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The value of hydrogen and carbon capture, storage and utilisation in decarbonising energy: Insights from integrated value chain optimisation

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Abstract

There is increasing interest in carbon capture, utilisation and storage (CCUS) and hydrogen-based technologies for decarbonising energy systems and providing flexibility. However, the overall value of these technologies is vigorously debated. Value chain optimisation can determine how carbon dioxide and hydrogen technologies will fit into existing value chains in the energy and chemicals sectors and how effectively they can assist in meeting climate change targets. This is the first study to model and optimise the integrated value chains for carbon dioxide and hydrogen, providing a whole-system assessment of the role of CCUS and hydrogen technologies within the energy system. The results show that there are opportunities for CCUS to decarbonise existing power generation capacity but long-term decarbonisation and flexibility can be achieved at lower cost through renewables and hydrogen storage. Methanol produced from carbon capture and utilisation (CCU) becomes profitable at a price range of £72-102/MWh, compared to a current market price of about £52/MWh. However, this remains well below existing prices for transport fuels, so there is an opportunity to displace existing fuel demands with CCU products. Nonetheless, the scope for decarbonisation from these CCU pathways is small. For investment in carbon capture and storage to become attractive, additional drivers such as decarbonisation of industry and negative emissions policies are required. The model and the insights presented in this paper will be valuable to policymakers and investors for assessing the potential value of the technologies considered and the policies required to incentivise their uptake.

Keywords: CO_2 utilisation; CO_2 storage; hydrogen; energy storage; value chains; optimisation.

1. Introduction

1.1. Background

Vast reductions in greenhouse gas emissions are required if the worst effects of climate change are to be prevented by keeping global temperature changes below 2°C or even 1.5°C [1, 2]. Primary energy use accounts for over 70% of global greenhouse gas emissions [1, 3], so our energy systems must be decarbonised. Additionally, there is an increasing need for low-carbon sources of flexibility for energy systems, where in

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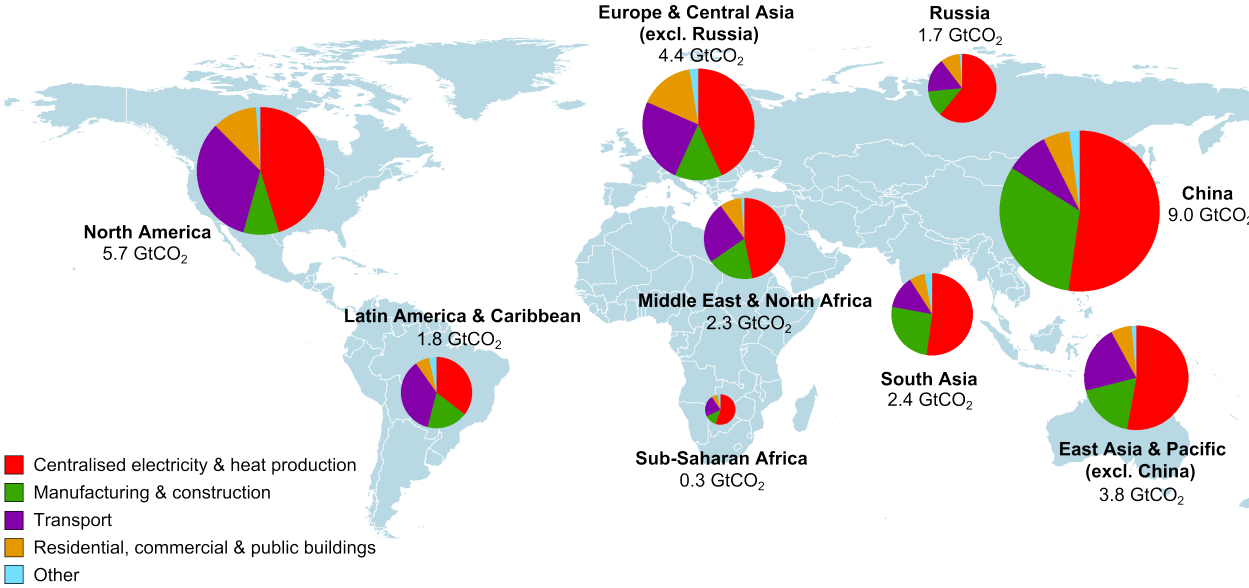


Figure 1: **Global CO_2 emissions from fuel combustion in 2014.** Data from the IEA [7] and the Carbon Dioxide Information Analysis Center [8], accessed using the World Bank DataBank [9]. Graphic inspired by Scott et al. [10].

the past systems have relied on fossil fuels to meet hourly, daily and seasonal demand variations, whether for heating, or in dispatchable power stations for electricity [4].

There is considerable interest in carbon capture and storage (CCS) for providing decarbonisation and flexibility to energy systems. Figure 1 shows the distribution of energy-based CO_2 emissions globally: almost half of these emissions arise from centralised heat and electricity production, well-suited to CO_2 capture. Further capturable emissions are available from industrial plants (both fuel combustion and process emissions). Fitting CO_2 capture to fossil fuel power plants could enable low-carbon, flexible electricity production. CCS solutions for "diffuse" emissions such as transport and buildings, which together make up 29% of energy-based emissions globally, are less obvious, although technologies such as Direct Air Capture and Storage (DACS) show interesting potential in this area [5]. Furthermore, technologies such as Biomass Energy CCS (BECCS) are gathering interest due to their potential to achieve net-negative emissions for the energy they deliver [5], although the wider environmental implications of biomass-based solutions must be considered carefully [6].

Beyond CCS, there is growing interest in alternative uses for captured CO_2, known as carbon capture and utilisation (CCU), that may enable emissions reductions whilst also delivering useful products and energy system flexibility. In CCU, rather than considering CO_2 emissions as an unwanted by-product, they are viewed as a resource for subsequent processes. CCU processes may involve use of CO_2 as an industrial feedstock, or conversion to synthetic fuels for use in energy systems. Hydrogen (H_2) is integral to many of these energy-based CCU pathways: for example, in Fischer-Tropsch synthesis, synthetic hydrocarbons are manufactured from CO_2 and hydrogen [11]. CCU has the potential to add economic incentive to CO_2 capture by creating a marketable final product from the CO_2 [12]. However, the potential of CCU for large-scale decarbonisation has been questioned [13].

Many other technologies exist that offer decarbonisation and flexibility potential without involving CO_2 capture. In the context of CO_2 capture, utilisation and storage (CCUS), it is also relevant to consider hydrogen technologies such as electrolysis and hydrogen storage [14]. With these technologies, it is possible to imagine a flexible energy system with no reliance on hydrocarbons or CO_2 at all [15, 16].

There is strong debate concerning the relative value of these various technologies for supporting a low-carbon, flexible energy system. For example, studies such as Mac Dowell et al. [13] and Bruhn et al. [17] have compared the merits of CCU and CCS, whilst others such as Ball and Weeda [18] and McPherson et al. [19] have assessed the potential of a future "hydrogen economy". However, these studies typically consider the technologies in isolation, not in their optimal configurations, and without considering the implications for the wider environment, energy system and economy.

The environmental impacts of these processes are complex, so require comprehensive analysis. Life cycle analysis (LCA) is valuable in this regard. Cuéllar-Franca and Azapagic [20] used LCA to assess CCS and CCU, whilst Parra et al. [21] performed LCA on power-to-gas. Both studies found several cases in which the processes being studied were less environmentally favourable than conventional fossil-fuel pathways. Assessing the environmental impacts of a single process can be treacherous, as decisions regarding where to apportion environmental "burden" may lead to a different result than when considering the system as a whole [22].

Some energy systems models have been applied to CCUS and hydrogen, attempting to quantify the system-level economic and environmental costs and benefits. For example, Blanco et al. [23] assessed the role of hydrogen in the EU using the JRC-EU-TIMES model, with various applications for the hydrogen including in CCU. Meanwhile Antenucci and Sansavini [24] assessed the potential of power-to-methane for recycling CO_2 through a coupled electricity planning and gas network simulation model. However, these models can still have system boundaries that do not account for the full impacts of the processes being modelled. Furthermore, these models lack the spatial, temporal and technological detail required to represent the interactions between technologies that may lead to different business cases or environmental impacts [25].

Value chain modelling and optimisation is a valuable method for representing the detailed interactions of energy processes, whilst also capturing the overall system effects. It can determine the most effective pathways for converting low-value primary resources and raw materials through a network of technologies to produce final products and services with high economic, social or environmental value [26]. Applying this methodology to CCUS and hydrogen processes enables the comparison of CCS and CCU, as well as alternative decarbonisation strategies, in their optimal configuration, taking into account CO_2 capture and purification, sourcing the energy and feedstocks (including hydrogen) required for the processes, logistics, and delivery of final products and energy services to customers. Value chain modelling and optimisation has been applied to many fields, including hydrogen value chains. For example Samsatli and co-workers have modelled hydrogen value chains for multiple applications in the UK [27, 28] and Welder et al. [29] modelled similar scenarios in Germany. Using the BeWhere model, Mesfun et al. [30] investigated the potential for hydrogen in the Alpine region, including using hydrogen in CCU, but they did not model the CO_2 value chain itself.

1.2. Contributions of this study

This paper presents new data, model and insights that provide crucial missing elements in the debate around CCS, CCU and hydrogen. Some of the novel and timely contributions are as follows:

- Whilst there have been studies made previously on CCS or CCU, none have considered them together within a comprehensive integrated value chain optimisation model with all of the supporting value chains and key enablers, such as hydrogen and energy storage. This study employs a whole-systems value chain optimisation approach that includes the key value chains that interact very tightly with CCS and CCU value chains. It quantifies the overall and relative worth of these technologies, in their optimal configuration in the value chain, for reducing carbon emissions and providing flexibility to the energy system.
- This study answers a question that has not yet been addressed: how will these technologies fit in and interact with existing and future infrastructures, and how effective will they be in helping to meet climate change targets? It determines, using optimisation, how much CO_2 emissions can be reduced by CCS, CCU and hydrogen technologies, as well as how the rest of the energy system can be designed and operated to meet CO_2 emissions reduction targets.
- This study considers the overall value of the technologies to the wider energy system, going beyond just quantifying cost or tonnes of CO_2 mitigated. Further factors that are explored include energy system flexibility and linking of different sectors, e.g. the heat, electricity, transport and chemicals sectors.

1.3. Structure of the paper

In Section 2, the key arguments in the CCUS debate are discussed. Section 3 provides an overview of hydrogen and CO_2 value chains. In Section 4, the comprehensive value chain optimisation model that was developed for this study is presented. Section 5 describes the scenarios that were modelled in this study. Great Britain (GB) was used as an exemplar of an energy system that faces decarbonisation and flexibility challenges. A number of different economic and policy assumptions were modelled in order to quantify and compare the value of CCS, CCU and hydrogen technologies over the next 40 years. Finally, Section 6 presents the results of these scenarios and discusses their implications.

2. The CCUS debate

There is strong debate regarding the relative merits of CCS and CCU for helping to enable a low carbon energy transition. However, considering these technologies as direct competitors can be problematic, as they often serve different purposes [17]. Furthermore, it is useful to consider hydrogen value chains in this debate, as they are both intrinsic to CCU, and also potential competitors. The discussion surrounding the technologies can be separated into six themes.

Scale. Assuming that CCUS technologies must sequester up to 160 $GtCO_2$ globally by 2050 in order to contribute to the 2050 2°C target, Mac Dowell et al. [13] argue that this would only require one sixth of the storage capacity of depleted oil and gas reservoirs and that there is considerably more capacity still in deep saline aquifers. They argue that the projected market size for CCU, however, allows for less than 3% of the 160 $GtCO_2$ to be sequestered for a significant duration. Nonetheless, there is some scope for demands for CCU products to grow in the future, for example if methanol were adopted at scale in the transport sector [31], and even if CCU is not capable of utilising all possible emissions, this is not a reason to prevent its uptake altogether.

Sustainability. CCS is inherently an unsustainable process: whilst the capacity for storage might be large, it is still finite. Additionally, since no CCS facilities have been operated for a long duration, the long-term effects are still uncertain [32]. Meanwhile performing environmental assessments of CCU is strewn with pitfalls, as all of the impacts in the system must be correctly accounted for and environmental "burdens" apportioned appropriately [22, 33]. In many CCU processes, CO_2 is only sequestered temporarily, being re-released into the atmosphere when the product is used. While CCU products may be able to replace fossil fuel usage to some extent, in some cases the life-cycle global warming potential of CCU products has been found to be higher than that of the fossil-fuel equivalent [20]. Nonetheless, there are scenarios in which the CO_2 emissions from the CCU product could be re-captured and re-utilised, creating a sustainable CO_2 cycle [34].

Economics and efficiency. CCU is capable of producing a product with an economic value, independent of any environmental benefits [12]. CCS meanwhile is merely an emissions mitigation strategy that without regulatory support has no clear business case [10]. Perhaps, there is potential to build CCU and CCS projects in unison, where CCU can provide some financial support to CCS [35]. Whilst both CCS and CCU already have examples of commercial operations, it is also difficult to determine how the economics of each would change if the scale of the operations were vastly increased [36, 37]. Despite the apparent economic incentive of CCU, concerns have been raised with regard to the efficiency of the processes, due to the levels of energy input required in both the capture and utilisation stages [10]. Of course, CCS processes also require energy inputs in addition to the capture processes, for example for compression and transportation.

Flexibility. Electricity systems have traditionally relied on fossil fuel fired generators such as CCGTs to provide system flexibility and stability, both through the spinning reserve they provide and the capability to ramp up or down generation in line with electricity demand. Some argue that in electricity systems with increasing penetrations of variable renewable sources such as wind and solar, these fossil fuel generation options will be even more essential [38]. If this is the case, then carbon capture technologies may be required to minimise the emissions of these generators. Others suggest that although the CCU processes are relatively energy intensive, it is possible that these energy requirements could be used to balance overall system supplies and demands, e.g. by using "power-to-liquids" processes [11]. For example, processes that utilise hydrogen as a feedstock can be used for load balancing if the hydrogen is produced from electrolysis, which can be ramped up and down in line with a variable electricity supply, and has been shown to be capable of providing frequency response services to electricity grids [39]. The hydrogen can be stored, then supplied at a constant rate to CCU processes. Moreover, the final products of CCU are often relatively easy to store, and could be used as fuels on the occasions when demand exceeds supply [34].

Infrastructure. A major challenge for CCS is that it requires a transport infrastructure connecting capture and storage facilities, particularly as this leads to a "chicken and egg problem" where capture plants, storage facilities and transport infrastructures all need to be invested in before any benefits of CCS are achieved [10]. This would require significant start-up investments and collaboration between all stakeholders. It is argued that if CCU were implemented effectively, utilisation facilities could be located near to large sources of CO_2 from capture plants, minimising the need for a costly CO_2 transport network [34]. However, this would also be likely to need significant stakeholder collaboration and encouragement to implement. Furthermore, CCU relies on additional feedstocks beyond CO_2 that will have their own production, distribution and storage requirements. Hydrogen, for example, whether used for CCU or other applications, requires a production infrastructure. "Power-to-gas" hydrogen production requires both electrolysers and sufficient (renewable) electricity production to power the process [14].

Diversification. Energy systems operators will look to diversify their sources of energy to ensure supply security. CCU could assist this through the production of a range of fuels that do not rely on specific natural resources (such as fossil fuels). Some argue meanwhile that CCS is only an enabling technology for the continuation of the fossil fuel industry, where supply security issues will only worsen over time [17], although this does not allow for the growing interest in BECCS.

Mathematical modelling can be used to help understand the issues discussed above and take a systematic account of the uncertainties associated with them. Furthermore, to ensure that CO_2 and hydrogen technologies are implemented in a manner that brings the greatest overall system benefit, a holistic approach is required. Policy-makers will need to identify the combination of technologies and networks that best satisfies economic, environmental and social objectives in order to devise suitable policy instruments (e.g. incentives, taxes, etc.). Value chain modelling and optimisation is a valuable tool that can examine these issues, at various scales from regional to national and trans-national scales, including how CO_2 and hydrogen technologies will fit into existing value chains in the energy and chemicals sectors and how effective they will be in helping to meet climate change targets.

3. Overview of hydrogen and CO_2 value chains

Many hydrogen and CO_2 technologies exist, and can be configured in various ways to create different value chains. In this section, the main technologies are described. Costs are provided in UK pounds sterling (£), but can be converted to US dollars at the 2018 average exchange rate of £1 = \$1.34 [40].

3.1. Hydrogen value chains

The following subsections describe the key components of a hydrogen value chain.

3.1.1. Hydrogen production

Conventionally, hydrogen is produced from reforming natural gas (e.g. steam methane reforming), or gasification of coal, oil or biomass feedstocks [41]. Currently, around 95% of hydrogen is produced from fossil fuels [42]. These processes are well established, so have relatively low costs and energy penalties. For example, through steam methane reforming (SMR), hydrogen can be produced for around £28-33 /$MWh_{H_2\text{-LHV}}$, with an efficiency of $76\%_{LHV}$ (1.3 $MWh_{CH_4\text{-LHV}}$ per $MWh_{H_2\text{-LHV}}$)[43, 44]. In the modelling carried out in this study, SMR was selected as the fossil-based technology for hydrogen production, due to its high level of development and the large, established gas industry in the UK. However, to produce low-carbon hydrogen from fossil fuels, CCS is required, which adds significantly to the cost and incurs an energy penalty. For example, with a CO_2 capture rate of 90%, SMR costs may increase to around £48/$MWh_{H_2\text{-LHV}}$ with an efficiency of $69\%_{LHV}$ (1.4 $MWh_{CH_4\text{-LHV}}$ per $MWh_{H_2\text{-LHV}}$) [43].

Alternatively, there is growing interest in power-to-gas for hydrogen production [14, 15, 45], wherein electrolysers are used to convert electricity (and water) to hydrogen (and oxygen). Energy losses through electrolysis could be significant: state-of-the-art PEM or alkaline electrolysers have a system efficiency of around $60\%_{\mathrm{LHV}}$ (1.7 $\mathrm{MWh_{Elec}}$ per $\mathrm{MWh_{H_2\text{-}LHV}}$) [46]. Arguments for power-to-gas often rely on the availability of cheap excess electricity [45], and consequently cost estimates vary widely. The other major challenge for power-to-gas is scalability, with the largest power-to-gas projects in operation today being only a few megawatts in size [45].

3.1.2. Hydrogen storage and conversion

Much of the interest in hydrogen as an energy vector arises from the relative ease with which it can be stored in large quantities and for long durations [28, 47]. Hydrogen can be stored underground in geological formations including salt caverns, saline aquifers and depleted oil and gas fields [48]. Cost estimates for underground hydrogen storage depend on the geological formation and the operating regime, but capital costs for salt cavern storage are in the region of £70-250 per MWh of hydrogen storage capacity [49, 50]. Energy losses for underground hydrogen storage are low, arising predominantly from the compression energy requirements [50]. Hydrogen can also be stored above ground, in purpose-built pressure vessels. In this study, both underground (salt cavern) and above ground (pressure vessel) storage technologies were modelled.

Finally, hydrogen must be converted into its final useful form. This might be through CCU, as described in Section 3.2.3. Alternatively, hydrogen can be used for heating, similarly to natural gas, provided that the infrastructure (boilers and distribution infrastructure) is in place [51, 50]. Hydrogen can be converted to electricity, either through open- or combined-cycle turbines or fuel cells [52, 42]. Due to relatively low conversion efficiencies for power-to-hydrogen and hydrogen-to-power, the overall performance of hydrogen energy (i.e. electricity) storage is low. For example, hydrogen power-to-power pathways may have round-trip efficiencies below 30% [52].

3.2. CO_2 value chains

This section describes the key components of a CO_2 value chain: capture, transportation, storage and utilisation of CO_2.

3.2.1. CO_2 capture and transportation

CO_2 capture can be carried out pre-combustion, post-combustion, or through oxy-fuel combustion [53]. Post-combustion capture through chemical absorption, for example amine scrubbing, is the most established technology and is well suited to capturing CO_2 from flue gases, e.g. from fossil power stations [54]. Several CO_2 capture installations are currently operational worldwide [54, 53]. Technology costs and energy penalties depend on the proportion of CO_2 that is captured from the flue stream. Rubin et al. suggest that for a CO_2 capture rate of 88%, a combined cycle gas turbine (CCGT) plant will require an additional 13-18% energy input for the same energy output, implying an energy penalty of around 870-1030 kWh of natural gas feedstock per tonne of CO_2 captured [55]. The additional CCGT plant cost would be £32-85 per tonne of CO_2 captured [55]. Achieving higher capture rates becomes increasingly expensive [53].

CO_2 transportation by pipeline is well established and is capable of transportation onshore and to offshore wells [54]. Currently there are over 4000 km of CO_2 pipelines in operation worldwide [56]. Costs of transportation by pipeline are estimated to be around £2.50 per tonne of CO_2 per 100 km onshore, and £2.90-4.40 per tonne of CO_2 per 100 km offshore, depending on the pipeline length [57]. Energy requirements are in the region of 1.3-4.5 kWh per tonne of CO_2 for each compression station (which are required every 100-200 km) [58]. CO_2 transport by ship is also a possibility [57].

3.2.2. CO_2 storage

CO_2 can be stored underground in geological formations [53]. Globally there is thought to be capacity for around 1,000 $GtCO_2$ in depleted oil and gas reservoirs, and up to 10,000 $GtCO_2$ in deep saline aquifers [13]. The processes for CO_2 storage are well understood, with several projects already injecting CO_2 into depleted oil and gas reservoirs to enhance hydrocarbon extraction (Enhanced Oil Recovery) [53].

Estimates for CO_2 storage costs have a large range, predominantly due to variations in the suitability of different sites. For offshore depleted oil and gas wells, the Zero Emissions Platform estimates costs of £2-14 per tonne of CO_2 stored [59]. Storage in offshore saline aquifers may cost £6-20 per tonne of CO_2 [59]. In this study, CO_2 storage was assumed to be in depleted oil and gas wells, in four suitable offshore locations around the UK [60].

3.2.3. CO_2 utilisation

CO_2 utilisation encompasses a range of possible uses for captured CO_2, including as a chemical feedstock, mineral carbonation, and direct usage (e.g. in the food and drink industry) [12, 20]. CO_2 utilisation as a chemical feedstock to produce synthetic fuels is the focus of this paper, due to the potential to re-use these fuels as energy vectors. Various fuels can be synthesised through CO_2 utilisation [26]: below, some of the more mature CCU value chains are described.

Liquid hydrocarbons such as diesel and petrol can be manufactured from syngas through Fischer-Tropsch synthesis [26], which is a well developed technology with several plants in operation worldwide producing liquid fuels from gas and coal deposits [26]. For Fischer-Tropsch to be used for CO_2 utilisation, captured CO_2 must first be converted into syngas using hydrogen. This can be done using the Reverse Water-Gas Shift (RWGS) reaction, where CO_2 and hydrogen are reacted at high temperature to produce carbon monoxide and water [26]. Alternatively, CO_2 and steam can be fed into a high temperature (solid oxide) electrolyser to produce hydrogen and carbon monoxide, as demonstrated by Sunfire at a plant in Germany [61]. Electricity requirements for the complete Fischer-Tropsch process (including for hydrogen production from electrolysis and other process requirements) are around 1.6-2.1 MWh_{Elec} per MWh_{LHV} of hydrocarbons produced [61, 62]. CO_2 utilisation is 0.43-0.56 tCO_2 per MWh_{LHV}.

An alternative CCU value chain is methanol production. Methanol is already used widely in the chemical industry and has potential as a fuel, e.g. in the transport sector [31]. Methanol can either be produced in a two-step process involving RWGS followed by methanol synthesis from syngas or produced from direct hydrogenation of CO_2 [63]. There is growing interest in "power-to-methanol", where hydrogen is produced from electrolysis and combined with captured CO_2. The George Olah plant in Iceland produces approximately 22,000 MWh of methanol per year through this process [26]. Based on modelling of a similar plant by Pérez-Fortes et al., the process would have a total electricity demand (including for electrolysis) of 2.0 MWh_{Elec} per MWh_{LHV} of methanol produced, utilising 0.22 tCO_2 per MWh_{LHV}[64].

Finally, captured CO_2 can be combined with hydrogen to produce methane through methanation. Most commonly, this process is carried out chemically, using the Sabatier process [26], but it is also possible to use biological methanation [14]. When the hydrogen is produced from electrolysis, this process is referred to as "power-to-methane" or sometimes "power-to-gas". In this work, "power-to-gas" is used to describe hydrogen production from electrolysis (as discussed in Section 3.1.1); the full process of electrolysis and methanation is named "power-to-methane". Depending on the CO_2 source, power-to-methane could be a fossil-free alternative to natural gas and has some advantages compared to power-to-hydrogen due to the availability of existing natural gas infrastructure. Several pilot plants use power-to-methane to convert electricity (e.g. from excess renewables) into methane that can be injected into the gas grid [45]. Power-to-methane has an overall efficiency of around $52\%_{LHV}$ (1.9 MWh_{Elec} per $MWh_{CH_4\text{-}LHV}$) [14], utilising 0.19 tCO_2 per $MWh_{CH_4\text{-}LHV}$ [65].

4. Integrated value chain optimisation

The Value Web Model (VWM) [66] was developed to optimise the integrated value chains for CCS, CCU and hydrogen in order to determine their roles in decarbonising an energy system over a 40 year period. The VWM is a mixed-integer linear programming (MILP) model, which can represent interconnected pathways for converting primary resources (e.g. natural gas and wind) to final products and services (e.g. electricity and heat), through various technologies that convert, store and transport resources. The optimisation determines the system design (e.g. where and when to invest in technologies and infrastructures) and the operating strategy for this system in order to optimise an objective function, which may include system costs, environmental impacts, and other indicators. Space and time are both explicitly represented in the VWM, in order to capture the spatial distribution of primary resource availability and demands for energy and products as well as their time-varying nature [67]. Space is represented by a discrete set of zones and time is represented on four levels of granularity: hourly intervals for fast dynamics associated with storage and intermittent renewables (e.g. wind), day types to represent different days of the week, seasons and yearly planning periods. The VWM is capable of modelling and optimising a wide range of different types of value chain and network such as a nationwide multi-carrier energy systems [28, 66] and urban energy systems [68].

Pathways are represented by a series of resources and technologies. Resources represent any type of material or energy involved in the pathway from primary resources to end products and energy vectors. Different technology types are included that can: (1) convert one or more resources to one or more other resources (e.g. a gas-fired CCGT that converts natural gas to electricity), (2) transport resources between zones or (3) store resources. Complex interconnected, linear and circular pathways can be constructed [68] by correctly defining resources and the technologies that inter-convert all of the resources.

The pathways can be represented graphically, as in Figure 2, which shows the value web representation for the CCUS and hydrogen value chains considered in this paper. The resources are represented by circles,

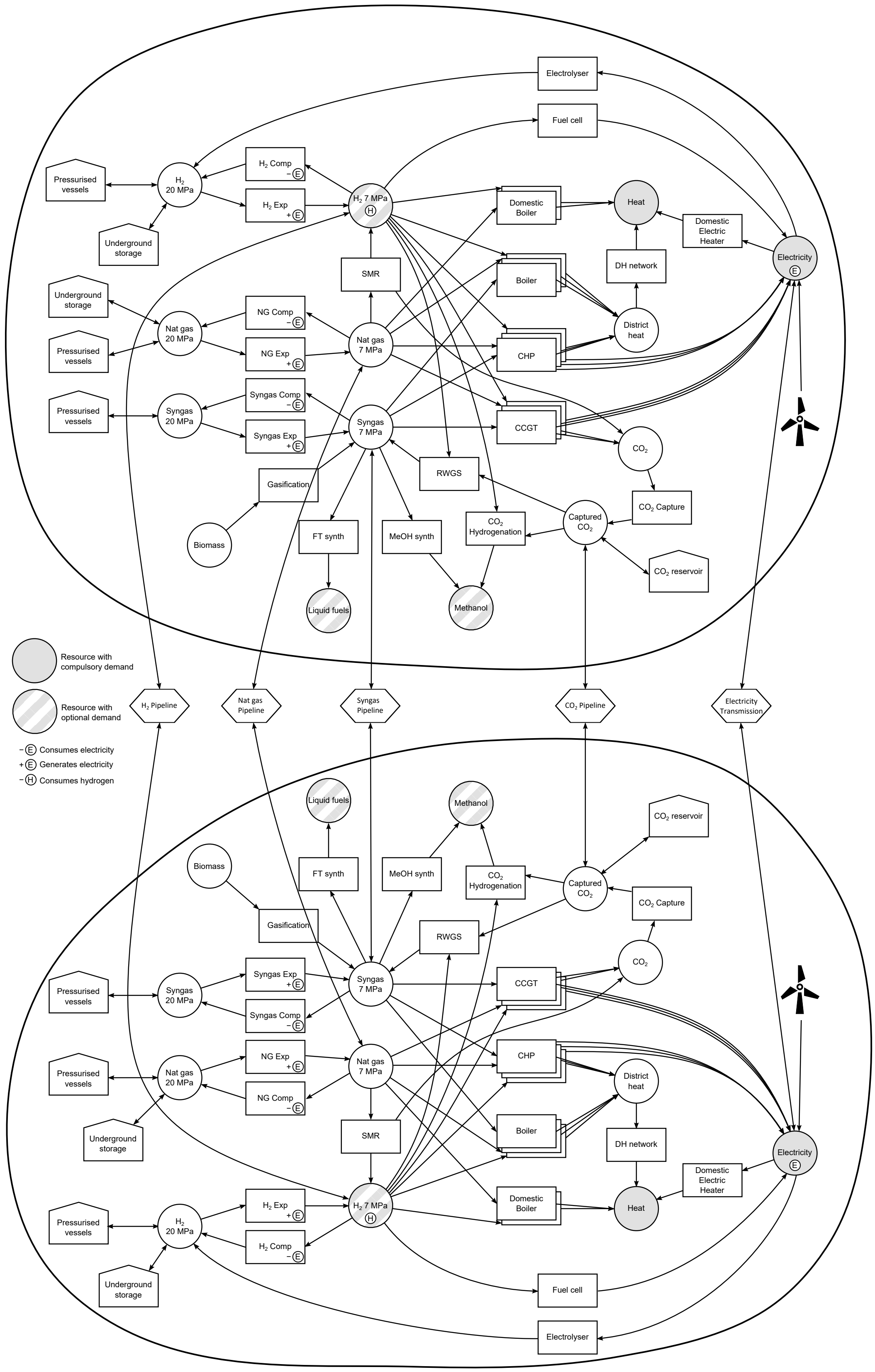


Figure 2: **Superstructure of the integrated hydrogen and CO_2 value chains in the Value Web Model.** The diagram shows the potential value chain pathways for two representative zones only. The model determines what pathways are used in each zone to maximise net present value.

some of which have demands that must always be met (grey circles in the diagram) and those that have demands that may optionally be met, if it is profitable to do so (striped circles). The rectangles represent the "conversion" technologies, which convert one set of resources to another set, as indicated by the arrows linking the resources to the technologies (to avoid too many crossed arrows, some links are indicated by a circle enclosed within the technology, with a + indicating that that resource is produced by the technology and a − indicating that the resource is consumed by the technology). Storage technologies are represented by pentagons with double-headed arrows (indicating flow in either direction for charging and discharging) connecting the stored resource. Transport technologies are represented by hexagons connected by double-headed arrows connected to the transported resource.

Overall, the diagram shows two typical zones in the problem (of which there may be many 10s or 100s of zones needed to represent the full area being considered). The transport technologies move resources from one zone to another, as shown by the hexagons. Within each zone the possible energy pathways are shown. Considering the zone at the bottom of the diagram (the one at the top is a mirror image), the three primary resources are: natural gas ("Nat gas 7 MPa") at the centre of the value web; biomass at the top left; and wind, represented by the wind turbine symbol on the right. When wind turbines are installed in the zone, electricity can be generated as shown by the arrow pointing to the Electricity resource on the right, which is grey to indicate there are demands for it. Below and to the right of the "Nat gas 7 MPa" resource is the wind/hydrogen/natural gas/heat/electricity value web: natural gas can be converted to heat and/or power via CCGT, CHP, boiler (industrial/district scale) and domestic boiler technologies. Natural gas can be converted to hydrogen, which has optional demands, using the SMR technology and hydrogen can also be produced from electricity using the electrolyser technology, though at a higher pressure of 20 MPa. Hydrogen can also be used to generate electricity via the fuel cell technology.

The CCUS value web is shown above the "Nat gas 7 MPa" resource: syngas can be produced by gasification of biomass or by the RWGS (reverse water-gas-shift) technology, which reacts hydrogen with captured CO_2. The syngas can then be converted to liquid fuels in the FT synthesis ("FT synth") technology or to methanol via the methanol synthesis ("MeOH synth") technology. Methanol can also be produced from hydrogen via the "CO_2 hydrogenation" technology, which also utilises captured CO_2. CO_2 can only be captured from certain technologies, e.g. SMR and CCGT, that are at a large enough scale to be equipped with a CO_2 capture technology. Any captured CO_2 that is not utilised by "utilisation" technologies must be stored in a CO_2 reservoir (i.e. it cannot be captured and then released to atmosphere). The CO_2 emissions from all technologies, including those that can have their CO_2 captured, are tracked through their operating impacts. Any CO_2 that is captured is then offset against these emissions as described in section 4.1.5.

Storage of resources other than CO_2 is possible: on the left of the value web can be seen the storage technologies for hydrogen, natural gas and syngas. These gases are stored at a pressure of 20 MPa and therefore need to be compressed from their normal pressures of 7 MPa (the maximum pressure in transmission pipelines) up to this level, which requires some electricity. Conversely, some energy can be recovered when the resources are taken out of storage by using a turbine to generate some electricity. In Figure 2, technologies ending in "Comp" or "Exp" represent compressors and expanders, respectively.

Finally, the transport technologies are shown as hexagons between the two typical zones. Pipelines can be built to transmit hydrogen, syngas or CO_2 between any pair of adjacent zones. Existing pipelines and electricity transmission lines can used to transport natural gas and power, respectively, as well as there being the possibility of extending/reinforcing these networks where necessary.

4.1. Model formulation

The Value Web Model consists of a large number of constraints governing the flows of resources, management of technologies (investments, operation etc.), satisfaction of demands and socio-enviro-techno-economic constraints, which are all solved simultaneously. The key constraints required to understand the model behaviour are presented here, and the nomenclature is included in Appendix B. The complete mathematical formulation of the model can be found in the supplementary material.

4.1.1. Objective function

The objective function in the Value Web Model is the minimisation of a weighted sum of all of the “impacts” of the value chain:

$$
\begin{aligned}
Z = \sum_{iy} \omega_i (\mathscr{I}_{iy}^{\mathrm{W}} + \mathscr{I}_{iy}^{\mathrm{P}} + \mathscr{I}_{iy}^{\mathrm{S}} + \mathscr{I}_{iy}^{\mathrm{Q}} + \mathscr{I}_{iy}^{\mathrm{w}} + \mathscr{I}_{iy}^{\mathrm{fp}} \\
+ \mathscr{I}_{iy}^{\mathrm{fs}} + \mathscr{I}_{iy}^{\mathrm{fq}} + \mathscr{I}_{iy}^{\mathrm{vp}} + \mathscr{I}_{iy}^{\mathrm{vs}} + \mathscr{I}_{iy}^{\mathrm{vq}} + \mathscr{I}_{iy}^{\mathrm{m}} + \mathscr{I}_{iy}^{\mathrm{x}} \\
+ \mathscr{I}_{iy}^{\mathrm{U}} + \mathscr{I}_{iy}^{\mathrm{IET}} - \mathscr{I}_{iy}^{\mathrm{CUS}} - \mathscr{I}_{iy}^{\mathrm{Rev}}) - \epsilon \sum_{y} E_y^{\mathrm{TOT}} n_y^{\mathrm{yy}} \qquad (1)
\end{aligned}
$$

Each impact, $\mathscr{I}_{iy}$, is the value of one of a number of key performance indicators, i, such as costs or CO_2 emissions, in yearly planning interval y for one of the activities in the value chain, signified by the superscript symbol. These include: capital investments into wind turbines (W), production technologies (P), storage technologies (S) and transport infrastructures (Q); fixed and variable operating impacts for wind turbines and the three different types of technology (w, fp, fs, fq, vp, vs, vq); imports and exports (m and x); utilisation of primary resources (U); CO_2 emissions and credits (IET and CUS); and revenues from satisfying demands for energy and fuels (Rev) – these are described in the subsequent subsections. The weighting factors ω_i represent the relative contribution of each key performance indicator to the weighted-sum objective function. Economic impacts are discounted back to present value based on a discount rate. The final term in the objective function is the total annual energy production in each planning period, E_y^{TOT}, so that if $\omega_i = 0 \; \forall i$ and $\epsilon = 1$ then the objective function is to maximise energy production.

4.1.2. 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:

$$U_{rzhdty} + M_{rzhdty} + P_{rzhdty} + S_{rzhdty} + Q_{rzhdty} = D^{\text{comp}}_{rzhdty} + D^{\text{sat}}_{rzhdty} + X_{rzhdty} + E_{rzhdty} \quad \forall r \in \mathbb{R},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{2}$$

U_{rzhdty} 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; P_{rzhdty} is resource production by conversion technologies; S_{rzhdty} is the net "production" of resources due to the operation of storage technologies (positive if resource is used from storage and negative if resource is stored); Q_{rzhdty} is the net transport rate of resource into the zone; M_{rzhdty} and X_{rzhdty} are the rates of resource import and export; D^{comp}_{rzhdty} and D^{sat}_{rzhdty} are the resource demands; and E_{rzhdty} is the excess resource production. Depending on the resource, any excess production can be curtailed for free or must be disposed of at an expense.

4.1.3. Utilisation of primary resources

Certain primary resources will be available in many or all zones and can be harvested if desirable. Three such resources are modelled in this study: natural gas, wind and biomass.

Natural gas availability, $u^{\text{max}}_{\text{NG},zhdty}$, is given as an input to the model with data obtained from the National Grid's gas transmission operational data [69]. This maximum availability is used to limit the amount of resources that can be utilised:

$$U_{rzhdty} \leq u^{\text{max}}_{rzhdty} \qquad \forall r \in \mathbb{R} - \mathbb{C},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{3}$$

which applies to all resources other than biomass, represented by the set $\mathbb{C}$, which is treated slightly differently.

For wind, the maximum amount of electricity that can be generated and utilised is given by the number and types of wind turbines installed in each zone, their characteristics and the wind speed:

$$u^{\text{max}}_{\text{Elec},zhdty} = \frac{\rho^{\text{air}}}{2 \times 10^6} \sum_w \left(\eta_w \left[N^{\text{W}}_{wzy} \pi \left(R^{\text{W}}_w \right)^2 + N^{\text{EW}}_{wzy} \pi \left(R^{\text{EW}}_w \right)^2 \right] \tilde{v}^3_{wzhdty} \right) \quad \forall z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{4}$$

where ρ^{air} is the density of air; η_w is the efficiency of wind turbine type w (which in this study includes onshore and offshore turbines); N^{W}_{wzy} and N^{EW}_{wzy} are the number of new and existing wind turbines in operation; R^{W}_w and R^{EW}_w are the radii of turbine rotors; and $\tilde{v}_{wzhdty}$ is the "effective" wind speed, which accounts for the cut-in, cut-out and rated wind speeds of the turbines and gives the correct electricity generation rate based on the actual wind speed (which is an input to the model) and the turbine rating. Installation of new wind turbines depends on the availability of suitable land (or seabed) area, $A^{\mathrm{W,max}}_{wzy}$, which is determined using a Geographic Information System (GIS) site-suitability analysis [28]. Assuming that new wind turbines will be erected on a hexagonal grid with a spacing of five rotor diameters, the number that can be installed in any zone is restricted by:

$$2\sqrt{3}\left(5R^{\mathrm{W}}_{w}\right)^{2} N^{\mathrm{W}}_{wzy} \leq A^{\mathrm{W,max}}_{wzy} \qquad \forall w \in \mathbb{W},\, z \in \mathbb{Z},\, y \in \mathbb{Y} \tag{5}$$

As biomass is seasonal and also depends on the area planted, the availability of biomass depends only on the season and is determined by the model, which chooses how much area to allocate to each crop, c. The availability is the product of the seasonal yield, Y^{Bio}_{czty}, and the area, A^{Bio}_{czy}, of land allocated to cultivating and harvesting each crop. The harvested biomass from each season is stored and can be utilised at any time during that season, provided the total utilisation over the season does not exceed the availability:

$$\sum_{hd} U_{czhdty} n^{\mathrm{hd}}_{h} n^{\mathrm{dw}}_{d} n^{\mathrm{wt}}_{t} \leq A^{\mathrm{Bio}}_{czy} Y^{\mathrm{Bio}}_{czty} \qquad \forall c \in \mathbb{C} \subseteq \mathbb{R},\, z \in \mathbb{Z},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{6}$$

where n^{hd}_{h}, n^{dw}_{d}, and n^{wt}_{t} define the length of each hourly interval h, number of each day type d in each week, and the number of weeks in season t. Thus, the sum on the left-hand side of equation 6 gives the total utilisation in each season t.

The area of land that is suitable for biomass production, $A^{\mathrm{Bio,max}}_{zy}$, is also obtained via a GIS site-suitability analysis, based on a number of constraints such as slope, elevation, topsoil organic carbon and other socio-political restrictions [70]. This is used to constrain the amount of area that can be allocated to biomass production, at local and national levels:

$$\sum_{c} A^{\mathrm{Bio}}_{czy} \leq f^{\mathrm{loc}}_{zy} A^{\mathrm{Bio,max}}_{zy} \qquad \forall z \in \mathbb{Z},\, y \in \mathbb{Y} \tag{7}$$

$$\sum_{cz} A^{\mathrm{Bio}}_{czy} \leq f^{\mathrm{nat}}_{y} \sum_{z} A^{\mathrm{Bio,max}}_{zy} \qquad \forall y \in \mathbb{Y} \tag{8}$$

where f^{loc}_{zy} is the fraction of suitable area that can be allocated to biomass production in zone z and f^{nat}_{y} is the fraction of the total suitable area that can be allocated.

The impacts associated with utilising resources are included in the objective function through the variables $\mathscr{I}^{\mathrm{U}}_{iy}$, which include impacts for planting and harvesting biomass, and impacts for extracting natural gas and other resources. The capital and operating impacts of wind turbines are also included: $\mathscr{I}^{\mathrm{W}}_{iy}$ and $\mathscr{I}^{\mathrm{w}}_{iy}$, respectively. All of these impacts are defined in the supplementary material.

4.1.4. Conversion technologies

Conversion technologies take resources as inputs and produce other resources as outputs. The net rate of production of a resource r by a conversion technology p is defined as follows:

$$P_{rzhdty} = \sum_p \mathscr{P}_{pzhdty}\alpha_{rpy} \qquad \forall r \in \mathbb{R},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{9}$$

where $\mathscr{P}_{pzhdty}$ is the operating rate of all technologies of type p, in zone z, at time $hdty$. The conversion factor α_{rpy} defines the rate at which resource r is consumed/produced by technology p per unit rate of operation of the technology – it is positive if resource r is produced by technology p and negative if it is consumed.

The operating rate of each technology is limited by the maximum rate of a single technology and the number of technologies present in each zone, as well as by a part-load constraint, as follows:

$$p_p^{\min} N_{pzy}^{\mathrm{PC}} \leq \mathscr{P}_{pzhdty} \leq p_p^{\max} N_{pzy}^{\mathrm{PC}} \tag{10}$$
$$\forall p \in \mathbb{P},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y}$$

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

$$N_{pzy}^{\mathrm{PC}} = \begin{cases} N_{pz}^{\mathrm{EPC}} + NI_{pzy}^{\mathrm{PC}} - NR_{pzy}^{\mathrm{PC}} & \forall p \in \mathbb{P}^{\mathrm{C}},\, z \in \mathbb{Z},\, y = 1 \\ N_{pz,y-1}^{\mathrm{PC}} + NI_{pzy}^{\mathrm{PC}} - NR_{pzy}^{\mathrm{PC}} - NR_{pzy}^{\mathrm{EPC}} & \forall p \in \mathbb{P}^{\mathrm{C}},\, z \in \mathbb{Z},\, y > 1 \end{cases} \tag{11}$$

A constraint is also included to limit the number of commercial technologies that can be built in a given planning period:

$$\sum_z NI_{pzy}^{\mathrm{PC}} \leq BR_{py} \qquad \forall p \in \mathbb{P}^{\mathrm{C}},\, y \in \mathbb{Y} \tag{12}$$

where BR_{py} is the maximum allowable build rate of technology p in planning period y. The impacts of investment in and operation of conversion technologies are a major contributor to the objective function. The total net present capital impact for building new conversion technologies is defined as follows:

$$\mathscr{I}_{iy}^{\mathrm{P}} = \varsigma \sum_{pz} D_{piy}^{\mathrm{C}} C_{piy}^{\mathrm{P}} NI_{pzy}^{\mathrm{PC}} \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \tag{13}$$

where C_{piy}^{P} is the technology capital impact; D_{piy}^{C} is a factor that discounts the capital cost back to start of the time horizon, taking account of how the capital is financed (for non-financial impacts, this factor is 1); and ς is a linear scaling factor to improve optimisation performance. The total net present O&M impact for conversion technologies is defined as follows:

$$\mathscr{I}^{\mathrm{fp}}_{iy} = \varsigma D^{\mathrm{OM}}_{iy} \sum_{pz} \phi^{\mathrm{P}}_{piy} N^{\mathrm{PC}}_{pzy} \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \tag{14}$$

where ϕ^{P}_{piy} is the technology fixed operating impact and D^{OM}_{iy} is a factor that discounts financial impacts, assumed to be made annually, back to the start of the time horizon or is equal to the number of years in period y, n^{yy}_{y}, for non-financial impacts. Finally, the total net present variable operating impact of conversion technologies depends also on the operating rates of the given technology:

$$\mathscr{I}^{\mathrm{vp}}_{iy} = \varsigma D^{\mathrm{OM}}_{iy} \sum_{pzhdt} \varphi^{\mathrm{P}}_{piy} \mathscr{P}_{pzhdty} n^{\mathrm{hd}}_{h} n^{\mathrm{dw}}_{d} n^{\mathrm{wt}}_{t} \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \tag{15}$$

where $\varphi^{\mathrm{P}}_{piy}$ is the variable (rate-dependent) operating impact.

4.1.5. CO_2 utilisation and storage

Whilst many conversion technologies generate CO_2 emissions, it is only possible for CO_2 capture technologies to capture emissions from large point sources. In the VWM, large technologies that can be coupled with CO_2 capture technologies produce a resource "CO_2" for the CO_2 that they emit. The capture technologies can convert this "CO_2" resource to "Captured CO_2", which can then be stored underground (CCS) or converted by other technologies to form useful products (CCU). The technologies that produce "capturable" CO_2 are denoted "industrial emitting technologies" (IET) and the following constraints are used to account for the amounts of CO_2 emitted, captured, utilised and stored.

The total rate of production of CO_2 from all industrial emitting technologies in each zone and at every time, $\mathscr{C}^{\mathrm{IET}}_{zhdty}$, is given by:

$$\mathscr{C}^{\mathrm{IET}}_{zhdty} = \sum_{p \in \mathbb{P}^{\mathrm{IET}}} \mathscr{P}_{pzhdty} \alpha_{p,\mathrm{CO_2}} \qquad \forall z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{16}$$

Some of this generated CO_2 can be captured by the CO_2 capture technologies (if any have been built – see Section 4.1.4) and the rate of capture of CO_2, which has to be utilised or stored, is given by:

$$\mathscr{C}^{\mathrm{US}}_{zhdty} = -\sum_{p \in \mathbb{P}^{\mathrm{CUS}}} \mathscr{P}_{pzhdty} \alpha_{p,\mathrm{CO_2^{cap}}} \quad \forall z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{17}$$

(Recall that $\alpha_{p,\mathrm{CO_2^{cap}}}$ is negative because CO_2 is consumed by the capture technologies.)

Economic penalties for emissions and rewards for capture and utilisation or storage are represented by the unit impacts V^{IET}_{iy} and V^{CUS}_{iy}, respectively. The two following components of the objective function are then defined for the CO_2-producing technologies (IET) and for CO_2 utilisation and/or storage:

$$\mathscr{I}^{\mathrm{IET}}_{iy} = \varsigma D^{\mathrm{OM}}_{iy} V^{\mathrm{IET}}_{iy} \sum_{zhdt} \mathscr{C}^{\mathrm{IET}}_{zhdty} n^{\mathrm{hd}}_h n^{\mathrm{dw}}_d n^{\mathrm{wt}}_t \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \tag{18}$$

$$\mathscr{I}^{\mathrm{CUS}}_{iy} = \varsigma D^{\mathrm{OM}}_{iy} V^{\mathrm{CUS}}_{iy} \sum_{zhdt} \mathscr{C}^{\mathrm{US}}_{zhdty} n^{\mathrm{hd}}_h n^{\mathrm{dw}}_d n^{\mathrm{wt}}_t \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \tag{19}$$

The values of the cost component ($i = \mathrm{cost}$) of V^{IET}_{iy} and V^{CUS}_{iy} may be different to allow CO_2 emissions to be penalised at a different rate to the rewards for CO_2 utilisation or storage.

CO_2 emissions are tracked as follows. All technologies that emit CO_2, including industrial emitters, contribute to the CO_2 component of the objective function through their impacts (C^{P}_{piy} and $\varphi^{\mathrm{P}}_{piy}$ in equations 13 and 15). Any CO_2 that is then captured, which can only be done for the "IET" technologies, is offset in the objective function by the term $\mathscr{I}^{\mathrm{CUS}}_{iy}$ for $i = CO_2$, which is exactly the amount of CO_2 captured and either utilised or stored. This requires that $V^{\mathrm{CUS}}_{CO_2,y}$ is set to 1 and $V^{\mathrm{IET}}_{CO_2,y}$ must be zero.

4.1.6. Storage technologies

Storage technologies are modelled similarly to production technologies: conversion factors define efficiencies and energy requirements for the operation of each storage technology, with the flows of resources being determined by the product of the operating rate and the conversion factor (cf. equation 9). However, storage technologies can either store excess resources, $\mathscr{S}^{\mathrm{put}}_{szhdty}$, or retrieve them from storage, $\mathscr{S}^{\mathrm{get}}_{szhdty}$. Thus, the equivalent of equation 9 for storage is:

$$S_{rzhdty} = \sum_{s} \left(\mathscr{S}^{\mathrm{put}}_{szhdty} \sigma^{\mathrm{put}}_{sr,\mathrm{src},y} + \mathscr{S}^{\mathrm{hold}}_{szhdty} \sigma^{\mathrm{hold}}_{sr,\mathrm{dst},y} + \mathscr{S}^{\mathrm{get}}_{szhdty} \sigma^{\mathrm{get}}_{sr,\mathrm{dst},y} \right)$$
$$\forall r \in \mathbb{R},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{20}$$

where there is also an operating rate equivalent to the amount of resource in storage, $\mathscr{S}^{\mathrm{hold}}_{szhdty}$, which allows the modelling of energy requirements for holding inventory (e.g. recondensing boiled-off natural gas in LNG storage) and losses (e.g. batteries losing charge over time). S_{rzhdty} is the net production of resource in a zone due to the operation of all storage technologies. For the resource being stored, it is negative if storage is being filled (the zone has to produce resource in order to store it) or it is positive if 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. Constraints equivalent to equations 10 and 11 restrict the rates of operation of the storage technologies, $\mathscr{S}^{\mathrm{put}}_{szhdty}$, $\mathscr{S}^{\mathrm{hold}}_{szhdty}$ and $\mathscr{S}^{\mathrm{get}}_{szhdty}$, as well as tracking the numbers of storage technologies in each zone, N^{S}_{szy}.

In addition to the above constraints, the overall inventory of a given storage technology s is also calculated:

$$I_{szhdty} = n^{\mathrm{hd}}_h \sum_{r} \left(\mathscr{S}^{\mathrm{put}}_{szhdty} \sigma^{\mathrm{put}}_{sr,\mathrm{dst},y} + \mathscr{S}^{\mathrm{hold}}_{szhdty} \sigma^{\mathrm{hold}}_{sr,\mathrm{src},y} + \mathscr{S}^{\mathrm{get}}_{szhdty} \sigma^{\mathrm{get}}_{sr,\mathrm{src},y} \right)$$
$$\forall s \in \mathbb{S},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{21}$$

and constrained to ensure that it remains within the maximum storage capacity of the technologies at all times, and also to ensure that an (optional) minimum level of storage is maintained for resilience. The full set of constraints are too numerous to show here but are all given in the supplementary material.

The rate at which the storage technology holds resource in storage, $\mathscr{S}^{\text{hold}}_{szhdty}$, is given by the inventory level at the end of the previous hourly interval:

$$\mathscr{S}^{\text{hold}}_{szhdty} = I_{sz,h-1,dty}/n^{\text{hd}}_{h} \quad \forall s \in \mathbb{S},\, z \in \mathbb{Z},\, h > 1 \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{22}$$

and $\sigma^{\text{hold}}_{sr,\text{src},y}$ is 1 minus the fraction of storage inventory lost in one hourly interval.

The impacts included in the objective function for the capital ($\mathscr{I}^{\text{S}}_{iy}$), fixed operating ($\mathscr{I}^{\text{fs}}_{iy}$) and variable operating ($\mathscr{I}^{\text{vs}}_{iy}$) impacts of storage technologies are defined in a similar way to the conversion technology impacts (equations 13 - 15).

4.1.7. Transport technologies

Transport of resources between zones is effected by transport technologies, which operate on transport infrastructures (e.g. trailer transport on roads, barges on inland waterways, power flows on electricity transmission lines of various types, etc.). The number and capacity of infrastructures in place between two zones limits the maximum rate of operation of each transport technology and further infrastructures can be invested in if required. Resource flows are calculated from the operating rate, $\mathscr{Q}_{lzz'hdty}$, of transport technology, l, and both distance-independent and distance-dependent conversion factors ($\bar{\tau}_{lrfy}$ and $\hat{\tau}_{lrfy}$, respectively – f = src or dst for the source or destination zone of the transport), which account for transmission losses and energy requirements for the transport (e.g. compression/pumping stations for fluid flows in pipes). Examples of how these are used to represent typical transport processes are given in the supplementary material, along with the full mathematical formulation. The net flow of resource into a zone due to the operation of transport technologies is:

$$\begin{aligned} Q_{rzhdty} = &\sum_{z'|\nu_{z'z}=1} \sum_{l\in\mathbb{L}} \left[\left(\bar{\tau}_{lr,\text{dst},y} + \hat{\tau}_{lr,\text{dst},y} d_{z'z} \right) \mathscr{Q}_{lz'zhdty} \right] \\ &\qquad + \sum_{z'|\nu_{zz'}=1} \sum_{l\in\mathbb{L}} \left[\left(\bar{\tau}_{lr,\text{src},y} + \hat{\tau}_{lr,\text{src},y} d_{zz'} \right) \mathscr{Q}_{lzz'hdty} \right] \\ &\qquad\qquad \forall r \in \mathbb{R},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \end{aligned} \tag{23}$$

where $\mathbb{L}$ is the set of all transport processes, $\nu_{zz'}$ is a binary parameter equal to 1 if a transport connection is allowed from zone z to zone z', $d_{zz'}$ is the distance between zones z and z', and the remaining symbols have been defined previously. The first term on the right-hand side accounts for transport into the zone, from all other zones, and the second term accounts for transport out of the zone. As with production and storage technologies, the conversion factors are signed quantities: for the resource being transported, they are negative for the source zone and positive for the destination zone; otherwise they are negative when they represent resource requirements to power the transport and positive if they represent emissions.

The number of transport infrastructures between each pair of zones in each planning interval is tracked, similar to conversion technologies (equation 11) and storage technologies. Impacts are included in the objective function for the capital ($\mathscr{I}_{iy}^{\mathrm{Q}}$), fixed operating ($\mathscr{I}_{iy}^{\mathrm{fq}}$) and variable operating ($\mathscr{I}_{iy}^{\mathrm{vq}}$) impacts of transport technologies and are defined in a similar way to the conversion technology impacts (equations 13 - 15).

4.1.8. Demand satisfaction

For some resources (e.g. heat and electricity), it is compulsory that demands are satisfied, so these are included in $D_{rzhdty}^{\mathrm{comp}}$. For others, a demand may exist that can be optionally satisfied, receiving a revenue for doing so (e.g. CCU products); the total level of optional demand (i.e. market size) is defined by $D_{rzhdty}^{\mathrm{opt}}$. The level of optional demand that is actually satisfied is the variable $D_{rzhdty}^{\mathrm{sat}}$, which appears in the resource balance (equation 2) along with $D_{rzhdty}^{\mathrm{comp}}$, and must be less than or equal to the optional demand:

$$D_{rzhdty}^{\mathrm{sat}} \leq D_{rzhdty}^{\mathrm{opt}} \qquad \forall r \in \mathbb{R},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{24}$$

Revenues from the sales of resources are included in the objective function using the following impact:

$$\mathscr{I}_{iy}^{\mathrm{Rev}} = \varsigma D_{iy}^{\mathrm{OM}} \sum_{rzhdt} V_{riy} \left(D_{rzhdty}^{\mathrm{comp}} + D_{rzhdty}^{\mathrm{sat}} \right) n_h^{\mathrm{hd}} n_d^{\mathrm{dw}} n_t^{\mathrm{wt}} \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \tag{25}$$

The parameter V_{riy} specifies the unit impact of the demand satisfaction (i.e. market price at which the resource is sold).

4.2. Model input data

In this study, 16 spatial zones, following the National Grid Seven Year Statement zones [71], were used to represent Great Britain. A 40-year time horizon, from 2017 to 2056, was modelled with four planning periods (decades); two season types to represent variabilities between the summer months (March – November) and the winter months (December – February); and four periods per day for modelling hourly variability.

Input data for the resources were acquired from various sources. Spatial heat and electricity data were acquired from Loughborough University data [72], and aggregated into the 16 spatial zones. The time profiles for heat and electricity demand were taken from Sansom [73] and the Gridwatch website [74] respectively, and then processed into the model time resolution. Wind speed data were obtained from the Renewables Ninja database [75, 76] and aggregated in space and time. Availabilities of natural gas production and imports were based on National Grid data [69]. For the scenarios that included availability of CO_2 from large industrial installations, this data was acquired from UK government data [77].

Input data for the properties of the conversion, storage and transport technologies shown in Figure 2 were also obtained from a variety of sources (all values and references are provided in the supplementary material).

These include: capital investment impacts; fixed and variable operating impacts; minimum and maximum rates of operation; maximum storage capacity, injectability and withdrawal rate; and conversion factors that represent the efficiencies of the technologies as well as resource requirements and losses for storage and transport technologies.

4.3. Implementation

The model was implemented in AIMMS (Advanced Interactive Multidimensional Modeling System) and solved using the CPLEX solver. A typical optimisation problem (or "scenario") consists of around 104,000 variables and around 163,000 constraints, taking about 2 hours to solve on a workstation with an Intel Xeon processor with 10 cores and 128 GB RAM. The problems are solved to an optimality tolerance of 5%, which ensures a good solution is obtained in a reasonable time.

5. Optimisation scenarios

A total of 135 scenarios were optimised to explore the potential contribution of CO_2 and hydrogen value chains to an energy system requiring decarbonisation and flexibility. The VWM was applied to the Great Britain (GB) energy system, as an example of a medium-sized, largely fossil-based energy system. The optimisation objective was to achieve the maximum overall net present value (NPV) for the system. Revenues can be obtained from the provision of useful services (heat and electricity), and the sale of products (e.g. methanol and liquid fuels). In all scenarios that were studied, the decarbonisation of the power and heating sectors was represented by a constraint on CO_2 emissions in the final decade. A level equivalent to a 90% reduction in emissions by 2050 compared to 1990 was chosen: whilst the UK Climate Change Act prescribes that national emissions should be reduced by 80% over this period [78], it is accepted that emissions from the power and heating sectors will require greater reductions in order to account for other harder-to-decarbonise sectors, such as the aviation sector [79]. Furthermore, emissions will need to be cut further still in order to meet the requirements of the Paris Agreement (net zero emissions by 2100) [80, 81]. Other than natural gas imports, energy imports and exports (e.g. via electricity interconnectors) are not included in this work. This interconnectivity can provide additional flexibility to energy systems but the focus of this study is to identify what technologies should be used to decarbonise a system, accounting for any flexibility services they may provide, and not on utilising imports/exports purely for flexibility.

Beyond the decarbonisation constraint, various scenarios were studied with additional policies and incentives to assess their influence on the energy system. These scenarios are summarised in Table 1, and detailed in sections 5.1 - 5.4. Additionally, a factorial analysis was performed to assess the effects of data uncertainties, and is described in section 5.5.

5.1. Baseline scenario

The baseline scenario was used to assess the GB energy system under present day policies and with median cost estimates for technologies.

Table 1: Details of the scenarios modelled and optimised

Scenario category	No. of runs in category	Constraint Payment (£/MWh)	Multiplying factor applied to storage costs	CO_2 trading price (£/tCO_2)	Methanol price (£/MWh)	Industrial CO_2 Included
Baseline	1	0	1	23	52	No
Flexibility	8	70	1 – 100	23	52	No
Economics	56	0	1	23 – 130	52 – 102	No
Industrial CO_2	6	0	1	23 – 130	52	Yes

A CO_2 trading price of £23/tCO_2 was included, equal to the average UK carbon price in 2017 (UK carbon support price of £18/tCO_2 [82] + average EU ETS price of £5/tCO_2 [83]). CO_2 "trading" was modelled to represent the European Union Emissions Trading Scheme (ETS) [84], penalising large emitters of CO_2 (e.g. CCGTs) by the trading price (a "cost" to the system). To further incentivise CCUS, CO_2 utilisation and storage plants are also rewarded at the same rate for the CO_2 they sequester (a "revenue" to the system). This goes beyond the existing EU ETS policy but is a useful tool for incentivising CCUS in the model: the significance of this incentive was explored through sensitivities on the CO_2 trading price.

Market prices for the CCU products were assigned based on present day prices. A price of £52 /MWh for methanol was used, based on the 2017 average (Methanex) market price [85]. Similarly, Fischer-Tropsch fuels could be sold at £55 /bbl, estimated from [86].

5.2. Flexibility

An area of interest for CCUS and hydrogen based technologies is their potential for providing energy system flexibility. The response of these technologies to different flexibility-based scenarios was assessed using two main inputs: the costs of hydrogen storage, and the cost of curtailed wind power. Hydrogen storage costs were increased by factors of up to 100, representing the wide range of cost estimates found in the literature [87, 88, 89] (the effects of hydrogen storage cost assumptions were also explored in the factorial analysis: see section 5.5). Additionally, penalties of up to £70 per MWh were applied for any unused wind power generation, representative of the average payment made by the UK grid operator in 2017 for unused wind power [90, 91].

5.3. Economics

As was discussed in section 3, the economic characteristics of CCUS technologies are complex. Two of the main drivers for the uptake of CCUS are the CO_2 trading price, and the market price available for the sale of CCU products. Therefore, a full range of scenarios was studied in which both the CO_2 trading price and the price of methanol were varied. Fifty-six scenarios were optimised with different combinations of CO_2 trading prices ranging between £23/tCO_2 and £130/tCO_2, and methanol prices ranging between £52/MWh and £102/MWh. Although there is significant uncertainty in the long term value of the CO_2 trading price, the UK government has indicated that the price could reach £70/tCO_2 by 2030 and £200/tCO_2 by 2050 [92, 93].

5.4. Industrial CO_2

This study focuses on the decarbonisation of domestic heat and electricity. However, industry is another major source of greenhouse gas emissions: in 2016, 32 $MtCO_2$ (equivalent) were attributed to large industrial installations in the UK, with further indirect emissions from the energy supplied to industry. Evidently, this could be a significant CO_2 feedstock for CCUS processes. Therefore, in the "industrial CO_2" scenarios, these emissions from large industrial installations were made available for capture and utilisation or storage. Although this would not count towards the decarbonisation constraints imposed on the domestic sector, the revenue from the CO_2 trading price was included in the objective function, and a range of trading prices were assessed with the industrial CO_2 feedstock in place.

5.5. Factorial analysis

Finally, a factorial analysis was performed to assess the effects of data uncertainty on the model results. A half-factorial (2^{k-1}) analysis was carried out, using seven factors, resulting in 64 optimisation runs. The analysis was carried out using Design-Expert version 11, published by Stat-Ease, Inc. [94]. The seven uncertain factors are: CO_2 capture cost, CO_2 utilisation cost, CO_2 storage cost, electrolyser cost, hydrogen storage cost, wind turbine cost, and average wind speed.

Six of the seven factors used in the analysis included multiple input parameters, for example CAPEX and OPEX costs, and technologies of all sizes. Sensitivity ranges were estimated from the literature for each factor, and applied to all input parameters in a given factor to calculate the "low" and "high" values in the factorial analysis. Details on the factors, sensitivity ranges (including references for the estimates), input parameters and final values used in the factorial analysis are provided in Appendix C.

A large sensitivity range was used for hydrogen storage costs, reflecting the wide range of data in the literature. This range is partly explained by different assumptions regarding the availability and usability of underground storage. The wind speed factor was included to reflect uncertainty in the availability of wind resource. All modelled wind speeds were scaled up/down by 20%.

6. Results and discussion

In the following sections, the results from the scenarios outlined in Section 5 are presented and their implications are discussed.

6.1. Renewables and hydrogen storage provide decarbonisation and flexibility

In the optimisation scenario with baseline policies, a transition occurs from the present day to a low-carbon, flexible energy system in 2056. However, no CCUS technologies are installed: decarbonisation and flexibility are provided at lower cost through renewables and hydrogen storage.

Figure 3 shows results for the optimal system design in 2056: 3a shows overall flows of energy and CO_2 and 3b shows maps of the system design. By 2056, all electricity generation is provided by wind turbines: all

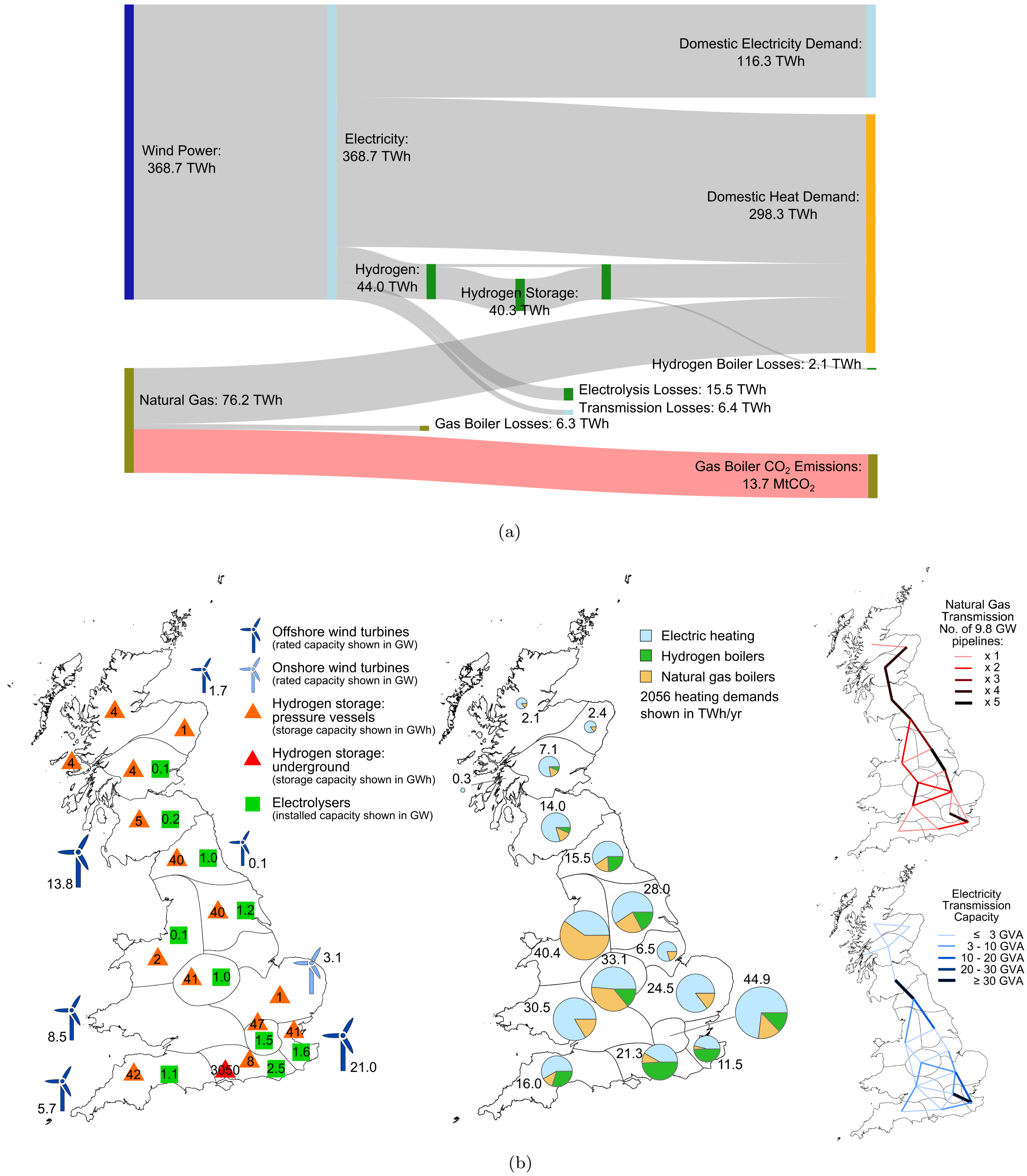


Figure 3: **Optimal energy system in the baseline scenario.** (a) Sankey diagram showing annual flows of energy (in TWh/yr) and CO_2 (in t/yr) in 2056. (b) Maps showing the optimal system configuration in 2056, including: installed capacities of key technologies (left); zonal heating demands and delivery method in 2056 (numbers give total annual demand in TWh/yr) (centre); and natural gas and electricity transmission networks (right). No other transmission infrastructures (i.e. hydrogen or CO_2 pipelines) were installed in this design.

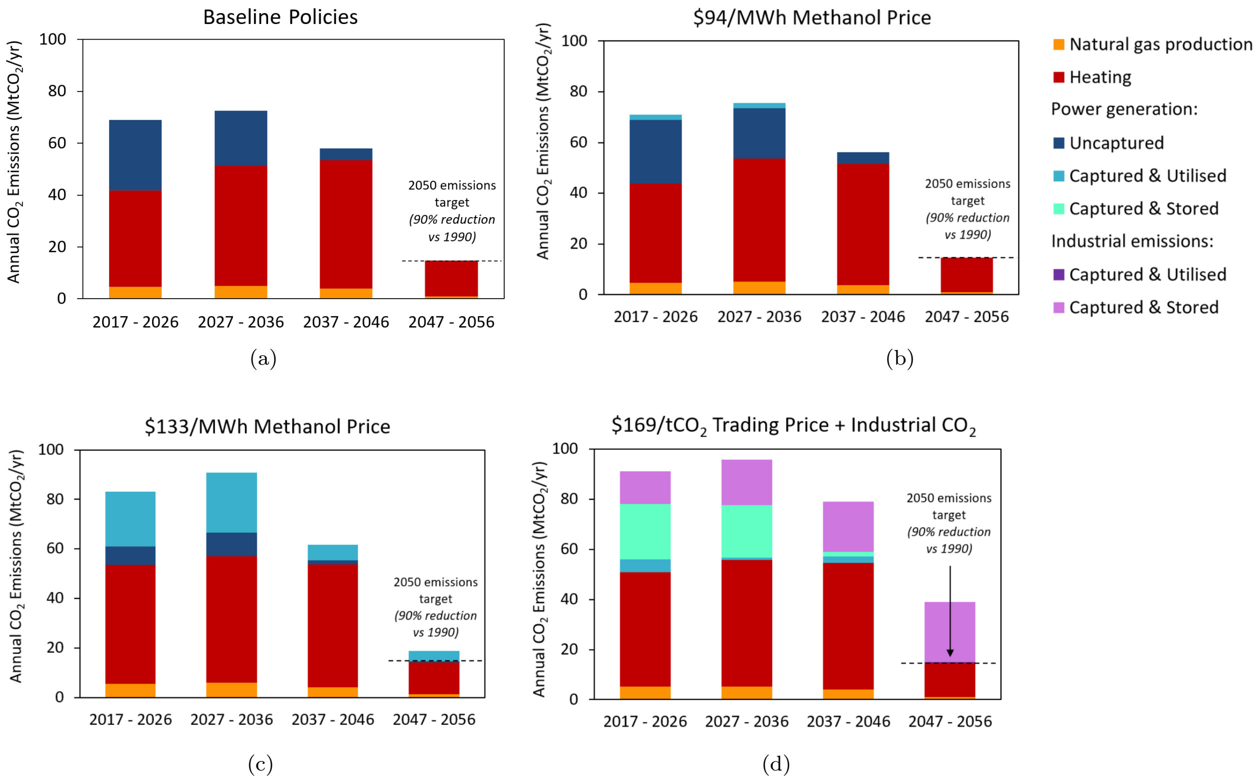


Figure 4: **Annual CO_2 emissions by source for four featured scenarios.** (a) Baseline policies, (b) CCU methanol price of £72/MWh, (c) CCU methanol price of £102/MWh, (d) CO_2 trading price of £130/tCO_2 and emissions from industry available for capture (but not included in emissions reduction target). For all scenarios, both captured and uncaptured emissions from power generation are shown: only uncaptured emissions are included in the net emissions level.

of the present day gas-fired power stations are retired over the four decades, and not replaced. The overall electricity generation base is significantly increased (by a factor of 1.6), to account for growth in electricity demand and electrification of heat. Figure 3a shows how domestic heating is satisfied in 2056: overall, 63% of heating demand is satisfied using electricity, and 23% using natural gas, with the remainder satisfied using hydrogen. Figure 3b shows the detail of how this heat is delivered in the 16 spatial zones that were modelled. As Figure 3a shows, all remaining CO_2 emissions in 2056 are from natural gas boilers in homes: complete decarbonisation of power generation and significant decarbonisation of heat is sufficient to achieve the emissions reduction target in the final decade. The annual CO_2 emissions for each of the four decades modelled are shown in Figure 4a.

The optimal system is highly reliant on intermittent wind power but system flexibility is provided by power-to-gas and hydrogen storage. The installed capacities of these technologies in 2056 are shown in Figure 3b. Electrolysers are installed in many locations across the country, with a total installed capacity exceeding 10 GW. Despite SMR facilities for hydrogen production being available to build, the optimal solution only includes hydrogen production from electrolysis. Hydrogen storage facilities are also installed: most significantly, a 3 TWh underground storage at Humbly Grove in southern England. Excess wind power generation is converted to hydrogen and either immediately distributed to homes for heating or stored to be used later. The amount of hydrogen in the Humbly Grove underground storage over the course of 2056 is shown in Figure 5, clearly showing both inter-seasonal storage and hourly balancing.

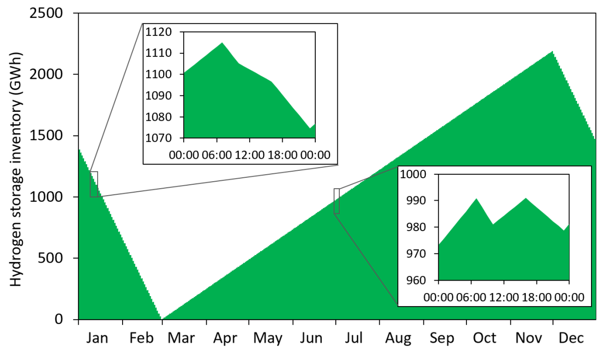


Figure 5: **Storage inventory for the Humbly Grove underground hydrogen storage facility throughout 2056 in the baseline scenario.** Insets show the inventory over a day in January and a day in July.

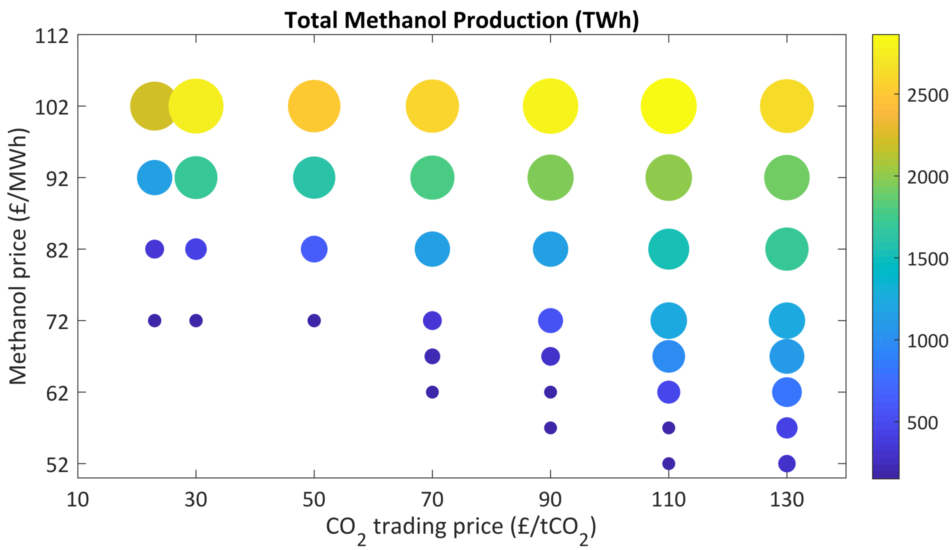


Figure 6: **Total methanol production (CO_2 hydrogenation) between 2017 and 2056, for a range of cases.** 56 scenarios were optimised, each with a unique combination of methanol price and CO_2 trading price. Total methanol production is represented by both the datapoint size and colour.

Under these baseline assumptions, CCUS is found to be less cost effective for providing system flexibility than energy storage. In order to investigate whether CCUS could have a flexibility-providing role in the energy system, a number of additional scenarios were modelled, focusing on increasing the costs of hydrogen storage (the main flexibility provider in the baseline scenario), and the cost of curtailed wind power.

Whilst these scenarios resulted in reduced levels of curtailment and storage, the results did not include any CCUS technologies operating in a flexibility-providing role (e.g. in conjunction with dispatchable CCGT plants). It is possible that due to the high capital costs associated with CCUS, high load factors are required to justify the initial expenditure, which is not suited to operating in conjunction with "peaking" fossil fuel power plants or, in the case of CCU, only utilising hydrogen produced from excess electricity.

6.2. Economic incentives for CCUS

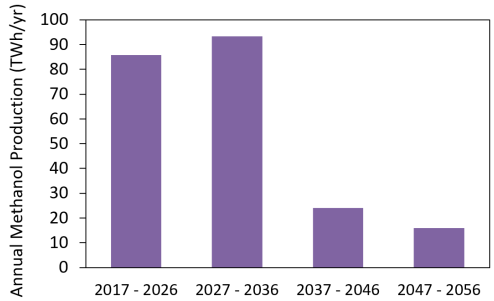


Figure 7: **Annual methanol production in each decade for the scenario with a methanol price of £102/MWh.**

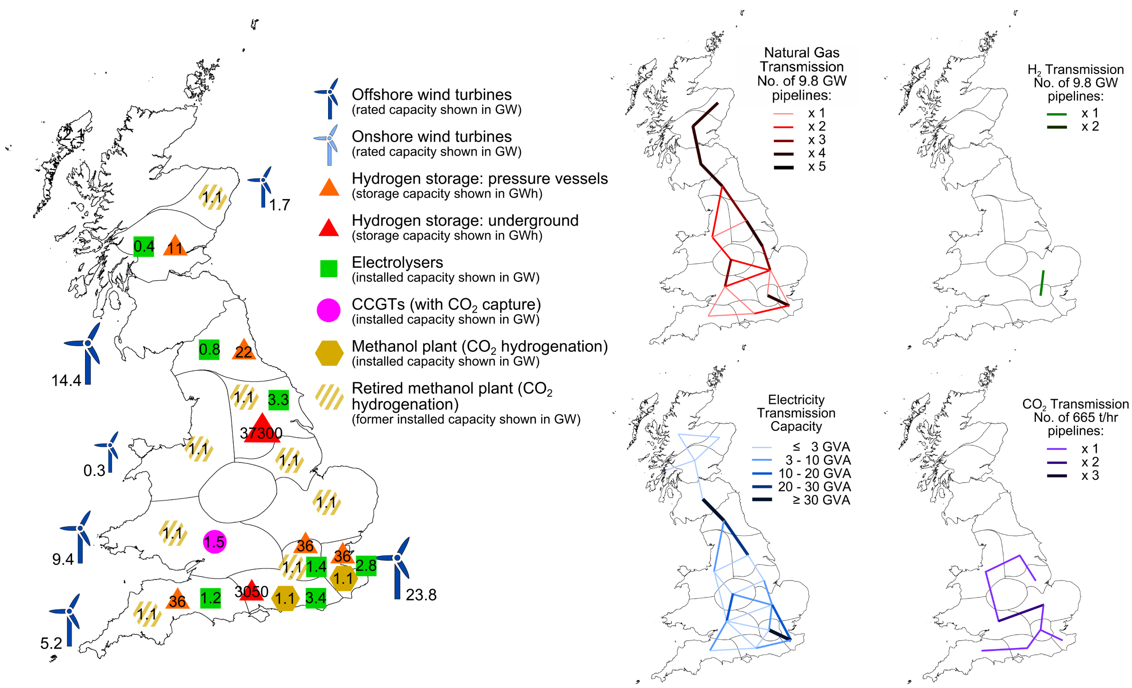


Figure 8: **Optimal energy system for the scenario with a methanol price of £102/MWh.** Maps show the system in 2056, including: installed capacities of key technologies (left); and natural gas, H_2, electricity and CO_2 transmission networks (right). Retired CCU plants are also displayed, indicating the scale of CCU during the early decades. In the final decade, 73% of heat demands are satisfied by electricity, 19% by natural gas and 9% by hydrogen. The hydrogen transmission pipeline in the east of England serves demands for hydrogen for heating in this region.

Given that under baseline assumptions, decarbonisation and flexibility constraints alone are insufficient to introduce CCUS technologies into the optimal system design, the economics of the technologies must also be explored. Primarily, this was done by varying two factors: the CO_2 trading price and the retail price of methanol. Additionally, a factorial analysis was performed, exploring the effects of different technology cost assumptions.

Figure 6 shows the total methanol production from CCU over the forty-year time horizon for each of the 56 scenarios that were assessed with different CO_2 trading prices and methanol prices.

Whilst a methanol market price of £52/MWh together with a CO_2 trading price of £23/tCO_2 were insufficient to incentivise methanol production from CCU, with a 40% increase in the methanol price (to £72/MWh) CCU becomes part of the optimal energy system. In this case, CO_2 capture facilities are installed at some existing CCGT plants, and the captured CO_2 is used with hydrogen from electrolysis to produce methanol in a single CO_2 hydrogenation plant. This plant produces 8.2 TWh per year, but as Figure 4b shows, the contribution of CO_2 utilisation to overall emissions reaches a maximum of only 2.1 MtCO_2 per year. The CCU plant operates only in the first two decades. In the later decades, as the existing CCGTs retire, they are replaced with wind power, rather than investing in new CCGTs with CCU. Consequently, by the final decade decarbonisation is achieved through renewables and heat decarbonisation. Although it may be optimal to the wider system to install and operate capital intensive CCU technologies for only two decades, in reality this strategy may be unattractive to potential investors.

With a 100% increase in the methanol price (to £102/MWh), CCU has a greater contribution, and CCU (along with new CCGTs) is sustained throughout all decades. Figure 4c shows the annual CO_2 emissions for this scenario and Figure 7 shows methanol production rates for each of the four decades. Although CCU is operated throughout all four decades, it still has its peak in the second decade, with some CCU plants retiring when existing CCGTs retire. However, in this scenario, it is now worthwhile in some locations to invest in new CCGTs with CCU, and consequently CCU has a significant contribution to the final decade emissions target (although it should be remembered that the emissions sequestered into the CCU products will be re-emitted when the product is consumed). Figure 8 shows the installed capacities of key technologies (including CCU) in 2056 in this scenario. A large capacity of hydrogen storage is required to match hydrogen supplies to the demands from both CO_2 hydrogenation and domestic heating.

The level of methanol production in the final decade of this scenario is 16 TWh/yr, compared with 93 TWh/yr produced in the second decade. The market size for methanol in Western Europe is currently around 40 TWh/yr [95], therefore it is likely that new demands for methanol would need to be found, such as displacement of existing fuels. For example, demand for petroleum for road transport in the UK in 2017 was 470 TWh [96], so this could provide a market for methanol. Furthermore, whilst methanol production is the key CCU pathway in this study, in reality a more diverse selection of CCU pathways exists, producing alternative products. A methanol price of £102/MWh is considerably higher than the current market price, so would be likely to require policy support. Petroleum has a retail price in excess of £130/MWh in the UK [97], so a methanol price of £102/MWh would be competitive, however this does not account for the significant levels of taxation applied to petroleum, and the subsequent loss in tax revenue.

CO_2 trading prices have some influence on the uptake of CCU for cases with a lower overall CCU uptake, but in cases with higher overall CCU uptake the influence is limited, as Figure 6 shows. The CO_2 trading price provides a strong incentive for CCUS in the early decades, when a large capacity of CCGTs producing by-product CO_2 still exists. These plants will be penalised by a CO_2 trading price, and only CCUS can reverse this penalty. In the later decades, once existing CCGTs have retired, the CO_2 trading price does not provide any incentive for installing CCGTs with CCUS over other types of low-carbon power generation (i.e. wind power). Hence, the CO_2 trading price has limited potential for incentivising large uptake of CCU, as this requires installation of new CCGTs with CCU once existing capacity has retired.

The limited incentive from the CO_2 trading price is also why CCS facilities, which lack an additional revenue stream, are not installed. Only with a CO_2 trading price of £130/tCO_2 does CCS become part of the optimal solution because, at this level, the costs of unabated emissions from the existing CCGTs are so high that building CCS for just the early decades is justified. This shows the importance of appropriate policies, if potentially valuable technologies such as CCUS are to be incentivised.

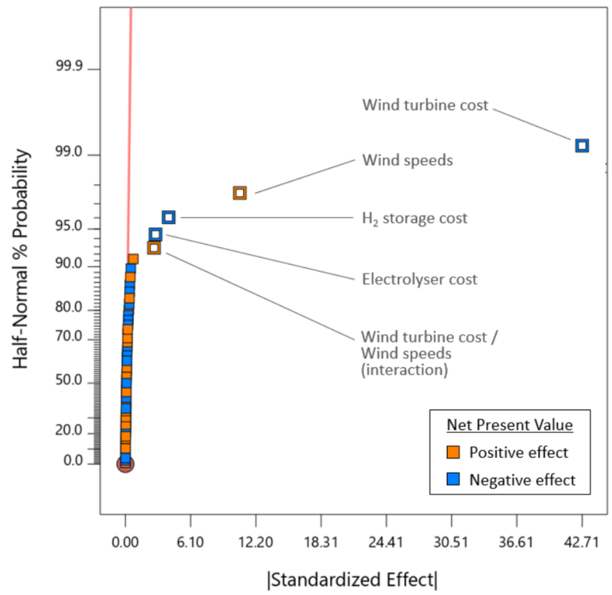
6.3. Factorial analysis

To assess the reliability of the baseline technology cost assumptions, a factorial analysis was performed consisting of 64 different optimisation scenarios. Half-normal plots of effects for four responses in the factorial analysis are shown in Figure 9 Selected results from all factorial analysis runs are provided in the supplementary material.

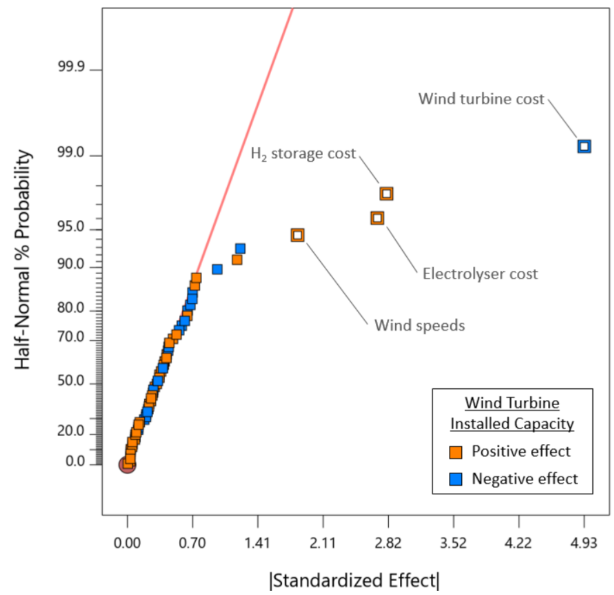
The results of the factorial analysis broadly support the robustness of the baseline data assumptions. For example, the contribution of CCUS to the optimal energy system remains limited, even in the scenarios with data sensitivities most favourable to CCUS (e.g. low CCUS costs, high hydrogen storage costs). CCS facilities continue to remain absent from all scenarios. The results show an increased uptake of CCU in the scenarios most favourable to CCU. However, this is predominantly only in the early decades, meaning that the final energy system design remains largely unchanged. A possible cause for this is the significant amount of supporting infrastructure that is required for CCUS: even with optimistic assumptions regarding the costs of CCUS itself, there are still the costs of the CCGTs, CO_2 transport and, in the case of CCU, hydrogen supply infrastructure. Figure 9d shows that the costs of CO_2 capture facilities and electrolysers were the dominant factors in the uptake of CCU, more than the cost of the CO_2 utilisation plant itself. This shows that CO_2 utilisation is quite reliant on its supply chain.

Overall, wind turbine data is the most influential on the optimisation results. Wind turbine cost is the factor with the greatest effect for many model responses, including net present value. The wind speed factor also has significant effect on several responses. The importance of wind turbine data is unsurprising given the strong role that wind turbines have in the majority of optimal networks. Confidence in data assumptions for wind turbines is relatively high, as the technology is well established. In fact, given that the baseline assumptions are based on present day technologies, it is possible that improvements in cost and performance will be achieved, increasing the case for wind turbines in the optimal system design.

The factorial analysis also revealed strong interdependence between wind turbines, electrolysers, and hydrogen storage. The costs for each of these technologies are all significant factors in the final installed capacities.



(a)



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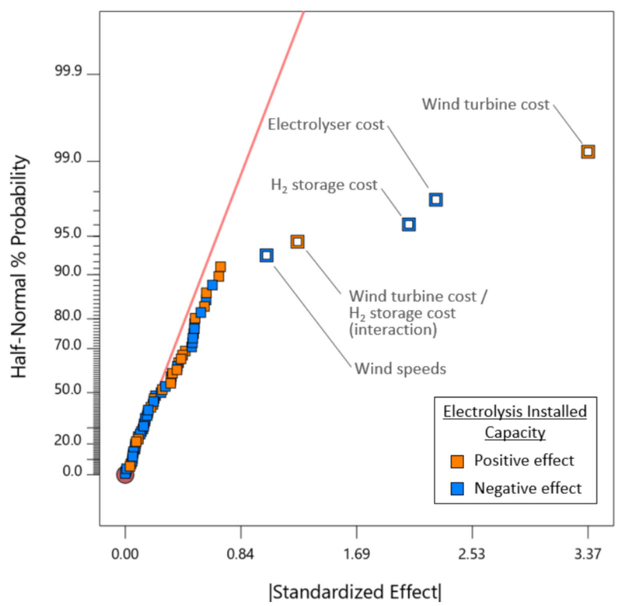
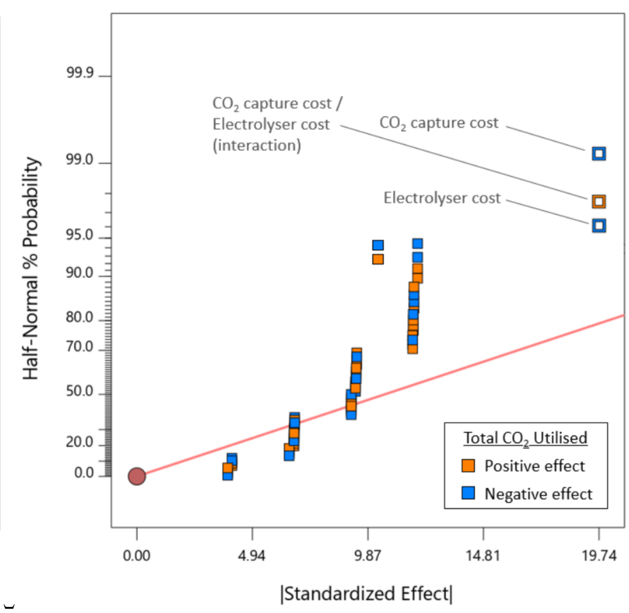


(c)



(d)

Figure 9: **Half-normal probability plots of effects for four responses in the factorial analysis.** (a) Net present value, (b) Installed capacity of wind turbines in 2056, (c) Installed capacity of electrolysers in 2056, (d) Total quantity of CO_2 emissions utilised over the time horizon. For each plot, the factors (and interactions between factors) with the most significant effects on the response appear further to the right, and are indicated. Orange denotes that the factor has a positive effect on the response, blue denotes negative.

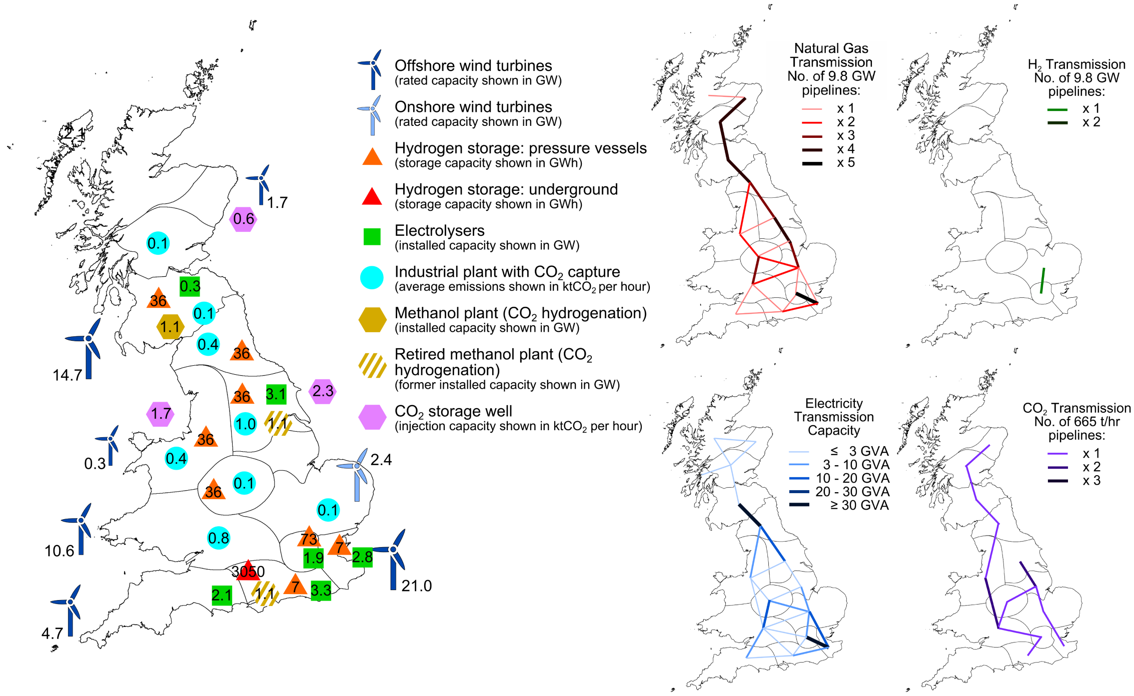


Figure 10: **Maps of the optimal energy system for the scenario with a CO_2 trading price of £130/tCO_2 and optional capture of CO_2 emissions from industry.** Maps show the system in 2056, including: installed capacities of key technologies (left); and natural gas, H_2, electricity and CO_2 transmission networks (right). Retired CCU plants are also displayed. In the final decade, 63% of heat demands are satisfied by electricity, 23% by natural gas and 14% by hydrogen.

For example in Figure 9c, it can be seen that the installed capacity of electrolysers in the final system design is most dependent on wind turbine costs, followed by electrolyser costs and hydrogen storage costs. This shows the reliance that each of these technologies has on the other stages of the value chain, and the importance of the costs of all of the technologies. Despite there being a significant level of uncertainty associated with hydrogen storage costs, they are found to have a relatively small effect on power-to-gas uptake, as shown in Figure 9c. This is due to the small contribution that storage costs have to the overall hydrogen supply chain.

6.4. Emissions from industry as an additional CO_2 feedstock

As CCGT plants are retired and replaced with renewable generation in the later decades, there becomes a lack of point source CO_2 emissions, and consequently there is limited opportunity for CCUS technologies. This is particularly challenging for CCS, which has high capital expenditure and long project times, meaning that a long term supply of CO_2 is necessary to justify investment.

To address this, additional CO_2 emissions from large industrial installations were included in the optimisation. These emissions were not included in the emissions reduction target, but could optionally be captured and utilised or stored, to obtain the revenue from the CO_2 trading price.

Whilst these additional emissions have little effect on the uptake of CCU, they do influence CCS. With a CO_2 trading price of £130/tCO_2, CO_2 capture is installed at many locations throughout the country, and CO_2 storage wells are installed at three locations. The optimal system design in this scenario is shown in

Figure 10. Annual CO_2 emissions for the scenario are shown in Figure 4d: in the early decades, CCS has a significant impact on emissions from power generation, but by 2056 power generation is again focused on wind power, and CCS is focused on emissions from industry.

7. Conclusions

Various CO_2 and hydrogen value chains exist that may offer potential for decarbonisation and flexibility in future energy systems. By modelling these value chains as integral components of the energy system, it has been possible to assess the merits of technologies including CCS, CCU, power-to-gas and hydrogen storage.

The results show that with baseline cost and policy assumptions, there are opportunities for CCUS to decarbonise existing power generation capacity. However, long-term decarbonisation can be achieved at lower cost through expansion of renewables, using hydrogen storage to ensure system flexibility. The high capital costs of CCUS technologies and their associated supply chains mean that it is challenging to find flexibility-based business cases, which are likely to involve low load factors for the technologies.

CCU pathways that combine captured CO_2 with renewable hydrogen are capable of producing synthetic fuels that are competitive with existing fuels. For example, methanol from CCU could be competitive with petroleum as a transport fuel, if it had a similar retail price, but it is not currently competitive with the existing market price for methanol from fossil-based sources. Despite the economic opportunity for CCU, based on existing market sizes it is unlikely that CCU will have a significant contribution to CO_2 emissions reductions, particularly considering the secondary emissions when the fuel is used.

The methodology and results presented in this study are valuable to both policymakers and potential investors for informing which technologies are likely to be valuable in future energy systems. The results also show the necessity of implementing appropriate policies if CCUS technologies are to be incentivised. This is particularly the case for CCS. In this study, it was found that a CO_2 trading price of £130/tCO_2 was required for CCS to become part of an optimal energy system, however there may be alternative policies that can incentivise this technology more efficiently.

Whilst this study found that the decarbonisation potential of CCUS for the power and heating sectors may be limited, it is likely that the contribution would be greater in scenarios where stringent decarbonisation targets are imposed on industry, much of which is reliant on fossil fuels. However, alternative decarbonisation options for industry should also be considered, such as efficiency savings, use of low-carbon fuels (e.g. renewable hydrogen and biofuels) and electrification.

This study assessed a national energy system over a forty year period, taking into account existing installed capacities of technologies, in order to model the rate of transition to a low-carbon system. The results showed a rapid transition to renewables and expansion of hydrogen supply chains. However, it remains to be seen whether power-to-gas can be scaled up sufficiently quickly. Alternative scenarios may see more hydrogen production from fossil fuels in the medium term; in this case, there would be a greater opportunity for CCUS technologies.

Finally, this study considered the optimal configuration for a low-carbon energy system in the 2050s. It is becoming increasingly important to look beyond this target, to possible zero-carbon energy systems. In this scenario, negative emissions technologies, such as BECCS and DACS may become more relevant, and hence there may be a greater role for CCUS in the long term.

Acknowledgements

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Appendix A. Abbreviations

BECCS	Biomass Energy Carbon Capture and Storage
CAPEX	Capital expenditure
CCGT	Combined Cycle Gas Turbine
CGH2S	Compressed gas hydrogen storage
CCS	Carbon Capture and Storage
CCU	Carbon Capture and Utilisation
CCUS	Carbon Capture, Utilisation and Storage
CH_4	Methane
CHP	Combined Heat and Power
CO_2	Carbon dioxide
DACS	Direct Air (carbon) Capture and Storage
Elec	Electricity
EU ETS	European Union Emissions Trading Scheme
FT	Fischer-Tropsch
GB	Great Britain
H_2	Hydrogen
LHV	Lower Heating Value
MeOH	Methanol
MILP	Mixed Integer Linear Programming
NPV	Net Present Value
OPEX	Operating cost
PEM	Proton Exchange Membrane
RWGS	Reverse Water-Gas Shift
SMR	Steam Methane Reforming
tCO_2	Tonnes of Carbon dioxide
US-H2	Hydrogen underground storage
VWM	Value Web Model

Appendix B. Model nomenclature

The following is the nomenclature for the mathematical formulation presented in Section 4.1.

As the majority of resources 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. In the scenarios considered here, the units for Fischer-Tropsch hydrocarbons are bbl and bbl/h (barrels and barrels per hour) and the units for CO_2 are t and t/h (tonnes and tonnes per hour); all other resource units are MWh and MW. In the following nomenclature section, the units for each resource are indicated by the unit "UoR", for "unit of resource", which stands for MWh for most resources in the scenarios presented in this paper, bbl for F-T hydrocarbons and t for CO_2. 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
$c \in \mathbb{C} \subset \mathbb{R}$	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
$l \in \mathbb{L}$	Transport technologies
$p \in \mathbb{P}$	Conversion technologies
$\mathbb{P}^{\mathrm{D}} \subseteq \mathbb{P}$	Domestic conversion technologies
$\mathbb{P}^{\mathrm{C}} \subseteq \mathbb{P}$	Commercial/industrial conversion technologies
$\mathbb{P}^{\mathrm{IET}} \subset \mathbb{P}^{\mathrm{C}}$	Industrial CO_2 emitting conversion technologies (large point source)
$\mathbb{P}^{\mathrm{CUS}} \subset \mathbb{P}^{\mathrm{C}}$	CO_2 utilisation or storage conversion technologies
$r \in \mathbb{R}$	Resources
$s \in \mathbb{S}$	Storage facilities
$t \in \mathbb{T}$	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

$A^{\mathrm{W,max}}_{wzy}$	Total area of land available for wind turbine type w in zone z in planning period y [m^2]
$A^{\mathrm{Bio,max}}_{zy}$	Total area of land available for growing biomass in zone z in planning period y [ha]
a_{sz}	Binary value determining whether there is availability for an underground 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)
$b^{\max}_{b}$	Maximum flow rate of transport infrastructure b [UoR/h]
C^{B}_{biy}	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^{P}_{piy}	System impact of the capital investment in a conversion technology p in planning period y [£ or tCO_2]
C^{S}_{siy}	System impact of the capital investment in a storage facility s in planning period y [£ or tCO_2]
C^{W}_{wiy}	System impact of the capital investment in wind turbine type w in planning period y [£ or tCO_2]
c^{Bio}_{city}	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^{M}_{rihdty}	System impact of importing a unit of resource r during hour h, day type d, season t and planning period y [£/UoR or $\mathrm{tCO_2}$/UoR]
c^{U}_{rihdty}	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 $\mathrm{tCO_2}$/UoR]
c^{X}_{rihdty}	System impact of exporting a unit of resource r during hour h, day type d, season t and planning period y [£/UoR or $\mathrm{tCO_2}$/UoR]
$D^{\mathrm{C}}_{\star iy}$	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 or storage technologies s.
D^{OM}_{iy}	Factor for discounting O&M impacts incurred in planning period y back to the beginning of the time horizon
D^{W}_{wiy}	Factor for discounting capital investments into new wind turbines made in planning period y back to the beginning of the time horizon
$D^{\mathrm{act}}_{rzhdty}$	Demand for resource r in zone z during hour h, day type d, season t and planning period y [UoR/h]
$D^{\mathrm{comp}}_{rzhdty}$	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]
$D^{\mathrm{opt}}_{rzhdty}$	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^{loc}_{zy}	Maximum allowable fraction of suitable biomass growing area in zone z that may be used in planning period y
f^{nat}_{y}	Maximum allowable fraction of suitable biomass growing area across the entire country that may be used in planning period y
LB_{lb}	Binary value that determines whether transport technology l can use infrastructure b, (= 1 if it can, 0 otherwise)
$m^{\max}_{rzhdty}$	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^{EW}_{wzy}	Number of pre-existing wind turbines of type w in zone z in planning period y (accounts for estimated retirement dates)
n^{hd}_{h}	Duration of hourly interval h [h]
n^{dw}_{d}	Number of occurrences of day type d in a week (e.g. 5 for a weekday, 2 for a weekend)
n^{wt}_{t}	Number of repeated weeks in season t
n^{yy}_{y}	Number of repeated years in planning period y
N^{EPC}_{pz}	Number of pre-existing commercial conversion technologies of type p in zone z
NR^{EPC}_{pzy}	Number of pre-existing commercial conversion technologies of type p in zone z that retire at the beginning of planning period y
N^{ES}_{sz}	Number of pre-existing storage technologies of type s in zone z
NR^{ES}_{szy}	Number of pre-existing storage technologies of type s in zone z that retire at the beginning of planning period y
$N^{\mathrm{EB}}_{bzz'}$	Number of pre-existing transport infrastructure connections of type b between zones z and z'
$p^{\max}_{p}$	Maximum operating rate of technology p [MW]

$p_p^{\min}$	Minimum operating rate of technology p [MW]
$q_l^{\max}$	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]
$RT_{py'y}^{\mathrm{P}}$	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)
$RT_{sy'y}^{\mathrm{S}}$	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)
$RT_{wy'y}^{\mathrm{W}}$	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)
$s_s^{\mathrm{get,max}}$	Maximum withdrawal rate from storage facility s [UoR/h]
$s_s^{\mathrm{hold,max}}$	Maximum storage capacity of a single storage facility s [UoR]
$s_s^{\mathrm{put,max}}$	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_{iy}^{IET}	Impact i of one tonne of CO_2 emissions from industrial emitting technologies (= the CO_2 trading price for cost; = 0 for emissions, which are counted through $\varphi_{piy}^{\mathrm{P}}$)
V_{iy}^{CUS}	Impact i of one tonne of CO_2 emissions utilised or stored (= the CO_2 trading price for cost; = 1 for emissions)
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_{czty}^{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
$\lambda_\star$	Economic lifetime of technologies [year] ($\star \in \{b, p, s\}$ for transport infrastructures, conversion technologies and storage technologies, respectively)
$\nu_{zz'}$	Binary parameter, 1 if zone z is adjacent to zone z'
ρ^{air}	Air density [kg/m^3]

$\sigma^{\text{get}}_{srfy}$	Conversion factor for performing "get" task with storage technology s on resource r in planning period y
$\sigma^{\text{hold}}_{srfy}$	Conversion factor for performing "hold" task with storage technology s on resource r in planning period y
$\sigma^{\text{put}}_{srfy}$	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)
$\bar{\tau}_{lrfy}$	Conversion factor for transport technology l transporting resource r in planning period y (distance-independent)
$\hat{\tau}_{lrfy}$	Conversion factor for transport technology l transporting resource r in planning period y (distance-dependent)
ϕ^{B}_{biy}	Annual O&M impact of transport infrastructure b in planning period y [(£ or tCO_2)/(connection-km-yr)]
ϕ^{P}_{piy}	Annual O&M (fixed) impact of conversion technology p in planning period y [£/yr or tCO_2/yr]
ϕ^{S}_{siy}	Annual O&M (fixed) impact of storage facility s in planning period y [£/yr or tCO_2/yr]
ϕ^{W}_{wiy}	Annual O&M (fixed) impact of wind turbines in planning period y [£/yr or tCO_2/yr]
φ^{P}_{piy}	Variable operating impact of conversion technology p in planning period y [£/UoR or tCO_2/UoR]
$\hat{\varphi}^{\text{Q}}_{liy}$	Distance-dependent variable operating impact of transport process l in planning period y [£/km/UoR or tCO_2/km/UoR]
$\bar{\varphi}^{\text{Q}}_{liy}$	Distance-independent variable operating impact of transport process l in planning period y [£/UoR or tCO_2/UoR] (e.g. flat rate freight charges)
$\varphi^{\text{SG}}_{siy}$	Variable operating impact of "get" task for storage facility s in planning period y [£/UoR or tCO_2/UoR]
$\varphi^{\text{SH}}_{siy}$	Unit variable operating impact of "hold" task for storage facility s in planning period y [£/UoR or tCO_2/UoR]
$\varphi^{\text{SP}}_{siy}$	Unit variable operating impact of "put" task for storage facility s in planning period y [£/UoR or tCO_2/UoR]
$\chi^{\max}_{rzhdty}$	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^{Bio}_{czy}	Area allocated to production of biomass (crop) c in zone z during planning period y [ha]
$\mathscr{C}^{\text{IET}}_{zhdty}$	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]
$\mathscr{C}^{\text{US}}_{zhdty}$	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^{sat}_{rzhdty}	Optional demands satisfied in zone z during hour h of day type d in season t of planning period y [UoR/h]
E_{rzhdty}	Excess production of resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]

I_{szhdty}	Inventory in storage facility s in zone z during hour h of day type d in season t of planning period y [UoR]
$I^{0,\text{act}}_{szdty}$	Inventory in storage facility s in zone z at the start of day type d of season t in planning period y [UoR]
$I^{0,\text{sim}}_{szdty}$	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]
$\mathscr{I}^{\text{P}}_{iy}$	Total net present impact of building new conversion technologies in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{S}}_{iy}$	Total net present impact of building new storage technologies in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{Q}}_{iy}$	Total net present impact of building new transport infrastructures in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{W}}_{iy}$	Total net present capital impact of building new wind turbines in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{m}}_{iy}$	Total net present impact of importing resources in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{fp}}_{iy}$	Total net present fixed O&M impact of conversion technologies in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{fq}}_{iy}$	Total net present fixed O&M impact of transport infrastructures in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{fs}}_{iy}$	Total net present fixed O&M impact of storage technologies in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{Rev}}_{iy}$	Total net present revenue from the sales of energy services for satisfying demands in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{U}}_{iy}$	Total impact of utilising natural resources in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{vp}}_{iy}$	Total net present variable operating impact of production facilities in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{vs}}_{iy}$	Total net present variable operating impact of storage facilities in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{vq}}_{iy}$	Total net present variable operating impact of transport technologies in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{w}}_{iy}$	Total net present O&M impact of wind turbines in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{x}}_{iy}$	Total net present impact of exporting resources in planning period y [£M or MtCO_2]
$\mathscr{I}^{\text{IET}}_{iy}$	Total net present impact of CO_2 emissions from industrial emitting technologies in planning period y
$\mathscr{I}^{\text{CUS}}_{iy}$	Total net present impact of CO_2 emissions which are utilised or stored in planning period y (i.e. credits)
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^{PD}_{pzy}	Millions of domestic conversion technology $p \in \mathbb{P}^{\text{D}}$ 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]
$u^{\max}_{rzhdty}$	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]
$\mathscr{P}^{\mathrm{h}}_{pzhdty}$	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]
$\mathscr{P}^{\mathrm{d}}_{pzdty}$	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]
$\mathscr{Q}_{lzz'hdty}$	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]
$\mathscr{S}^{\mathrm{get}}_{szhdty}$	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]
$\mathscr{S}^{\mathrm{hold}}_{szhdty}$	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]
$\mathscr{S}^{\mathrm{put}}_{szhdty}$	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]

Free variables

P^{h}_{rzhdty}	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^{d}_{rzdty}	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]
Q_{rzhdty}	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_{rzhdty}	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
$\delta^{\mathrm{d}}_{szdty}$	Net surplus put into storage s in zone z over one day in day type d in season t of planning period y [UoR]
$\delta^{\mathrm{t}}_{szty}$	Net surplus put into storage s in zone z over one week in season t of planning period y [UoR]
$\delta^{\mathrm{y}}_{szy}$	Net surplus put into storage s in zone z over one year in planning period y [UoR]

Integer variables

$N^{\mathrm{B}}_{bzz'y}$	Number of transport infrastructure b installed between zones z and z' during planning period y
N^{PC}_{pzy}	Total number of commercial conversion technology $p \in \mathbb{P}^{\mathrm{C}}$ in zone z during planning period y
N^{S}_{szy}	Total number of storage technology s in zone z during planning period y
N^{W}_{wzy}	Total number of wind turbines of type w in zone z during planning period y
$NI^{\mathrm{B}}_{bzz'y}$	Number of new transport infrastructure b invested in at the beginning of planning period y between zones z and z'

NI^{PC}_{pzy}	Number of new commercial conversion technology $p \in \mathbb{P}^{\mathrm{C}}$ invested in at the beginning of planning period y in zone z
NI^{S}_{szy}	Number of new storage facility s invested in at the beginning of planning period y in zone z
NI^{W}_{wzy}	Number of new wind turbines of type w invested in at the beginning of planning period y in zone z
NR^{PC}_{pzy}	Number of commercial conversion technology $p \in \mathbb{P}^{\mathrm{C}}$ retired in zone z at the beginning of planning period y
NR^{S}_{szy}	Number of storage facility s retired in zone z at the beginning of planning period y
NR^{W}_{wzy}	Number of wind turbines of type w retired in zone z at the beginning of planning period y

Appendix C. Values used in the factorial analysis

Table 7: **Details of the factors used in the factorial analysis, included baseline, lower and upper values**

Factor	Name	Sensitivity range	Range ref.	Parameter	Baseline Value	Low Value	High Value
A	CO_2 capture cost (£m)	+ 10% – 50%	[55]	CO_2 Capture - CAPEX	555	278	611
				CO_2 Capture - OPEX	55.5	27.8	61.1
B	CO_2 utilisation cost (£m)	+ 30% – 30%	[64]	Hydrogenation plant - S - CAPEX	22.3	15.6	29.0
				Hydrogenation plant - M - CAPEX	89.9	62.9	117
				Hydrogenation plant - L - CAPEX	358	251	465
				Hydrogenation plant - S - OPEX	1.23	0.861	1.60
				Hydrogenation plant - M - OPEX	4.95	3.47	6.44
				Hydrogenation plant - L - OPEX	19.7	13.8	25.6
C	CO_2 storage cost (£m)	+ 50% – 50%	[59, 57]	CO_2 Well - S - CAPEX	95.3	47.7	143
				CO_2 Well - M - CAPEX	137	68.5	206
				CO_2 Well - L - CAPEX	231	116	347
				CO_2 Well - S - OPEX	6.10	3.05	9.2
				CO_2 Well - M - OPEX	6.49	3.25	9.7
				CO_2 Well - L - OPEX	7.67	3.84	11.5
D	Electrolyser cost (£m)	+ 50% – 50%	[45]	Electrolyser - S - CAPEX	8.04	4.02	12.1
				Electrolyser - M - CAPEX	20.4	10.2	30.7
				Electrolyser - L - CAPEX	31.6	15.8	47.3
				Electrolyser - S - OPEX	0.402	0.201	0.603
				Electrolyser - M - OPEX	1.02	0.511	1.53
				Electrolyser - L - OPEX	1.58	0.789	2.37
E	H_2 storage cost (£m)	+ 1000% – 90%	[87, 88, 89]	CGH2S - S - CAPEX	4.07	0.407	44.8
				CGH2S - M - CAPEX	23.5	2.35	258
				CGH2S - L - CAPEX	135	13.5	1,489
				US-H2 - Ald - CAPEX	429	42.9	4,719
				US-H2 - Hum - CAPEX	61.0	6.10	671
				US-H2 - Rou - CAPEX	280	28.0	3,080
				US-H2 - War - CAPEX	200	20.0	2,198
				CGH2S - S - OPEX	0.0815	0.00815	0.896
				CGH2S - M - OPEX	0.469	0.0469	5.16
				CGH2S - L - OPEX	2.71	0.271	29.8
				US-H2 - Ald - OPEX	8.58	0.858	94.4
				US-H2 - Hum - OPEX	1.22	0.122	13.4
				US-H2 - Rou - OPEX	5.60	0.560	61.6
				US-H2 - War - OPEX	4.00	0.400	44.0
F	Wind turbine cost (£m)	+ 30% – 30%	[98]	Turbine - Offshore - CAPEX	10.8	7.56	14.0
				Turbine - Onshore - CAPEX	2.50	1.75	3.25
				Turbine - Offshore - OPEX	0.235	0.165	0.306
				Turbine - Onshore - OPEX	0.0545	0.0382	0.0709
G	Wind availability	+ 20% – 20%	[76]	Wind Speed Factor	1	0.8	1.2

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