by D_{rzhdt}^{opt} . The level of optional demand that is then actually satisfied is constrained as follows:

$$D_{rzhdt}^{\text{sat}} \leq D_{rzhdt}^{\text{opt}} \quad \forall r \in \mathbb{R}, z \in \mathbb{Z}, h \in \mathbb{H}, d \in \mathbb{D}, t \in \mathbb{T}, y \in \mathbb{Y} \quad (99)$$

3.9.1. Impacts of demand satisfaction

Revenues from the sale of resources and energy services (satisfying demands) may be included in the objective function using the following impact. The parameter V_{riy} specifies the unit impact of the demand satisfaction (i.e. market price at which the resource is sold):

$$\mathcal{J}_{iy}^{\text{Rev}} = \varsigma D_{iy}^{\text{OM}} \sum_{rzhdt} V_{riy} \left(D_{rzhdt}^{\text{comp}} + D_{rzhdt}^{\text{sat}} \right) n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} \quad \forall i \in \mathbb{I}, y \in \mathbb{Y} \quad (100)$$

References

- [1] Christopher J. Quarton and Sheila Samsatli. Resource and technology data for spatio-temporal value chain modelling of the Great Britain energy system. *Data in Brief*, 31:105886, 2020.
- [2] Department for Energy and Climate Change. RHI biomethane injection to grid tariff review. Consultation document, Department for Energy and Climate Change, 2014. Available online at www.gov.uk/government/consultations/rhi-biomethane-injection-to-grid-tariff-review.
- [3] Goran Strbac, Danny Pudjianto, Robert Sansom, Predrag Djapic, Hossein Ameli, Nilay Shah, Nigel Brandon, Adam Hawkes, and Meysam Qadrdan. Analysis of alternative UK heat decarbonisation pathways. Report, Imperial College London, 2018. Available online at www.theccc.org.uk/wp-content/uploads/2018/06/Imperial-College-2018-Analysis-of-Alternative-UK-Heat-Decarbonisation-Pathways.pdf.
- [4] Department for Business, Energy and Industrial Strategy. Greenhouse gas reporting: conversion factors 2019. Dataset, 2019. Available online at www.gov.uk/government/publications/greenhouse-gas-reporting-conversion-factors-2019.
- [5] R. Ray, S. Ferguson, and A. Tarrant. Assessing the Cost Reduction Potential and Competitiveness of Novel (Next Generation) UK Carbon Capture Technology. Report, BEIS and Wood, 2018.
- [6] Committee on Climate Change. Biomass in a low-carbon economy. Report, 2018. Available online at www.theccc.org.uk/publication/biomass-in-a-low-carbon-economy/.
- [7] Sheila Samsatli and Nouri J. Samsatli. A multi-objective MILP model for the design and operation of future integrated multi-vector energy networks capturing detailed spatio-temporal dependencies. *Applied Energy*, 220:893 – 920, 2018.
- [8] Felix Creutzig, N H Ravindranath, Göran Berndes, Simon Bolwig, Ryan Bright, Francesco Cherubini, Helena Chum, Esteve Corbera, Mark Delucchi, Andre Faaij, Joseph Fargione, Helmut Haberl, Garvin Heath, Oswaldo Lucon, Richard Plevin, Alexander Popp, Carmenza Robledo-Abad, Steven Rose, Pete Smith, and Anders Stromman. Bioenergy and climate change mitigation: an assessment. *Global change biology*, 7(5):916–944, 2015.
- [9] Mathilde Fajardy and Niall Mac Dowell. Can BECCS deliver sustainable and resource efficient negative emissions? *Energy Environ. Sci.*, 10:1389–1426, 2017.
- [10] E4Tech. The Fuel Cell Industry Review 2019. Report, E4Tech, 2019. Available online at www.fuelcellindustryreview.com/.
- [11] FuelCell Energy. Suresource 4000. Factsheet, FuelCell Energy, 2020. Available online at www.fuelcellenergy.com/wp-content/uploads/2013/11/Product-Spec-SureSource-4000.pdf.
- [12] International Energy Agency. Technology roadmap: Hydrogen and fuel cells. Report, 2015. Available online at [http://ieahydrogen.org/pdfs/TechnologyRoadmapHydrogenandFuelCells-\(1\).aspx](http://ieahydrogen.org/pdfs/TechnologyRoadmapHydrogenandFuelCells-(1).aspx).
- [13] Ofgem. Website: Breakdown of a gas bill. Available at www.ofgem.gov.uk/data-portal/breakdown-gas-bill, 2019. Updated August 2019.
- [14] National Grid. Future Energy Scenarios. Report, 2019. Available online at www.fes.nationalgrid.com/fes-document/.

- [15] HM Treasury. The Green Book: Central Government Guidance on Appraisal and Evaluation. Guidance document, UK Government, 2018. Available online at www.gov.uk/government/publications/the-green-book-appraisal-and-evaluation-in-central-government.
- [16] Sophie Lyons, Emrah Durusut, and Ian Moore. Industrial fuel switching market engagement study. Report, Element Energy and Jacobs, 2018. Available online at https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/824592/industrial-fuel-switching.pdf.
- [17] Sheila Samsatli and Nouri J. Samsatli. A general mixed integer linear programming model for the design and operation of integrated urban energy systems. *Journal of Cleaner Production*, 191:458 – 479, 2018.