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Technical, economic and life cycle assessments of low-carbon fuel and chemical technologies

Written

by

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Thesis abstract

Low-carbon fuel and chemical technologies, such as biomass-to-liquids, direct air capture and power-to-X, are essential for achieving net-zero emissions and mitigating climate change. First, advanced "drop-in" biofuels from biomass-to-liquids, partly derived from H_2, are compatible with existing fuel and vehicle infrastructures, and when produced sustainably, they could play a crucial role in mitigating greenhouse gas (GHG) emissions from transportation, particularly in hard-to-decarbonise sectors like freight and aviation. However, there is a need to understand the availability of biomass resources for advanced biofuels use and the potential challenges associated with utilising these feedstocks, including supply chain issues related to feedstock types and production configurations. Second, achieving net zero emissions by 2050 will require the development of cost-effective and CO_2-efficient direct air capture (DAC) technology to remove atmospheric CO_2. DAC CO_2 can be integrated into fuel and chemical technologies for producing low-carbon synthetic fuels and chemicals, thereby enabling a circular economy, or it can function as a standalone low-carbon technology for permanent CO_2 storage. However, the current cost of DAC is expensive, and there is limited technical information available to chart the development routes that will facilitate its cost reduction and enable its wider deployment, while maintaining its emission benefits. Third, there is consensus that achieving net zero emissions will require the use of power-to-X technologies, such as electricity-based H_2 and its derivatives, particularly in the hard-to-abate areas of the transport sector, to complement biofuels, CO_2 capture and storage in reservoirs and battery electric vehicles. Other applications of power-to-X technologies are expected in domestic and industrial heating, and in chemical manufacturing, where they could serve as fuels for heating or as starting chemicals for producing higher-value chemical products. However, due to the various production and downstream operations that can be employed in low-carbon fuel and chemical supply chains, this necessitates the development of global supply chains, which can be complex given limited global experience, especially for H_2 supply chains. Therefore, it is essential to understand the technical, economic and life cycle environmental impacts of biomass-to-liquids, direct air capture and power-to-X technologies to facilitate their deployment.

Hence, first, this thesis presents a critical review of non-food biomass and advanced biofuels production, covering biomass availability (in the UK), the production of advanced biofuels via thermochemical routes, estimated fuel prices and production volumes, and life cycle GHG impacts. The thesis examines several factors influencing fuel production, including energy and H_2 requirements, as well as supply chain considerations, to estimate the potential for advanced biofuels in the UK. The availability of biomass resources is crucial for the deployment of biofuels and sustainable product operations. It was estimated that volumes of non-food biomass resources in the UK ranged from 167–205 Mtpa (wet) [839–1033 PJ per year], as more than 50% of these volumes are from high moisture content feedstocks, such as biogenic municipal waste and sewage sludge. Other biomass feedstocks that are produced in significant quantities include straw and wood waste. Additionally, it was estimated that the total UK advanced biofuels production potential ranged from 269–563 PJ per year. When used to displace fossil fuels in road transport, this could lead to a reduction in GHG emissions of 18.8–64.7% (18.7–64.4 $MtCO_2e$ per year) relative to the UK's 2021 road transport emissions.

Second, this thesis presents techno-economic and life cycle GHG emission assessments of advanced biofuels production via hydrothermal liquefaction to assess economic viabilities, CO_2 mitigation potentials, and prospects for scale-up, specifically within the UK context. Currently, more than 50% of the UK's non-food biomass resources are from high moisture content feedstocks, with hydrothermal liquefaction offering a viable fuel production option. The innovative approach in this work integrates key production factors, including the regional availability of main feedstocks (digestates, food waste, biodegradable municipal waste, and sewage sludge), plant configurations (centralised vs

decentralised), and H_2 sources (grey, blue, green). The study demonstrated the economic trade-off between economies of scale and feedstock transport distances in centralised and decentralised configurations, as well as the economic and emissions trade-offs associated with the use of different H_2 sources. It is found that co-processing of different waste feedstocks is an important strategy to minimise fuel selling price by enabling better economies of scale and feedstock transport, resulting in a fuel price of $19.92–27.40 per GJ. The corresponding GHG emissions from the co-processing case range from 11.4–24.9 $kgCO_2e$ per GJ in 2021, based on the consequential life cycle assessment approach. Furthermore, it is estimated that the utilisation of key UK wet feedstocks could only provide 4.5% of current fuel consumption and reduce emissions by 4.5–5.4 $MtCO_2e$/year, which translates to 3.4–4.0% reductions in the UK's 2021 transport emissions. However, the volumes from biofuels, including those produced from dry biomass feedstocks, will not be sufficient to meet the high demand for transport fuels, given the current and projected estimates of transport fuel demand volumes. Hence, the use of other low-carbon fuels and alternative transport technologies, including direct air capture and vehicle electrification, is required for achieving net zero emissions.

Third, this study presents a comprehensive assessment of five solid sorbents under different technology scenarios to determine the design, operations, costs and GHG emissions of DAC technologies. This was aimed at identifying low-cost, low-carbon options for DAC and charting DAC's commercialisation pathways. The cost and GHG emissions of the five sorbent types assessed ranged from $1,200–40,400/t and 3.1–12.3 tCO_2e/t sorbent in 2024, respectively, mainly driven by the raw materials used for sorbent manufacture. Cost estimates for the best capture technologies ranged from $97–168/gross tCO_2 captured [$126–170/net tCO_2 captured] in 2025 and can be further reduced to $87–140/gross tCO_2 captured [$93–142/net tCO_2 captured] in 2050. The costs of DAC are heavily influenced by: (i) economic factors (e.g., capital expenses and energy costs), (ii) design elements (e.g., plant scale and energy capacity factors) and (iii) operational parameters (e.g., sorbent's adsorption rate and time). Conversely, the GHG emissions of DAC are mostly determined by the source of energy. Price signals in existing carbon markets are inadequate to support a DAC project, but a forecasted carbon price increase to $140–240/$tCO_2$ by 2030–2050 could make DAC commercially viable.

Fourth, this study assessed the supply chains of gaseous synthetic fuels across various supply chains, with applications in the transport, heating, and manufacturing sectors. It summarised key insights drawn from over 10,000 cases, analysing the supply of H_2 and synthetic natural gas (SNG) from six renewables-rich regions and transporting them via different modes to markets, using six different chemical forms, including compressed-H_2 (CH2), liquefied-H_2 (LH2), SNG, methylcyclohexane (MCH), ammonia (NH_3), and methanol (MeOH). The study discussed the implications on the overall energy efficiency, product losses throughout the supply chains, and life cycle GHG emissions from technological, geospatial, and temporal perspectives. The total loss and energy efficiencies of H_2 and SNG throughout the supply chains were estimated to range from 0.8–11.0%/kg and 1.8–3.6 MJ/MJ of gaseous fuel delivered, respectively. The lifecycle GHG emissions (without embodied emissions) ranged from 5–86 gCO_2e/MJ in 2025, and this could reduce to 2–40 gCO_2e/MJ in 2050, due to changes in technological, design and operational factors. Minimising the impact of fuel/carrier production, H_2/CH_4 losses, and fuel and electricity emissions factors by combining centralised and decentralised supply chain approaches could result in a lower GHG estimate. The use of chemical carriers could increase GHG emissions due to the H_2 liberation step at the destination. Even when starting with a low carbon intensity H_2 at the plant gate, the emissions associated with the supply chain can drive the emissions above the EU and UK regulatory limits. This paper further adds to the body of evidence pointing to the need for life cycle assessment-based certification that is asset-specific and supply chain-specific for demonstrating compliance against regulatory limits or H_2 standards globally.

Fifth, this study examined the supply chains of liquid electro-fuels and chemicals for applications in the transport, heating, and manufacturing sectors. It presents key insights drawn from over 10,000 cases, analysing the supply chains of NH_3, MeOH, synthetic gasoline, synthetic diesel and synthetic kerosene produced via various hydrogenation processes. It assessed the life cycle H_2 losses, energy efficiencies, water consumptions and GHG emissions of liquid low-carbon electro-fuels supply chains in transport and manufacturing applications using a dynamic Excel-based tool that analyses over 10,000 supply chain scenarios. The total loss of H_2 to the environment, energy efficiencies and water consumptions in liquid electro-fuel supply chains typically ranged from 0.2–2.6% H_2 per kg fuel, 1.9–4.0 MJ per MJ fuel and 0.41–5.04 kg H_2O per kg fuel delivered, respectively. The GHG emissions (excluding embodied emissions) of renewable electricity-based liquid electro-fuel supply chains typically ranged from 1–21 gCO_2e per MJ in 2025, and could reduce to 1–10 gCO_2e per MJ in 2050, due to technological, design and operational factors. Using approaches that minimise the impact of fuel/carrier production methods, H_2 losses and fuel emissions factors by combining centralised and decentralised processes efficiently offered the lowest GHG emissions estimates with liquid electro-fuels, making the scenarios using centralised fuel production approaches perform well due to the high mass and energy density of the liquid electro-fuels, which favours both short and long supply chain distances. Overall, the GHG emissions of all the renewable electricity-based liquid electro-fuels assessed were within EU/UK emission limits for transportation, which exclude embodied emissions. Furthermore, the analysis also shows that policy definitions of low-carbon fuels across different jurisdictions should encompass a broad range of viable low-carbon fuels production pathways that could considerably aid emission reductions and wider decarbonisation goals.

The thesis findings emphasise that technological factors, including fuel production methods as well as centralised and decentralised production and reconversion configurations, alongside economic factors, emission factors, and assessment methodologies, affect the designs, operations, costs, and environmental impacts of low-carbon technologies. Given the wide range of low-carbon technologies that could be used to achieve emission reductions and climate targets, policies should encompass viable pathways across low-carbon technologies, taking into account resource availability, technology design and operations, environmental, costs and social impacts in their development. Consequently, for the effective deployment of low-carbon fuel and chemical technologies, both general strategies and supply chain-specific approaches are vital for successful implementation.

Publications

First author publications (included in this thesis):

Lilonfe, S., Dimitriou, I., Davies, B., Abdul-Manan, A. F. N., & McKechnie, J. (2024). Comparative techno-economic and life cycle analyses of synthetic "drop-in" fuel production from UK wet biomass. *Chemical Engineering Journal*, *479*, 147516. https://doi.org/10.1016/j.cej.2023.147516.

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Lilonfe, S., Rodgers, S., Abdul-Manan, A. F. N., Dimitriou, I., & McKechnie, J. (2025). Technical, economic and lifecycle greenhouse gas emissions analyses of solid sorbent direct air capture technologies. *Carbon Capture Science & Technology*, *15*, 100380. https://doi.org/10.1016/J.CCST.2025.100380.

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Presentations

Oral presentation (June 2023) at *European Biomass Conference and Exhibition (EUBCE)* on "Techno-Economic and Life Cycle Analyses of Renewable Hydrocarbon Fuels from UK Wet Biomass Feedstocks."

Poster presentation (September 2023) at *UKRI Chemical Circular Summer School* on "Comparative techno-economic and life cycle analyses of synthetic 'drop-in' fuel production from UK wet biomass."

Oral presentation (July 2024) at *Glasgow 2024 Engineering Convention* on "Techno-Economic and Life Cycle Analyses of Renewable Hydrocarbon Fuels for Road Transport Applications."

Poster presentation (March 2025) at *UKCCSRC Spring 2025 Conference* on "Technical, economic and lifecycle greenhouse gas emissions analyses of solid sorbent direct air capture technologies."

Oral presentation (April 2025) at *ChemEngDayUK Sheffield 2025* on "Technical, economic and lifecycle greenhouse gas emissions analyses of solid sorbent direct air capture technologies."

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1 Introduction

1.1 Background

Climate change is a global issue, primarily driven by the release of greenhouse gases into the atmosphere. In 2023, human activities alone released a total of 36 $GtCO_2e$ into the atmosphere from fuel combustion, mainly to meet the energy and material demands of the transport and industrial sectors (Ritchie, 2020; IEA, 2025). There is no silver bullet to addressing this greenhouse gas emissions issue, but there is consensus that low-carbon technologies, such as biofuels, battery electric vehicles, direct air capture and electro-fuels, are essential approaches to mitigating greenhouse gas emissions (European Commission, 2019; IEA, 2022b; DfT, 2024). While battery electric vehicles can offer significant greenhouse gas reductions in transportation, their effectiveness greatly depends on the accessibility of critical battery materials (Zhang, Yan and You, 2023), charging infrastructures and the widespread availability of renewable electricity to support a more ambitious battery electric vehicle uptake. Furthermore, in the hard-to-electrify transport sectors, like heavy-duty trucks, marine and aviation, there is consensus that low-carbon fuels will have to play a more significant role in decarbonising these sectors. However, they also face challenges. Biofuels, the most commonly used low-carbon fuel today, can be limited by biomass and land availability, as well as sustainability concerns arising from land management practices in biomass production (Searchinger *et al.*, 2008; IEA, 2019; DESNZ, 2023). Hence, electro-fuels, often obtained from renewable electricity, are considered complementary solutions to battery electric vehicles and biofuels in the transport sector's climate change mitigation strategies. Additionally, some electro-fuels and their chemical equivalents, such as e-H_2 and blue H_2 and e-methanol and blue methanol, can be used as fuels or base chemicals in manufacturing industries for enabling a low-carbon circular economy and sustainability.

Generally, biofuels can be produced from biochemical processes, as in the case of conventional biofuels, e.g., bioethanol produced from fermentation. They can also be produced from thermochemical processes, often referred to as biomass-to-liquids when the products are liquids, as in the case of advanced "drop-in" biofuels, e.g., bio-kerosene produced by Fischer-Tropsch synthesis. Direct air capture technology is an engineering-based method of removing CO_2 from the atmosphere through chemical or physical processes, allowing the captured CO_2 to be stored permanently or utilised to produce high-value chemical products. Power-to-X technologies, which include power-to-gases and power-to-liquids, convert electricity into fuels and chemical products, often referred to as electro-fuels and chemicals, e.g., e-H_2. Other low-carbon technologies utilise different designs and operations, e.g., battery electric vehicles, which use electricity stored in batteries for transportation.

However, despite the environmental benefits of low-carbon technologies, their deployment is below the targets set by different stakeholders, including the EU (European Commission, 2019; European Court of Auditors, 2023; IEA, 2023c) and IEA (IEA, 2022a, 2022b). This is primarily due to technical, economic, environmental, policy and social challenges, such as the limited availability of resources [e.g., biomass and battery materials (DESNZ, 2023; Zhang, Yan and You, 2023)], process design and operational issues (especially for renewable electricity-based technologies) (IEA, 2023b; Concawe and Aramco, 2024) and high production costs (Dimitriou, Goldingay and Bridgwater, 2018; Concawe and Aramco, 2024). Therefore, a strong justification exists for assessing the technical, economic, environmental and policy implications of low-carbon technologies. Furthermore, existing technical, economic, environmental and policy literature have failed to address many issues associated with production, e.g., using centralised vs decentralised production approaches and modelling integrated manufacturing; transformations for transport and storage, e.g., using centralised vs decentralised reconversion approaches; product delivery modes, e.g., using ships, rail, trucks and pipelines across different supply chains; the use of low-carbon technologies, e.g., the transition from natural gas for

heating to low-carbon synthetic natural gas, H_2 or grid electricity; and policies implications, e.g., the implications of the different energy policies and emissions limits of fuels. Hence, to address these challenges, this work assessed over 30,000 low-carbon fuel and chemical supply chains, including biomass-to-liquids, direct air capture and power-to-X, using process modelling, techno-economic and life cycle assessment methodologies, taking into account technology, geographical, temporal and policy perspectives. Additionally, existing policies were critically reviewed, and novel strategies were developed to support the deployment of low-carbon fuel and chemical technologies.

Techno-economic assessment, which is a tool for analysing the technical and economic performances of industrial plants, processes or products (Zimmermann *et al.*, 2020), is widely used to assess the technical requirements, capital, operating, revenue, and product costs of fuel and chemical products. These technical and economic data are crucial as they provide preliminary insights that inform the design, construction, and operations of successful production plants. Additionally, techno-economic assessment supports stakeholders (including policymakers) with opportunities to select the most economical process that will significantly impact the production and competitiveness of technologies. The techno-economic performances of industrial plants, processes or products are mainly influenced by 1) Design and operational approaches, such as production method, product states (e.g., compressed or liquid H_2), plant size, plant commissioning year and system boundary (Valente, Iribarren and Dufour, 2021; IEA, 2023a; Concawe and Aramco, 2024) 2) Economic factors, such as the cost of raw materials, transportation expenses, capital expenses, discount and tax rates (Zhu *et al.*, 2014; Rodgers *et al.*, 2021; Concawe and Aramco, 2024) and 3) techno-economic methodologies (Green, 2007; Feng and Rangaiah, 2011; Rodgers, 2024). Therefore, it is important to assess and control the impacts of these factors for deploying cost-competitive low-carbon products.

On the other hand, the sustainability of processes and products is usually evaluated, reviewed, and improved using tools such as life cycle assessment. Life cycle assessment is an assessment technique that is used to assess environmental impacts associated with all the stages of a product's life or service's life, which include upstream processes, such as raw material extraction, to downstream processes, such as waste disposal (Sphera, 2020). The greenhouse gas emissions of fuels and chemicals from various sources are reported to vary over a wide range, from emissions of less than -100 gCO_2e per MJ to those exceeding 94.7 gCO_2e per MJ product (the fossil fuel benchmark for applications in the transport sector). This significant variation is due to many factors, such as feedstocks and associated land use change impacts (Searchinger *et al.*, 2008; BEIS, E4tech and LBST, 2021), production techniques (de Jong *et al.*, 2017; McQueen *et al.*, 2020; Concawe and Aramco, 2024), allocation methods used to attribute impacts across multiple product outputs (Shonnard, Williams and Kalnes, 2010; de Jong *et al.*, 2017), system boundary (Kolosz *et al.*, 2020; Fernanda Rojas Michaga *et al.*, 2022), and energy sources (Hsu, 2012; Concawe and Aramco, 2024). Hence, understanding and mitigating the impacts of these factors is important in improving the sustainability of low-carbon technologies.

Therefore, to address the issues associated with low-carbon fuels and chemicals, such as product prices and life cycle environmental impacts, this thesis presents process modelling, techno-economic and life cycle assessments of low-carbon fuel and chemical technologies, including biomass-to-liquids, direct air capture and power-to-X systems. Process modelling, techno-economic and life cycle assessment methodologies are developed in this study to model the designs, operations, costs and environmental impacts of low-carbon fuels and chemicals supply chains, with the goal of developing strategies that would enable their successful deployment. Due to the diverse areas of assessment and the depth of each area covered in this research, this chapter provides a general background on the various technologies assessed. Specific information, including the limitations of the existing literature in specific technologies and the novelty of this work, is further explored in the succeeding chapters.

Chapter 2 critically reviews the literature and presents findings on biomass-to-liquids, direct air capture and power-to-X technologies. Chapter 3 presents an extended study on biomass-to-liquids technology to address the challenges of biomass resource availability and competing applications. Chapter 4 presents the general insights into the methodologies adopted in the thesis. Chapters 5–8 present this study's publications on process modelling, techno-economic and life cycle assessments of biomass-to-liquids, direct air capture, power-to-gases and power-to-liquids technologies. Lastly, Chapter 9 presents conclusions and recommendations from this study. Additional details on the outline of the thesis can be found in Section 1.3 and the Table of Contents.

1.2 Thesis aims and scope

The thesis aims to develop and apply techno-economic and life cycle assessment methodologies to evaluate key low-carbon fuel and chemical technologies, including biomass-to-liquids, direct air capture, and power-to-X technologies. The study assesses economic viabilities, CO_2 mitigation potentials, and prospects for scale-up of key low-carbon fuel and chemical technologies to chart commercialisation pathways for low-cost, low-carbon solutions, including bioproducts, direct air capture, and power-to-X technologies. These technologies are complementary to each other (for example, diesel and kerosene), or their products are chemical equivalents (for example, bio-kerosene produced via biomass-to-liquids and e-kerosene via power-to-X technologies). Hence, these justify the aim and scope of the work, which includes integrated and comparative assessments of low-carbon fuel and chemical technologies. Additionally, biomass-to-liquids, direct air capture, and power-to-X technologies were assessed in this work because of their (i) compatibility with existing infrastructure and markets, including direct air capture, which can help offset emissions from hard-to-abate areas, (ii) potential for significant volume uptake and emissions reductions due to the availability of renewable resources (e.g., biomass and wind energy) and CO_2 storage options (IPCC, 2005, 2024; Welfle *et al.*, 2020), (iii) commercial feasibility, with each of the technology categories in Technology Readiness Level ranging from 5–9, and (iv) potential for some supply chain options, which are not well understood in terms of design and operations, to have significant environmental impacts (see Section 2.2, and Chapters 3–8 for additional information). The assessment of other low-carbon technologies, such as conventional biofuels, biomass-to-gases, bioenergy with carbon capture, battery electric vehicles and hydrothermal carbonisation, is outside the scope of this project. This is mainly due to the extensive research already available on the production methods of these technologies. Nevertheless, many products of these technologies and their downstream processes were studied here, e.g., the delivery options for H_2 produced from fermentation, power-to-X and biomass-to-gases, as well as the delivery options for CO_2 into reservoir or manufacturing applications. The study's objectives are presented in various chapters of the thesis (e.g., Chapters 3 and 5–8) and are summarised here, while Figure 1.1 provides a map of the thesis structure and the connections between the objectives.

i. **Critically review biomass-to-liquids supply chains, including biomass feedstock availability, competing uses and biomass-to-liquids methods**. This review aims to understand existing technologies and competing biomass uses, while also mitigating key challenges.
ii. **Develop appropriate techno-economic and life cycle assessment frameworks for evaluating biomass-to-liquids-related supply chains.** These frameworks should tackle key challenges associated with biomass-to-liquids supply chains, such as feedstock availability and competing uses, as well as centralised and decentralised production and reconversion methods**.**
iii. **Determine the cost, environmental impacts, and available volumes of advanced biofuels across the UK market, and whether advanced biofuels may or may not meet the transport fuel demand.** This will assist in understanding how advanced biofuels and other low-carbon fuel and chemical technologies could be utilised in decarbonising the transport sector.

iv. **Develop appropriate techno-economic and life cycle assessment frameworks for evaluating the supply chains of non-biomass-based low-carbon fuel and chemical technologies for primary use in the transport sector, if biofuel volumes are inadequate to achieve transport sector fuel demand and decarbonisation targets.** These frameworks should tackle key challenges related to supply chains for other low-carbon fuels and chemicals, such as centralised and decentralised production and reconversion methods.

v. **Determine the costs and/or environmental impacts of other low-carbon fuel and chemical technologies that could complement biofuels in meeting transport sector fuel demand and decarbonisation targets.**

1.3 Thesis outline

The structure of the thesis, which can be grouped into biomass-to-liquids, direct air capture and power-to-X technologies, consists of five journal publications, which have been indexed as key thesis chapters, as shown in Figure 1.1. The publications in this thesis all contribute towards the technical, economic and life cycle assessments of low-carbon fuel and chemical technologies.

Chapter 1 presents general information on the thesis, including the background and aims of the study.

Chapter 2 presents a critical literature review of supply chain processes relating to low-carbon fuel and chemical technologies, with a particular focus on the techno-economic and life cycle assessments of biomass-to-liquids, direct air capture, and power-to-X technologies.

Chapter 3 provides an in-depth critical review of biomass-to-liquids supply chains, giving the significant variability and concerns surrounding biomass resources and their competing uses. It also evaluates the life cycle environmental impacts of utilising dry and wet non-food biomass feedstocks. This has been published in Sustainable Production and Consumption as "A review of techno-economic analyses and life cycle greenhouse gas emissions of biomass-to-hydrocarbon "drop-in" fuels." Some of the assessment methodologies and results for wet non-food biomass feedstocks in Chapter 5 were used alongside data for dry non-food biomass feedstocks obtained from the literature to perform an extended analysis of the UK non-food biomass feedstocks utilisation for advanced biofuels production. Additionally, the findings from the work were used to select and assess other complementary solutions that could be deployed to meet decarbonisation targets.

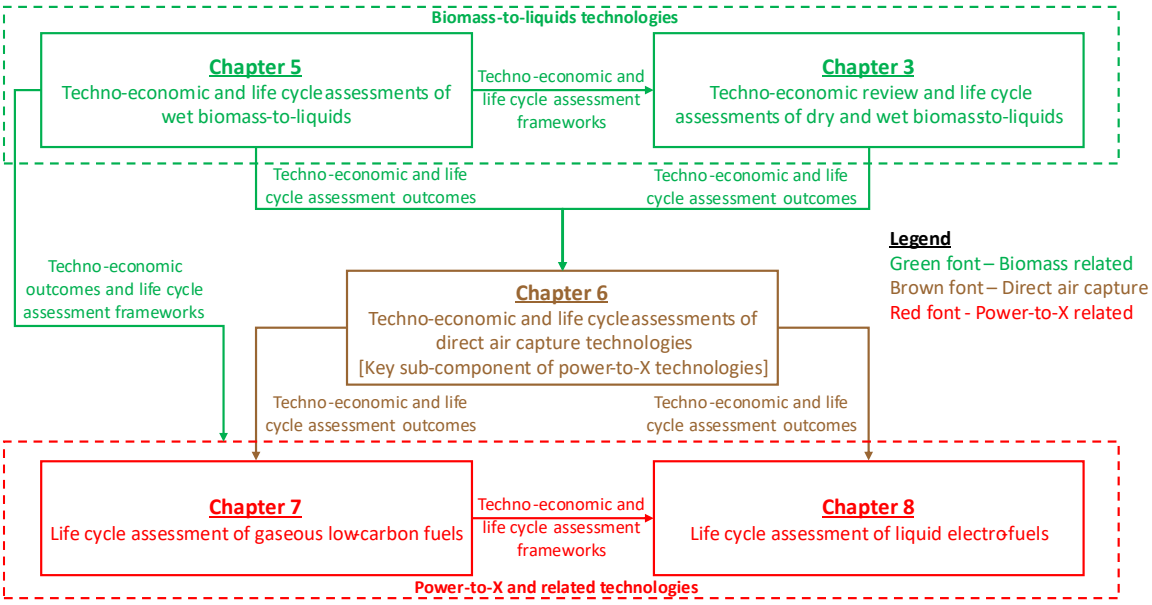

Figure 1.1: Outline of the thesis results' headings and the links between them.

Chapter 6 presents the techno-economic and life cycle assessment of direct air capture technologies, including the technical, economic and life cycle assessments of solid sorbent manufacturing and CO_2 capture plants. It charts development routes for sorbent and direct air capture technologies towards commercialisation. This has been published in Carbon Capture Science & Technology as "Technical, economic and lifecycle greenhouse gas emissions analyses of solid sorbent direct air capture technologies." The techno-economic and life cycle assessment outcomes from the work were utilised to assess the life cycle environmental impacts of power-to-X-related technologies in Chapters 7 and 8.

Chapter 7 presents the life cycle assessment of gaseous low-carbon fuels, including power-to-gases technologies, from different design, operational, geographical and temporal perspectives. It assesses the life cycle environmental impacts associated with the production and delivery of gaseous low-carbon fuels, including H_2 (transported in various forms such as compressed-H_2, liquefied-H_2, methylcyclohexane, ammonia, and methanol), as well as synthetic natural gas. This has been published in Energy Conversion and Management as "Life cycle greenhouse gas implications of low-carbon gaseous fuel supply chains from technological, geospatial, and temporal perspectives." The techno-economic and life cycle assessment frameworks from Chapters 3, 5 and 6 were utilised to assess the life cycle environmental impacts of gaseous low-carbon fuels and chemicals.

Chapter 8 presents the life cycle assessment of liquid electro-fuels, including ammonia, methanol, gasoline, diesel and kerosene, across different technical, geographical and temporal perspectives. This work is currently undergoing internal review for publication in a peer-reviewed journal as "Life cycle assessment of global liquid electro-fuels and chemicals supply chains from technological, geospatial, and temporal perspectives." The techno-economic and life cycle assessment frameworks from Chapters 3 and 5–7 were utilised to assess the life cycle environmental impacts of power-to-liquids.

Chapter 9 covers the conclusions and recommendations from this study.

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2 Literature review

This chapter presents a critical literature review of supply chain processes related to low-carbon fuel and chemical technologies, with a particular focus on the techno-economic and life cycle assessments of biomass-to-liquids, direct air capture, and power-to-X technologies. It discusses fuel production methods, techno-economic assessment frameworks and outcomes, life cycle assessment frameworks and outcomes, centralised and decentralised production and reconversion approaches, and key policies on low-carbon fuels and chemicals. Due to serious concerns about the availability of biomass resources and competing uses, an in-depth critical discussion and analysis are provided in Chapter 3.

2.1 Low-carbon technologies

Low-carbon technologies are defined as technologies that emit a low overall (positive, negative or zero) amount of CO_2 into the environment in their life cycle. They include a range of technologies, such as biofuels, solar power, electric vehicles, direct air capture, and electro-fuels. Low-carbon technologies that remove CO_2 from the environment are often referred to as CO_2 removal technologies, e.g., direct air capture and hydrothermal carbonisation. Typically, CO_2 removal technologies may also emit some CO_2 while removing it from the environment in their life cycle. This is often termed carbon efficiency. Hence, this highlights the importance of life cycle assessments to ensure minimal environmental impacts from low-carbon technologies. The supply chains of important low-carbon fuel and chemical technologies utilised in transport and industrial sectors are summarised in Figure 2.1, with the scope of this work shown. The assessment of other technologies, such as conventional fuels (fossil fuels and first-generation biofuels), biomass-to-gases, bioenergy with carbon capture, battery electric vehicles, and hydrothermal carbonisation, is outside the scope of this study.

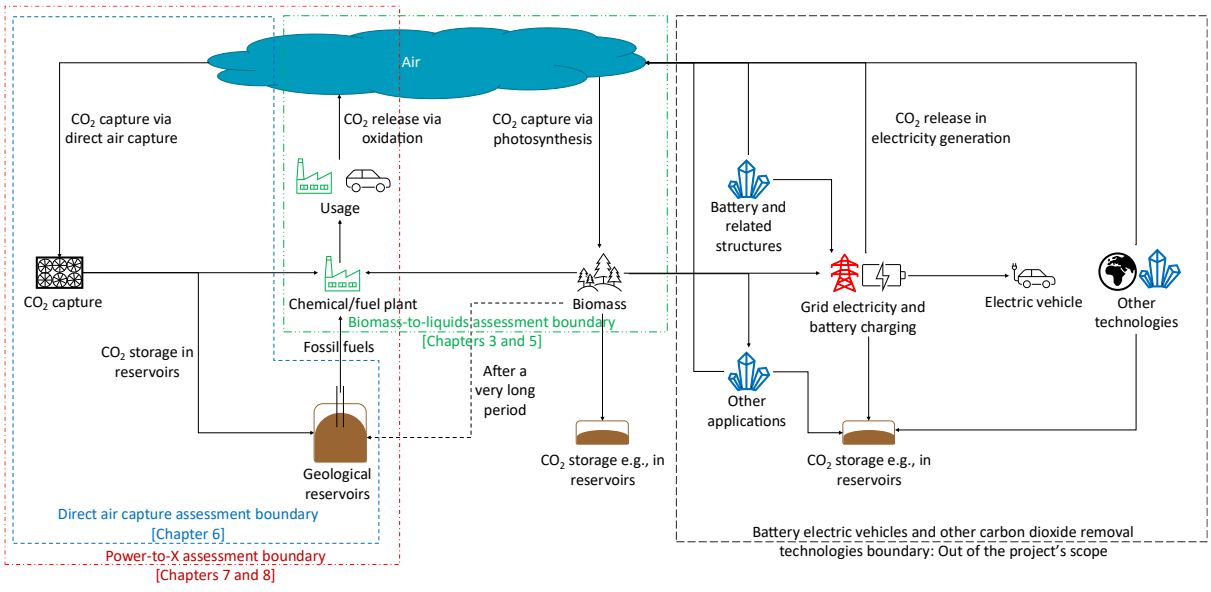

Figure 2.1: Simplified life cycle of key low-carbon technologies, showing an overview of this study.

The use of low-carbon fuel and chemical technologies, including biofuels, direct air capture and electro-fuels, is deemed essential for achieving net zero emissions and combating climate change (IEA, 2022a; DESNZ, 2023c; European Union, 2023b; Government Office for Science, 2023; IPCC, 2023). This is because there is no silver bullet to addressing the issue of climate change arising from the release of greenhouse gas into the atmosphere, given the complexity of anthropogenic systems.

In the transport, heating and manufacturing applications, first-generation biofuels and biochemicals – the most commonly used low-carbon fuel and chemical technologies today – can be limited by the

availability of biomass and land, as well as sustainability concerns arising from land management practices in biomass production (Searchinger *et al.*, 2008; Plevin *et al.*, 2010; DESNZ, 2023a). The food vs fuel debate has strongly intensified since the global food crisis of 2008, which was partly attributed to the use of first-generation biofuels (European Commission, 2011). First-generation biofuels and biochemicals are typically produced from food-based biomass, such as the fermentation of starch and sugar and the transesterification or hydrogenation of fats and oils. Additionally, first-generation biofuels, such as bioethanol and biodiesel (transesterified), can only be used in blends with petroleum fuel up to a certain percentage in current engines without requiring costly engine modifications. These current limitations not only impact the production of first-generation biofuels but also their utilisation, and therefore, the development of alternative fuels and chemicals, such as renewable hydrocarbon biofuels and electro-fuels, is considered a key innovation for addressing these issues.

Advanced "drop-in" biofuels, which are hydrocarbon fuels, such as bio-gasoline and advanced biodiesel, are designed as drop-in solutions that can be used as direct replacements for petroleum fuels, thereby allowing for broader biofuels use in transportation. Additionally, drop-in biofuels are typically produced from second and third-generation biomass feedstocks such as agricultural waste (Anex *et al.*, 2010) and algae (Jones *et al.*, 2014). They can also be produced from waste bio-CO_2 (d'Amore *et al.*, 2023). Drop-in biofuel production allows the utilisation of non-food biomass resources and can improve the sustainability of biofuels by addressing issues such as land use change, indirect land use change and the availability of biomass resources. Non-food biomass, which includes lignocellulosic biomass and waste biomass, typically has zero land use change emissions, especially for residues and wastes. However, the utilisation of non-food biomass for drop-in biofuel applications may come with other consequential indirect emissions, which may arise from diverting these materials from existing streams (Ou *et al.*, 2022). These consequential emissions, which may vary significantly by feedstock, technology and market, can be either positive or negative, depending on the competing applications, such as diverting food waste from landfilling or anaerobic digestion. Additionally, the methods for producing drop-in biofuels, often referred to as second-, third-, and fourth-generation biofuels, differ substantially from those of first-generation biofuels. Hence, it is essential to conduct technical, economic, and life cycle assessments of drop-in biofuels to understand the key strategies, including cost and greenhouse gas emissions, for their successful production and delivery.

Furthermore, second-, third-, and fourth-generation biofuels and biochemicals face challenges too, such as limited biomass availability and varying biomass feed composition, which may lead to operational difficulties during their production. Consequently, power-to-X derived from renewable electricity is considered a complementary solution for achieving net zero emissions strategies. This is due to their advantages, such as compatibility with today's technologies and infrastructures, a ready-to-be-used solution, which can be implemented in today's fossil fuel pools to achieve a steady increase in share, and their functionality as chemicals for long-term energy storage of renewable electricity (BEIS, 2021; Concawe and Aramco, 2024). However, despite the potential of power-to-X to be low-carbon, with their plant gate emissions usually low when renewable electricity is used, the life cycle (well-to-user) emissions of power-to-gases could vary significantly, from 2–25 gCO_2e/MJ for a short national distance of 150 km (BEIS, E4tech and LBST, 2021). Since current decarbonisation strategies requiring power-to-X may involve long-distance fuel delivery, the regulatory limits (legal obligation) for life cycle emissions of 32.9 gCO_2e/MJ by the UK Renewable Transport Fuel Obligation (RTFO) (DfT, 2024a) and 28.2 gCO_2e/MJ by the EU (European Union, 2023b, 2023a) could be exceeded under some supply options. Additionally, many regulatory standards, such as the UK Low Carbon Hydrogen Standard (DESNZ, 2023d) and EU Renewable Energy Directive (RED) II (European Union, 2023a), do not account for embodied emissions from infrastructure, including production equipment and transport vehicles. As a result, even H_2-based supply chains that comply with regulatory limits may

still incur significant emissions from infrastructure, thereby increasing overall greenhouse gas emissions and potentially impacting decarbonisation targets. Furthermore, the cost of power-to-X is currently high, making it not competitive with conventional fuels and chemicals (IEA, 2022b; Martin, Neumann and Ødegård, 2023; Concawe and Aramco, 2024). Part of this cost, which includes the CO_2 capture cost, could be reduced if the cost of carbon capture is significantly lowered. Generally, power-to-X supply chains differ by design and operations, namely: H_2 production method; transformations for transport and storage; transportation modes and distances; and the form of fuel and dispensing method at the point of delivery to the user. Hence, it is essential to mitigate the impacts of these factors using comprehensive technical, economic and life cycle assessment approaches.

2.2 Synthetic fuels and chemicals production technologies

Generally, synthetic fuels and chemicals can be produced via a range of production processes, including electrolysis, CO_2 or biomass hydroprocessing to methanol or methane, hydroprocessing of methanol to gasoline and kerosene and hydroprocessing of syngas to Fischer-Tropsch liquids via Fischer-Tropsch synthesis. Hence, synthetic fuels and chemicals production processes can be classified into gaseous synthetic fuels and chemicals (e.g., e-H_2) and liquid synthetic fuels and chemicals approaches (e.g., e-methanol). The production of gaseous fuels and chemicals from biomass is outside the scope of this study due to the maturity of biogas and the developments in biohydrogen technologies. The details of synthetic fuels and chemicals production methods can be found below.

2.2.1 Gaseous synthetic fuels and chemicals production technologies

2.2.1.1 H_2 production

The simplest synthetic fuel is e-H_2, which is usually produced from water electrolysis using renewable electricity. In water electrolysis, water is separated into H_2 and O_2 by a current flowing between two electrodes positioned apart and immersed in an electrolyte. The overall reaction equation is shown in Equation (2.1). H_2 electrolysis can be performed using low-temperature processes (at 40 to 80 °C) or high-temperature processes (at 700 to 1000 °C) (Concawe and Aramco, 2024). The water demand for electrolytic H_2 is reported to be negligible compared to that in energy crops (a few litres of water versus several thousand litres of water per litre of energy equivalent (Concawe and Aramco, 2024). Presently, H_2 production from water electrolysis accounts for less than 1% of global H_2 production volumes (CertifHy, no date; Wood Mackenzie, no date). In transport, heating, power generation, and manufacturing applications, H_2 can be used as a fuel in gas burners, gas turbines, and new transport engines (e.g., fuel cells and combustion engines), or as a base chemical for producing other chemicals (Hydrogen UK, no date; GE, 2022; Chu and Cui, 2023; Concawe and Aramco, 2024; World Bank, 2025).

H_2 production: $2\ H_2O \rightarrow 2\ H_2 + O_2 \qquad \Delta H = +286\ kJ/mol$ (2.1)

Generally, there are three widely used e-H_2 production technologies, namely, 1) alkaline electrolysis cells, 2) proton exchange membrane (or polymer electrolyte membrane) electrolysis cells, and 3) solid oxide electrolysis cells.

Alkaline electrolysis, which is in commercial application, is currently the most established water electrolysis technology (Brynolf *et al.*, 2018; Concawe and Aramco, 2024; Environment Agency, 2024). A typical alkaline electrolyser cell consists of two electrodes coated with Ni as catalysts and immersed in an electrolyte (20–40% potassium hydroxide solution). Alkaline electrolysis can be performed at ambient pressure or at pressures of up to 30 bars (Concawe and Aramco, 2024). The efficiencies of alkaline electrolysers are reported to be in the range of 43–69% on an H_2 lower heating value basis. This is due to design and operation factors, such as electrolyte concentration, temperature, current

density, and material types (de Groot, Kraakman and Garcia Barros, 2022). Their costs, which depend on their size and efficiency, currently vary from €600–2600/kW_{el}, while the future alkaline electrolysers' costs have been estimated to reduce to €250–1000/kW_{el} (Table 2.1). The main advantages of alkaline electrolysers, compared to polymer electrolyte membrane and solid oxide electrolysers, include their low capital costs, suitability for large-scale H_2 production, and long lifespan (Ursua, Gandia and Sanchis, 2012; Brynolf *et al.*, 2018). Conversely, the main disadvantages of alkaline electrolysers include their low current density, lower operating pressure limits of 30 bars compared with the other electrolysers, a limitation on operational production rates of 25–100% due to the formation of flammable gas mixtures, and high maintenance costs due to the corrosive nature of the electrolyte (Ursua, Gandia and Sanchis, 2012; Brynolf *et al.*, 2018).

Polymer electrolyte (or proton exchange) membrane electrolysis cells, also available for commercial applications, are relatively new compared to alkaline electrolysis cells (IEA, 2023b; Concawe and Aramco, 2024). In contrast to the alkaline electrolysis cells, polymer electrolyte membrane electrolysers do not have a liquid electrolyte. Instead, the electrolyte is a solid plastic material, usually Niafon (Ursua, Gandia and Sanchis, 2012). The electrodes are usually made from noble metals like platinum or iridium. Polymer electrolyte membrane electrolysers can operate at a higher pressure than alkaline electrolysers, with design pressures of up to 100 bars (Brynolf *et al.*, 2018; Concawe and Aramco, 2024). The efficiencies of polymer electrolyte membrane electrolysers are comparable to alkaline electrolysers (Brynolf *et al.*, 2018; IEA, 2023b). However, their costs, which also depend on their size and efficiency, are higher than alkaline electrolysers as they currently vary from €750–3700/kW_{el}. The future costs of polymer electrolyte membrane electrolysers are estimated to reduce to €240–1100/kW_{el} (Table 2.1). The main advantages of polymer electrolyte membrane electrolysers include their ability to operate at variable power feeding regimes, making them also suitable for dynamic operations, the absence of corrosive electrolytes, and the ability to accommodate high pressures of up to 100 bars. However, they are very expensive due to their association with proprietary membranes and metal noble-based electrodes. In addition, noble metals, such as platinum or iridium, used for the metal electrolytes are critically scarce materials.

Solid oxide electrolysis cells, currently in the development stage, are widely considered to have the best potential, particularly due to their high efficiencies. The design and operations of solid oxide electrolysers consist of the electrodes (often made up of zirconia doped with yttria) in contact with a vapour phase (steam), solid electrolytes (ceramic membranes), and steam is reduced to H_2 by high-temperature (600–1000 °C) electrolysis (Ursua, Gandia and Sanchis, 2012; Götz *et al.*, 2016; Ballal *et al.*, 2023; Concawe and Aramco, 2024). Solid oxide electrolysers' ability to use heat energy input to reduce electricity requirements allows them to be thermally integrated with exothermic fuel production processes, thereby offering benefits, such as co-electrolysis, where steam and CO_2 can be used to produce renewable syngas in only one process step (Ballal *et al.*, 2023; Concawe and Aramco, 2024). Their disadvantage is in their long-term degradation and unsuitability for dynamic systems (Laguna-Bercero, 2012; Götz *et al.*, 2016). The efficiencies of solid oxide electrolysers are higher than those of alkaline and polymer electrolyte membrane electrolysers, with estimates ranging from 75–85% on an H_2 lower heating value basis (Ursua, Gandia and Sanchis, 2012; Ballal *et al.*, 2023; Concawe and Aramco, 2024). Currently, their cost is higher, €1200–3100/kW_{el}, due to their lack of maturity, but this cost is forecasted to decrease to €250–1500/kW_{el} in the future as they become more developed.

Table 2.1 : Key electrolysers techno-economic data based on 1–100 nominal power (MW_{el}) capacity *(Götz* et al*., 2016; Brynolf* et al*., 2018; Zauner* et al*., 2019; BEIS, 2021; Ballal* et al*., 2023; Concawe and Aramco, 2024; Environment Agency, 2024)*.

Electrolyser Technologies	**Efficiencies on H_2 LHV basis**	**Investment cost (€/kW_{el})**			**O&M cost [% invest. cost]**	**Present TRL**
		2020	**2030**	**2050**		
Alkaline	43–75%	600–2600	400–1200	250–1000	2–5	TRL 9
Polymer electrolyte membrane	40–79%	750–3700	300–1400	240–1100	2–5	TRL 6–8
Solid oxide	75–85%	1200–3100	400–2000	250–1500	2–3	TRL 5–7
Note: TRL – Technology Readiness Level						

Low-carbon H_2 can also be produced using fossil fuels with carbon capture and storage, such as steam methane reforming with carbon capture and storage, see Equation (2.2). Steam methane reforming is a well-established process for producing H_2 by the reforming of methane (in natural gas) and steam at operating temperature and pressure (typically 700–1000 °C and 15–50 bar) (Dincer, Rosen and Al-Zareer, 2018; Concawe and Aramco, 2024). By capturing the fossil CO_2 from the reforming of natural gas and permanently storing it, the greenhouse gas emissions of current steam methane reforming can be significantly reduced (Longden *et al.*, 2022; IEA, 2023a). Other low-carbon H_2 production technologies include biomass gasification and fermentation. However, the discussion of these technologies is out of the scope of this work, as highlighted in Sections 1.2 and 2.2.

Steam methane reforming (overall): $CH_4 + 2\,H_2O \leftrightarrow 4\,H_2 + CO_2 \qquad \Delta H = +165\,kJ/mol$ (2.2)

2.2.1.2 Methane production

Methanation, which can be achieved through reverse steam methane reforming (also known as the Sabatier reaction), can be used to produce methane from H_2. This is due to the reversibility of the steam methane reforming reaction, as shown in Equation (2.2). The Sabatier reaction, which is exothermic, typically occurs at 400 °C, under 30 bars, and in the presence of a nickel or ruthenium catalyst (Concawe and Aramco, 2024). Hence, this allows for the production of synthetic natural gas from low-carbon H_2. Currently, methane is used directly as a fuel (e.g., in boilers and vehicles) or a base chemical to produce other chemicals (CertifHy, no date; Persson and Svensson, 2012).

2.2.1.3 CO_2 production

CO_2 is often considered a chemical feedstock used directly to make products, such as carbonated drinks and fire extinguishers, or as a starting chemical for producing higher-value chemicals, such as urea and methanol (IEA, 2019). Current CO_2 production is typically a byproduct of industrial processes, most notably H_2, ammonia, and ethanol production, as well as natural gas processing. However, CO_2 can be produced directly using technologies like direct air capture. Direct air capture is an engineered technology that captures CO_2 from the air using chemical or physical processes. It captures CO_2 by using sorbents that selectively adsorb or absorb CO_2 from the air. The captured CO_2 is then released during sorbent regeneration and collected for further actions as the sorbent is replenished. The CO_2 captured from the air can be used to produce other higher-value products, such as low-carbon synthetic fuels and chemicals, to meet society's growing demand for energy and materials in our existing carbon-based economy, or it can be stored permanently (e.g., in geological reservoirs).

The removal of CO_2 from the air can be achieved using various direct air capture techniques. Generally, direct air capture can be classified into four main groups, namely: (i) Liquid sorbent, which captures

CO_2 from the air through selective absorption using a liquid sorbent; (ii) solid sorbent, which captures CO_2 from the air through selective adsorption using a solid sorbent; (iii) cryogenic, which is based on air liquefaction and (iv) membrane, which captures CO_2 from air through selective permeation using a membrane. However, only the thermal solid and liquid sorbent direct air capture are presently commercially proven (Climeworks, no date; Fasihi, Efimova and Breyer, 2019). Generally, the energy demands of solid sorbent direct air capture are reported to be lower than those of liquid sorbent direct air capture (Ozkan *et al.*, 2022; IEA, 2023c). Also, the quality of heat in the two processes differs significantly. Solid sorbent direct air capture requires thermal energy at about 80–130 °C, offering the opportunity to exploit low-grade heat for sorbent regeneration. In addition, solid sorbent direct air capture offers low operating costs and applicability across a wide range of scales, owing to its modular nature. Conversely, liquid sorbent direct air capture requires a wide range of solvent regeneration temperatures, from as low as 80–130 °C with amines to as high as 800–900 °C for hydroxides (e.g., KOH) (Keith *et al.*, 2018; Fasihi, Efimova and Breyer, 2019; McQueen *et al.*, 2021). Liquid sorbent direct air capture allows the contactor to be operated continuously. This helps allow very long contactor lifetimes, even in the presence of dust and atmospheric contaminants (Keith *et al.*, 2018).

Liquid sorbent direct air capture technologies use liquid sorbents to capture CO_2 from the atmosphere. Many models of liquid sorbent direct air capture technologies are mature and typically at Technology Readiness Level 6–9. Liquid sorbent direct air capture, based on amine sorbents, is the oldest direct air capture technology. It has been used for CO_2 capture from flue gas since 1930 (Wang *et al.*, 2022). Aqueous amines such as monoethanolamine and diethanolamine have typically been used for CO_2 capture due to their suitable properties such as high adsorption rates, low regeneration temperatures, and relatively lower cost (Aghel *et al.*, 2022; Wang *et al.*, 2022). However, amine capture could be faced with many problems, such as corrosion due to the corrosive nature of liquid amines and evaporative (capacity) loss due to amines' high vapour pressure (Erans *et al.*, 2022; Wang *et al.*, 2022; Singh *et al.*, 2024). Hence, other forms of liquid sorbents, such as KOH and NaOH, have seen strong interest recently with demonstration and commercial plants currently in operation (Keith *et al.*, 2018; Fasihi, Efimova and Breyer, 2019; An, Farooqui and McCoy, 2022). The operations of liquid sorbent direct air capture by start-up company Carbon Engineering consist of two connected chemical cycles (Figure *2.2*). The first cycle (adsorption cycle) captures CO_2 from the atmosphere using an aqueous KOH sorbent. In the second cycle (regeneration cycle), carbonate ions (from K_2CO_3) are precipitated by reactions with $Ca(OH)_2$ to regenerate KOH and produce solid $CaCO_3$ simultaneously. The captured CO_2 and $Ca(OH)_2$ are then recovered from solid $CaCO_3$ by heating the $CaCO_3$ up to around 900 °C in a kiln (calciner unit) to release CO_2 and CaO. CO_2 is collected as a pure stream while the CaO is hydrated or "slaked" to produce $Ca(OH)_2$, thereby closing the second cycle.

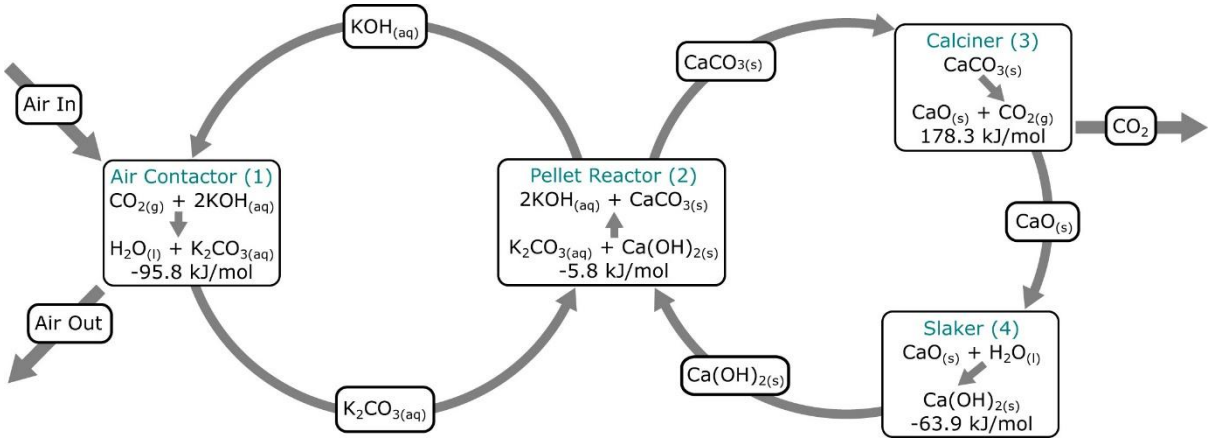

Figure 2.2: Carbon Engineering's liquid sorbent direct air capture operation principle, based on Keith et al. *(Keith* et al.*, 2018)*. Reprinted under the Creative Commons Attribution License (CC BY NC ND).

On the other hand, solid sorbent direct air capture technologies use solid sorbents to capture CO_2 from the atmosphere. Several solid sorbents have been used for direct air capture, ranging from pure physically-modified to chemically-modified sorbents, such as activated carbon, amine-modified silica, zeolites, and metallic organic frameworks (MOFs) (Sinha *et al.*, 2017; Deutz and Bardow, 2021; Jiang *et al.*, 2023; Bahmanzadegan and Ghaemi, 2024). Solid sorbents are usually modified, physically and chemically, to improve their performance, such as adsorption rates, corrosion effect and amine stability. For example, different amines were reported to improve the adsorption rates of amine-modified zeolites and MOFs, up to 7 mol CO_2/kg sorbent (Lin *et al.*, 2013; Sinha *et al.*, 2017; Bahmanzadegan, Pordsari and Ghaemi, 2023). Amine-modified sorbents have also seen great interest by several start-ups, including Climeworks (Climeworks, no date) and Hydrocell (An *et al.*, 2023), which operate demonstration and commercial plants at Technology Readiness Level 6–9, with solid sorbents functioning as their desired direct air capture sorbents. Generally, amine-modified zeolite and silica materials are frequently favoured for their low cost and high adsorption rates, while amine-modified MOFs are often considered in direct air capture applications for their durability and high adsorption rates (Sinha *et al.*, 2017; Jiang *et al.*, 2023; Bahmanzadegan and Ghaemi, 2024). In solid sorbent direct air capture, the sorbents contained in monoliths capture the CO_2 from the air and the CO_2-depleted air is released back into the atmosphere. The sorbent is then regenerated based on pressure, vacuum, pressure-vacuum, temperature, electric, temperature vacuum or hybrid swing adsorption processes (Sinha *et al.*, 2017; Jiang *et al.*, 2023; Bouaboula *et al.*, 2024). A widely used regeneration method is the temperature vacuum swing adsorption (Figure *2.3*) described by Sinha et al. (Sinha *et al.*, 2017), which has five key steps that are used in sorbent regeneration, to manage the oxidation of the amines at high temperatures by limiting the temperature and oxygen concentration in the monolith channels (Sinha *et al.*, 2017). These steps are 1) Adsorption: Air is passed through the channel at ambient conditions for CO_2 capture by the sorbents, 2) Evacuation: CO_2-depleted air is evacuated from the channel at the end of the adsorption step, since it contains oxygen. This is achieved by sealing the channel's front end ($z = 0$) and evacuating it at the rear end ($z = L$) with the aid of a vacuum pump. 3) Pressurisation: The channel is pressurised to 1 atm to prevent the backflow of air (oxygen) from the rear end ($z = L$) of the channel. 4) Desorption: The rear end ($z = L$) of the channel is opened and saturated steam at 1 atm is passed into the channel from the front end ($z = 0$) to desorb CO_2 by temperature swing and 5) Cooling: The system temperature is cooled after evacuating the rich-CO_2 mixture and prior to feeding air containing oxygen (Step 1) to prevent oxidation of amines (Sinha *et al.*, 2017). Generally, in the regeneration processes of solid sorbents, steam is passed through the monolith channels during the adsorption and desorption cycle to release the CO_2 in the sorbent.

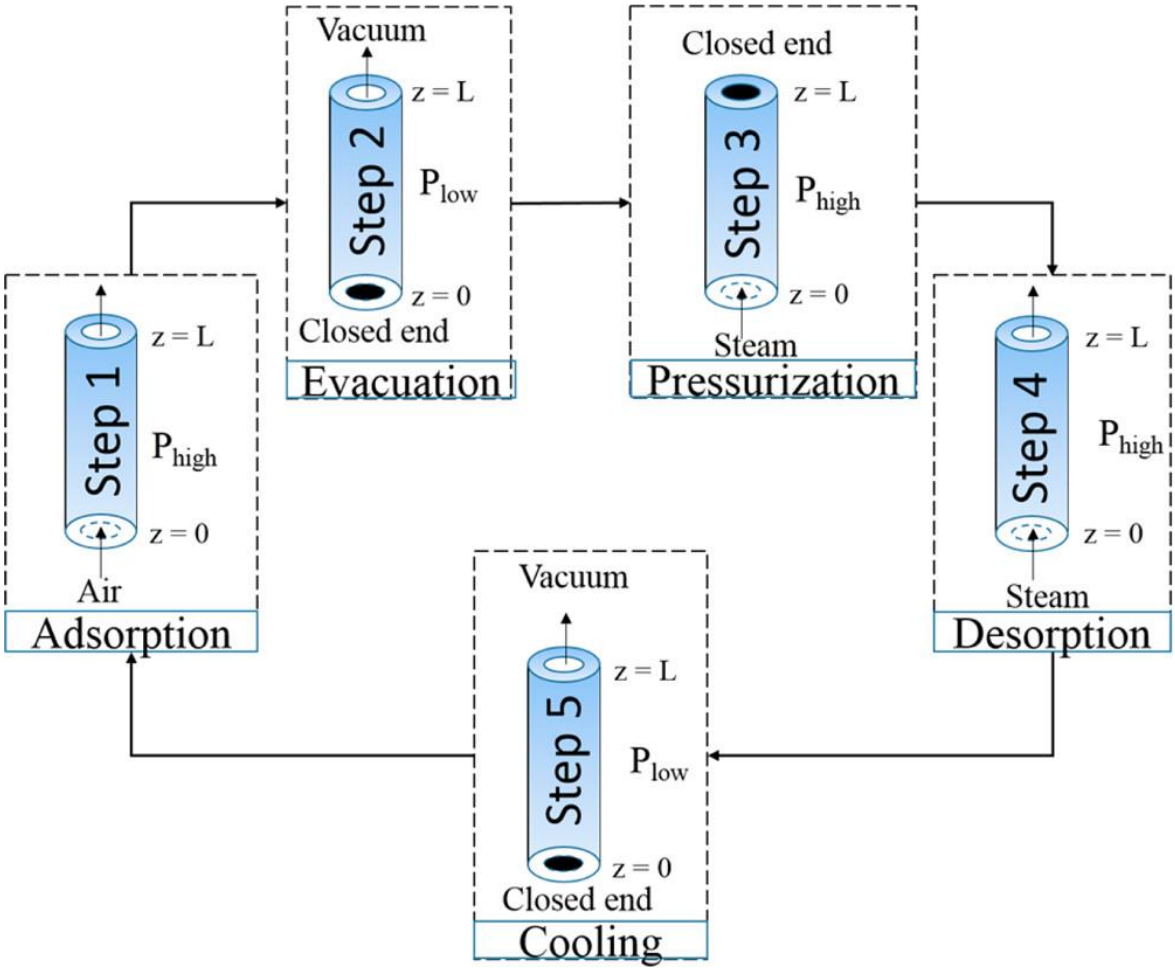

Figure 2.3: The overview of temperature vacuum swing adsorption by Sinha et al. *(Sinha* et al.*, 2017)*. Reprinted with permission from *(Sinha* et al.*, 2017)*. Copyright 2017 American Chemical Society.

2.2.2 Liquid synthetic fuels and chemicals production technologies

2.2.2.1 Ammonia production

Ammonia is produced via nitrogen hydrogenation, mainly the Haber-Bosch process, as shown in Equation (2.3). The Haber-Bosch process is well-matured, at Technology Readiness Level 9, while a modified Haber-Bosch process using e-H_2 is at Technology Readiness Level 7–9 (Sterner *et al.*, 2024). The Haber-Bosch thermochemical process is an exothermic process that occurs at high pressure (100–1000 bar) and elevated temperatures (400–550°C) in the presence of a catalyst (Concawe and Aramco, 2024). It is the most widely used method for ammonia synthesis, accounting for almost all ammonia produced currently. Other options that have found interest recently include the electrochemical-driven Haber-Bosch process (Hochman *et al.*, 2020; Liu, Elgowainy and Wang, 2020). Ammonia is a base chemical in manufacturing industries, such as the fertiliser industry, where it has found most of its current utilisation. It can also be used directly as a transport fuel. However, its combustion poses some technical challenges, such as the slow combustion rate (Erdemir and Dincer, 2021; Tornatore *et al.*, 2022) and nitrous oxides emissions (Pedersen *et al.*, 2023), which can result in issues like lower engine performance, ammonia slip, and higher greenhouse gas emissions. In the future, these issues are expected to be resolved as ongoing research has shown promising development. Ammonia is toxic and corrosive, which can be a potential issue, especially in the event of an ammonia leak. Because of these issues, ammonia's use as a transport fuel is often limited to ship transportation.

Ammonia synthesis: $N_2 + 3\ H_2 \leftrightarrow 2\ NH_3$ $\Delta H = -92\ kJ/mol$ (2.3)

2.2.2.2 Methanol production

Methanol can be produced via CO_2 hydrogenation, as shown in Equation (2.4). CO_2 hydrogenation to methanol is typically done at 200–300 °C and 10–100 bar in the presence of a catalyst (e.g., Cu-based catalyst). Synthetic methanol production is currently at Technology Readiness Level 8–9, with some commercial plants in operation (European Energy, no date; Concawe and Aramco, 2024; Sterner *et al.*, 2024). Methanol is an important industrial feedstock for producing a wide range of products, e.g., plastic and hydrocarbon fuel. Due to its high-octane rating of 114, it can also be used directly as a transport fuel in blended ratios with other fuels and in unblended form (Methanol Institute, no date).

Methanol synthesis: $CO_2 + 3\ H_2 \leftrightarrow CH_3OH + H_2O$ $\Delta H = -49.4\ kJ/mol$ (2.4)

2.2.2.3 Methanol-to-gasoline and methanol-to-kerosene

Synthetic gasoline and kerosene can be produced via methanol hydrogenation to olefins and their subsequent oligomerisation (Dimitriou, 2013; Concawe and Aramco, 2024), as shown in Equations (2.5)–(2.7). Methanol-to-gasoline, first developed by Mobil, utilises a multistage process to convert methanol into gasoline at 300–400°C and 15–20 bar in the presence of a zeolite catalyst. Methanol-to-gasoline is at Technology Readiness Level 6–9 (ExxonMobil, no date; Breuer *et al.*, 2022). Methanol-to-kerosene operates similarly to methanol-to-gasoline; however, it is not well-developed and commercially proven like methanol-to-gasoline (Dimitriou, 2013; Concawe and Aramco, 2024). Synthetic gasoline and kerosene can be used directly in existing combustion engines without the need for fuel blending or costly engine modifications (Concawe and Aramco, 2024).

Dimethyl ether synthesis: $2n\ CH_3OH \leftrightarrow n\ CH_3OCH_3 + n\ H_2O$ $\Delta H = -10\ kJ/mol$ (2.5)

Olefin oligomerisation: $n\ CH_3OCH_3 \rightarrow 2\ (CH_2)_n, olefins + n\ H_2O$ $\Delta H = -18.7\ kJ/mol$ (2.6)

Hydrocarbon synthesis: $2\ (CH_2)_{n,olefins} \rightarrow C_{2n}H_{4n,hydrocarbons}$ $\Delta H = -16\ kJ/mol$ (2.7)

2.2.2.4 Fischer-Tropsch synthesis

Fischer-Tropsch synthesis can be used to hydrogenate CO_2 (that is reduced to CO) into hydrocarbons. By converting CO_2 to CO using reverse water-gas shift reactions and subsequently converting CO to hydrocarbons using Fischer-Tropsch reactions, synthetic "drop-in" fuels are produced from CO_2. Fischer-Tropsch reactions are typically carried out at a pressure of 20–40 bar and a temperature of 200–350 °C, depending on the desired product, as the product distribution is heavily influenced by temperature and catalyst (Dimitriou, 2013; Concawe and Aramco, 2024). The overall Fischer-Tropsch synthesis reaction is shown in Equation (2.8) (Dimitriou, 2013; Concawe and Aramco, 2024). Currently, Fischer-Tropsch synthesis is at Technology Readiness Level 6–9 (Concawe and Aramco, 2024; Paulsen *et al.*, 2024). Additionally, Chapter 3 provides more information on synthetic fuels production.

FTS: $n\ CO + (2n+1)\ H_2 \rightarrow H(CH_2)_nH + n\ H_2O$ $\Delta H = -152\ kJ/mol$ (2.8)

2.3 Techno-economic assessment

Techno-economic assessments assess the technical and economic performances of industrial plants, processes or products (Zimmermann *et al.*, 2020) and are widely used to assess the technical requirements, capital, operating, revenue, and product costs associated with full system designs and scale-up technologies. Generally, techno-economic assessment commences at a Technology Readiness Level 3, denoting technical proof of concept, and undergoes modifications until reaching

the early commercialisation stage of Technology Readiness Level 9 (Humbird, 2018; Rodgers, 2024). Techno-economic assessment results can be significantly affected by Technology Readiness Level and techno-economic assessment methodologies, with expected cost variations of up to 100% (Green, 2007; Feng and Rangaiah, 2011; AACE International, 2020; Rodgers, 2024). Techno-economic assessment data are crucial as they provide preliminary insights that inform the design, construction, and operation of successful production plants. Additionally, techno-economic assessment supports stakeholders (including policymakers) by identifying opportunities to select the most economical process that will significantly impact production and competitiveness. Generally, the methods for techno-economic assessments include mass and energy balance analysis and cost analysis.

2.3.1 Technical (mass and energy balance) analysis

Mass and energy balance analysis is typically conducted using process modelling, where original plant data are generated, or by using data from previous literature, including process models, experimental rigs, pilot plants and commercial plants. Process modelling is a technique used in chemical engineering to design and simulate processes. These simulations are typically performed using commercial software, such as Aspen HSYSY or CHEMCAD (Rodgers, 2024). The technical data, especially mass and energy balance, used in techno-economic assessments typically originates from process modelling. Hence, this has led to the widespread applications of process modelling tools in process plant design.

2.3.2 Economic analysis

Economic or cost analysis of processes and products is often based on the assessment of capital costs, operating costs, and investment parameters (such as discount rates and tax rates). Cost modelling analysis generates performance metrics, such as cash flow, net present value and product price.

Capital costs are typically based on the total equipment cost and other project cost components, such as contingency, Outside Battery Limit (OSBL), and working capital. Generally, in the literature, capital costs of new technologies are usually obtained using data from process modelling and equipment cost correlation equations and charts. This approach is used because it is somewhat difficult and unrealistic to obtain exact equipment costs, especially for equipment that has not been built. Other methods for estimating capital costs include rapid cost estimation methods, which scale original equipment or overall plant costs using proposed design capacities, scaling factors, and historical costs, e.g., as shown in Equation (2.9). Consequently, total capital costs obtained using various methodologies often differ significantly, with up to a 100% difference (Green, 2007; Feng and Rangaiah, 2011; Rodgers, 2024).

$$Scaled\ equipment\ cost\ = Cost\ at\ original\ scale\ \times \frac{Scale\ up\ capacity^{n}}{Original\ capacity} \qquad (2.9)$$

Operating costs, including fixed and variable types, are generally estimated using capital and market costs. This is due to the fact that annual operating costs are often smaller compared to the capital costs of commercial-scale plants. Furthermore, fixed operating costs, such as labour expenses, can be directly estimated through design and operational procedures, as well as the market cost of labour (Green, 2007; Rodgers *et al.*, 2022). The costs of materials and energy can be obtained from the market and market forecasts (Snowden-Swan *et al.*, 2017; Rodgers *et al.*, 2022; DESNZ, 2023b).

Generally, product prices are often determined using the minimum selling price and the levelised cost approaches. The minimum selling price, also known as the break-even price, is the selling price of a product or process at the plant gate or market that makes the project's net present value (NPV) equal to zero over the plant life [Equation (2.10)]. The minimum selling price approach is often used for final products that go into consumer markets, e.g., fuels and chemicals, and could include downstream costs such as taxes, product transportation costs and retailers' margins. On the other hand, the

levelised cost of a product or process is the discounted lifetime cost of constructing and operating a process plant or producing a product [Equation (2.11)]. The levelised cost approach is often used for intermediate industrial products and processes, such as renewable electricity, H_2 and CO_2. The levelised cost does not often account for downstream cost factors, such as taxes, product transportation and retailers' margins, which can be key in determining a project's profitability.

$$Selling\ price\ subject\ to\ NPV = \sum \frac{net\ cash\ flow}{(1+discount)^{years}} = 0 \quad (2.10)$$

$$Levelised\ cost\ = \frac{\sum \frac{annual\ cost}{(1+discount\ rate)^{years}}}{\sum \frac{annual\ production\ rate}{(1+discount\ rate)^{years}}} \quad (2.11)$$

2.3.3 Techno-economic assessment studies of synthetic fuels and chemicals

Numerous studies have examined the economics of synthetic fuels and chemicals, as shown in Table 2.2. However, despite these numerous assessments, the costs of these technologies are currently high. The prices of synthetic fuels and chemicals technologies from various production approaches, including biomass-to-liquids, direct air capture, power-to-X and blue fuels, were estimated to range from \$0.6–10.0 per diesel litre equivalent (and \$100–400 per tCO_2 captured gross for CO_2) [Table 2.2]. According to the various authors in Table 2.2, several factors can significantly influence the prices of synthetic fuels and chemicals technologies, including (a) Design factors, such as feedstock types, plant scale and capacity factors (b) operational factors, such as transport distances, feedstock sources and energy sources and (c) economic factors, such as capital expenses, transportation cost, energy costs, tax rate and discount rates. Some authors estimate that the cost of these technologies could decrease significantly by 2050, to \$40–130 per tonne CO_2 captured for CO_2 and \$0.7–2.2 per litre diesel equivalent for fuels. However, these costs are still expensive for some key synthetic fuel and chemical options, e.g., H_2 derivatives. Additionally, some of the methodologies used in these estimates, especially those presenting capture costs of less than \$40 per tonne of CO_2 captured, are often based on learning-by-doing. These underscore the importance of understanding design parameters and strategies that have the greatest impact on synthetic fuels and chemicals technologies, enabling targeted research and development to facilitate cost reduction and promote the broader deployment of synthetic fuels and chemicals. Furthermore, many studies do not assess the impacts of key design, operational and economic factors, such as novel production approaches, location factors and transportation costs, which could significantly impact the costs of synthetic fuels and chemicals technologies. Hence, it is crucial to understand and mitigate the impacts of critical factors in synthetic fuels and chemicals supply chains using comprehensive economic assessment approaches. Table 2.2 summarises the costs of synthetic fuels and chemicals from key sources as found in the literature.

Table 2.2: Summary of some important economic studies on synthetic fuels and chemicals.

Source	**Product**	**Technique**	**Plant type**	**Levelised or minimum selling price) [$\$_{2021}$/l diesel equiv. for fuel or $\$_{2021}/tCO_2$ for CO_2]**
(Michailos, Parker and Webb, 2017)	Advanced biofuels	▪ Feed input of 2200 t/d cane bagasse ▪ Gasification with FTS	Commercial	0.61
	Advanced biofuels	▪ Feed input of 2200 t/d cane bagasse ▪ Fast pyrolysis with upgrading	Commercial	0.66

Source	Product	Technique	Plant type	Levelised or minimum selling price) [$2021/l diesel equiv. for fuel or $2021/tCO2 for CO2]
(Li, Zhang and Hu, 2015)	Advanced biofuels	▪ Feed input of 2000 t/d biomass/bio-oil ▪ Fast pyrolysis, bio-oil gasification and FTS	Commercial: nth	1.66
(Zhu and Valkenburg, 2011)	Advanced biofuels	▪ Feed input of 2200 t/d wood chips ▪ Gasification with FTS ▪ Different gasifier heating scenarios considered	Commercial: nth	1.42–1.64
	Advanced biofuels	▪ Feed input of 2200 t/d wood chips ▪ Gasification, methanol conversion and MTG ▪ Different gasifier heating scenarios considered	Commercial: nth	1.08–1.37
	Advanced biofuels	▪ Feed input of 2200 t/d wood chips ▪ Fast pyrolysis with upgrading ▪ Different gasifier heating scenarios considered	Commercial: nth	0.84
(Swanson *et al.*, 2010)	Advanced biofuels	▪ Feed input of 2000 t/d corn stover ▪ Gasification with FTS ▪ Two scenarios were considered-low and high temp. gasification, ▪ Nth and first-of-its-kind plant	Commercial: nth	1.56–1.72
	Advanced biofuels		Commercial: first-of-a-kind	2.74–2.93
(Carrasco *et al.*, 2017)	Advanced biofuels	▪ Feed input of 2000 t/d forest residues ▪ Fast pyrolysis with upgrading ▪ Laboratory demonstration and TEA of liquid fuels from forest residue via pyrolysis	Commercial: first-of-a-kind	1.85
(Tanzer *et al.*, 2019)	Advanced biofuels	▪ Feed input of 500 t/d various agricultural residues ▪ Gasification with FTS	Commercial: first-of-a-kind	1.90–3.88
	Advanced biofuels	▪ Feed input of 500 t/d various agricultural residues ▪ Fast pyrolysis with upgrading	Commercial: first-of-a-kind	1.61–3.35
	Advanced biofuels	▪ Feed input of 500 t/d various agricultural residues ▪ HTL with upgrading	Commercial: first-of-a-kind	1.50–4.27
(Dimitriou, Goldingay and Bridgwater, 2018)	Advanced biofuels	▪ Feed input of 2000 t/d woody biomass ▪ Gasification with FTS ▪ Various BTL pathways	Commercial	0.82–0.84
	Advanced biofuels	▪ Feed input of 2000 t/d woody biomass ▪ Gasification, methanol conversion and MTG ▪ Various BTL pathways	Commercial	1.08–1.19

Source	Product	Technique	Plant type	Levelised or minimum selling price) [$$_{2021}$/l diesel equiv. for fuel or $$_{2021}$/t$CO_2$ for CO_2]
	Advanced biofuels	▪ Feed input of 2000 t/d woody biomass ▪ Gasification, TIGAS ▪ Various BTL pathways	Commercial	0.90–0.92
(Rahbari *et al.*, 2019)	Advanced biofuels	▪ Feed input of 16000 t/y algae ▪ SCWG with FTS ▪ Solar-driven SCWG-reforming and FTS	Commercial: nth	2.69
(Campanario and Gutiérrez Ortiz, 2017)	Advanced biofuels	▪ Feed input of 60 t/h bio-oil aqueous phase ▪ SCWG with FTS	Commercial	1.08
(Zhu *et al.*, 2014)	Advanced biofuels	▪ Feed input of 2000 t/d woody biomass ▪ HTL with upgrading ▪ Nth and first-of-its-kind plant	Commercial: first-of-a-kind	1.60
	Synthetic biofuels		Commercial: nth	0.90
(Pedersen *et al.*, 2018)	Advanced biofuels	▪ Feed input of 1000 t/d organic matter ▪ HTL with upgrading ▪ Heat integration of model using pinch analysis	Commercial	0.90–1.23
(Tews *et al.*, 2014)	Advanced biofuels	▪ Feed input of 2000 t/d forest residue ▪ HTL with upgrading ▪ Comparative studies of fast pyrolysis and HTL	Commercial: nth	0.60
(Jones *et al.*, 2014)	Advanced biofuels	▪ Feed input of 1349 t/d algae ▪ HTL with upgrading	Commercial: nth	1.40
(An, Farooqui and McCoy, 2022)	Direct air capture CO_2	▪ Liquid sorbent (potassium hydroxide) direct air capture with a capacity of 1 Mtpa of CO_2 captured ▪ Capital cost based on Carbon Engineering estimates ▪ Primary energy source: Natural gas with flue gas capture or grid electricity	Commercial	240–440
(Keith *et al.*, 2018)	Direct air capture CO_2	▪ Liquid sorbent (potassium hydroxide) direct air capture with a capacity of 1 Mtpa of CO_2 captured ▪ Capital cost for Carbon Engineering plants ▪ Primary energy source: Natural gas or Natural gas with grid electricity	Commercial	100–250
(McQueen *et al.*, 2020)	Direct air capture CO_2	▪ Generic solid sorbent direct air capture with a capacity of 100 ktCO_2/year	Commercial	220–250

Source	Product	Technique	Plant type	Levelised or minimum selling price) [$2021/l diesel equiv. for fuel or $2021/tCO2 for CO2]
		▪ Primary energy source: Natural gas, waste heat from geothermal, or slip steam from nuclear		
(Fasihi, Efimova and Breyer, 2019)	Direct air capture CO_2	▪ Generic solid and liquid sorbents direct air capture, with large-scale CO_2 systems ▪ Heavy use of learning rates to estimate future capital cost ▪ Primary energy sources include wind power, solar power, hybrid PV-Wind-battery plants and heat pumps, and waste heat	Commercial	40–270
(Sievert, Schmidt and Steffen, 2024)	Direct air capture CO_2	▪ Generic solid and liquid sorbents direct air capture, with large-scale CO_2 systems ▪ Heavy use of learning rates to estimate future capital cost ▪ Primary energy sources include solar PV with storage for electricity and natural gas for heat, as well as electricity from geothermal and nuclear power plants	Commercial	226–835
(Franco *et al.*, 2021)	e-H_2	▪ Electrolysers: Generic electrolysers with capacity of 100 MW ▪ Fuels: H_2 using CH2, LH2 and LOHC ▪ Different timeline 2020–2050. ▪ Electricity source: Renewable electricity scenarios ▪ No information on renewable electricity location factors ▪ Short delivery distances	Commercial	1.7–2.3
(BEIS, 2021)	e-H_2 and blue H_2	▪ Electrolysers: Alkaline, polymer, solid oxide electrolysers ▪ Fuels: H_2 ▪ Timeline: 2020 to 2050. ▪ Electricity source: Renewable and grid electricity scenarios ▪ No information on renewable electricity location factors ▪ Short delivery distances	Commercial	0.7–3.0
(Concawe and Aramco, 2024)	e-H_2, e-methane, e-methanol, e-NH_3, OME_x, e-gasoline, e-diesel and e-kerosene	▪ Electrolysers: Alkaline and solid oxide electrolysers ▪ Fuels: H_2, methane, methanol, NH_3, OME_x, gasoline, diesel and kerosene ▪ Timeline: 2020–2050	Commercial	1.4-4.5

Source	Product	Technique	Plant type	Levelised or minimum selling price) [$$_{2021}$/l diesel equiv. for fuel or $$_{2021}$/tCO$_2$ for CO$_2$]
		▪ Electricity source: Renewable and grid electricity scenarios. Yearly resolutions on renewable electricity location factor. ▪ Long distance from Middle East to Europe		
(Giampieri, Ling-Chin and Roskilly, 2024)	e-H_2	▪ Electrolysers: Polymer electrolyte membrane electrolyser ▪ Fuels: H_2 using different H_2 states and carriers: CH2, LH2, NH_3 and MCH ▪ Timeline: 2020–2050 ▪ Electricity source: Renewable electricity scenarios, with capacities of 1320 MW. Hourly resolutions on renewable electricity of Hornsea Project Two (UK) ▪ Short delivery distances	Commercial	0.6–3.8
(Niermann *et al.*, 2021)	e-H_2	▪ Electrolysers: Polymer electrolyte membrane electrolysers ▪ Fuels: H_2 using different H2 states and carriers (CH2, LH2, dibenzyltoluene, toluene and methanol). Capacity of 182,500 t/a. ▪ Timeline: 2020. ▪ Electricity source: Renewable electricity scenarios. Yearly resolutions on renewable electricity from Algeria ▪ Long-distance supply chains (Algeria to Germany)	Commercial	3.2–5.5
(Raab and Dietrich, 2023)	e-LH2, e-methane, e-SAF	▪ Electrolysers: Alkaline electrolysers ▪ Fuels: LH2, synthetic natural gas, SAF (225 kt_{H_2}/a) ▪ Timeline: 2020 ▪ Electricity source: Renewable and grid electricity scenarios. Yearly resolutions on renewable electricity from Morocco ▪ Long-distance supply chains (Morocco to Germany)	Commercial	1.8–3.5
(Martin, Neumann and Ødegård, 2023)	e-H_2, e-NH_3, e-FT-liquids	▪ Electrolysers: Generic electrolysers ▪ Fuels: H_2, NH_3, FT-liquids ▪ Timeline: 2020–2050 ▪ Electricity source: Renewable electricity scenarios. No details	Commercial	0.9–5

Source	Product	Technique	Plant type	Levelised or minimum selling price) [$$_{2021}$/l diesel equiv. for fuel or $$_{2021}$/tCO$_2$ for CO$_2$]
		on renewable electricity location factors ▪ No details on distance of supply chains		
(Peacock *et al.*, 2023)	e-FT-liquids	▪ Electrolysers: Polymer and solid oxide electrolysers ▪ Fuel: FT-liquids. Plant capacity of 1 Mt/a CO_2 captured ▪ Timeline: 2020–2050 ▪ Electricity source: Renewable electricity and nuclear scenarios. No details on renewable electricity location factors ▪ No details on distance of supply chains	Commercial	1.5–8.6
(Nizami, Slamet and Purwanto, 2022)	e-H_2 and e-methanol	▪ Electrolysers: Polymer electrolyte membrane electrolysers ▪ Fuel: H_2 and methanol ▪ Timeline: 2020–2050 ▪ Electricity source: Renewable and grid electricity scenarios (1,000 MW). Hourly resolution details on renewable electricity location factors ▪ Cradle-to-gate analysis (downstream supply chain not considered)	Commercial	1.5–3.1
Key for processes: BTL for biomass-to-liquids, FTS for Fischer-Tropsch synthesis, HTL for hydrothermal liquefaction, MTG for methanol-to-gasoline, SCWG for supercritical water gasification, TIGAS for Topsøe Improved Gasoline Synthesis, PV for photovoltaics. Key for products: CH2 for compressed H_2, LH2 for liquefied H_2, LPG for liquified petroleum gas, SAF for sustainable aviation fuels, FT-liquid for Fischer-Tropsch liquids, OME_x for polyoxymethylene dimethyl ethers.				

2.4 Life cycle assessment

Life cycle assessment is an assessment technique used to evaluate the environmental impacts associated with all the stages of a product's or service's life, including upstream processes, such as raw material extraction, to downstream processes, such as waste disposal (Sphera, 2020). It has been crucial in assessing the environmental impact and sustainability of emerging technologies, as well as reviewing and improving the environmental impact and sustainability of existing processes. Life cycle assessment covers all relevant inputs from the environment and outputs (e.g., raw materials and products emissions) (Muthu, 2020a). It can measure a list of impacts on the environment, such as global warming potential (GWP), abiotic depletion (ADP), ozone layer depletion potential (ODP), eutrophication potential (EP), acidification potential (AP), and human toxicity potential (HTP) (Muthu, 2020b). The International Organisation for Standardisation (ISO) provides principles for performing a life cycle assessment through ISO 14 040 and 14 044. These principles divide the process of life cycle assessment into four stages, namely; (i) Goal and scope definition, which defines the object, aim, and

scope of the analysis, including functional units of the analysis; (ii) Inventory analysis, which contains data analysis of all the relevant resource, energy consumption, or emissions of the process or product to the environment; (iii) Impact assessment, which analyses the impacts of the data obtained from the inventory analysis in terms of environmental burdens or impacts such as carbon and water footprints; (iv) Interpretation stage where the results of the analysis are evaluated and interpreted into useful information (Arvanitoyannis, 2008; H. Scott Matthews, Chris T. Hendrickson and Deanna Matthews, 2014; Reijnders, 2021). These processes are interrelated, as shown in Figure 2.4.

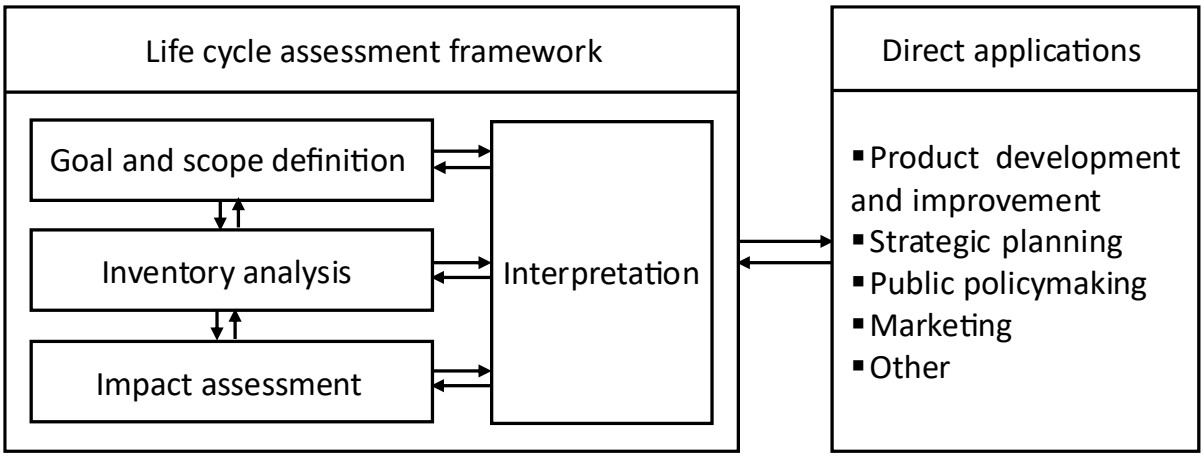

Figure 2.4: Overview of the International Organisation for Standardisation (ISO) life cycle assessment framework (ISO, 2006b, 2006a; H. Scott Matthews, Chris T. Hendrickson and Deanna Matthews, 2014).

2.4.1 Forms of life cycle assessment

Life cycle assessments can be carried out in various forms, and thus, they can be classified by several criteria, such as by boundary conditions into cradle-to-grave, cradle-to-gate, cradle-to-cradle, gate-to-gate, and well-to-wheel; by emissions allocation into attributional and consequential life cycle assessments; and by time horizons into conventional and prospective life cycle assessments.

2.4.2 Boundary types in life cycle assessment

By boundary conditions, life cycle assessments can be classified into i) Cradle-to-grave: a full life cycle assessment that includes all the stages of a product, process, or service life; ii) Cradle-to-gate: a partial life cycle assessment of a product which covers the stages from raw material extraction to the production, manufacturing, and packaging processes; iii) Cradle-to-cradle: a special type of cradle-to-grave assessment, where the end-of-life disposal step for the product is a recycling process; iv) Gate-to-gate: a partial life cycle assessment looking at only one value-added process in the entire production chain; (v) Well-to-wheel: a specific life cycle assessment used to evaluate the production and use of transport fuels, which covers the emissions associated with the production and use of fuels from the well or raw material origin to the fuel used in vehicles, and this may sometimes exclude embodied emissions of infrastructures (such as vehicles) depending on the study's methods.

Depending on the boundary set for life cycle assessment, life cycle emissions can differ substantially. For example, the UK BEIS reported that the emissions from renewable electricity and blue H_2 supply chains in 2020 could change from 0–25 gCO_2e/MJ to 2–50 gCO_2e/MJ when the boundary changed from the plant gate (well-to-gate) to the product user (well-to-wheel) (BEIS, E4tech and LBST, 2021). This highlights the need to define the boundaries of life cycle assessments clearly.

2.4.3 Emission allocation

2.4.3.1 Attributional and consequential life cycle assessment

The methods for performing life cycle assessments can be classified into attributional and consequential life cycle assessments. In attributional life cycle assessment, the impact of emissions directly associated with a process or product over its life cycle is analysed. In contrast, consequential life cycle assessment analyses the emissions impacts that are directly and indirectly associated with using a process or product. Usually, attributional life cycle assessment allocates an estimate of the share of global environmental burdens to a process or product, while consequential life cycle assessment allocates an estimate of how a process or product impacts the global environmental burdens (Ekvall, 2019). These different methodologies can significantly impact the results of life cycle assessments (Searchinger *et al.*, 2008; Kolosz *et al.*, 2020; Fernanda Rojas Michaga *et al.*, 2022). This is because attributional life cycle assessment analyses the emissions impact directly associated with a process or product, while consequential life cycle assessment analyses the direct and indirect emissions associated with using a process or product. The direct impacts of a product or process could include land use change, crop cultivation, process catalyst, and electricity consumption emission factors. Meanwhile, the indirect emissions from a product or process could encompass indirect land use change, avoided landfill emissions, foregone energy benefits, and foregone fertiliser benefits. Often, attributional life cycle assessment is a subset of consequential life cycle assessment, as shown in Figure 2.5. A more detailed attributional life cycle assessment that includes land use change and consequential life cycle assessment is typically undertaken when there is a strong potential competition for resources or for the product itself with other existing or emerging supply chains, e.g., the use of biomass resources, which could serve as feedstocks for synthetic fuels and chemicals synthesis. Consequently, many government documents, such as the UK Biomass Strategy (DESNZ, 2023a) and EU derivatives (European Union, 2018), require that emissions associated with land use change and indirect land use change are accounted for in biofuels applications. Currently, there is no regulation on emissions from the use of biomass as a starting feedstock for chemical production in manufacturing sectors and downstream-related applications.

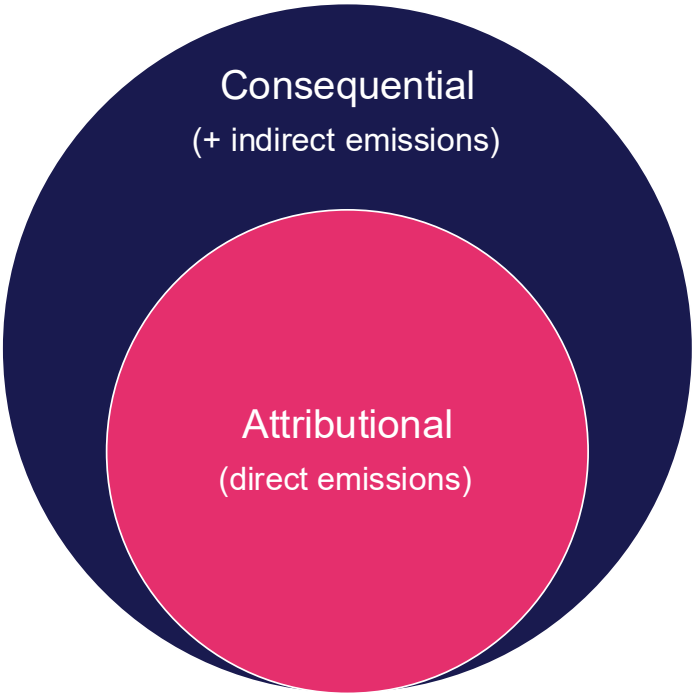

Figure 2.5: The scope of attributional and consequential life cycle assessments.

Generally, the use of biomass resources for biofuel production is often associated with competing applications, such as food, paper, furniture and digestate production. Hence, some studies on this subject have often assessed the impacts of diverting food-based biomass (such as corn and sugarcane) and land resources for biofuels production (Searchinger *et al.*, 2008; Plevin *et al.*, 2010; Valin *et al.*, 2015). According to Searchinger et al. (Searchinger *et al.*, 2008), when accounting for the impact of land use change in corn cultivation, the greenhouse gas emissions of corn-based ethanol could double over 30 years, rather than achieving the initially estimated 20% savings without land use change. Although other studies have published smaller estimates for the land use change effect of corn ethanol, the greenhouse gas emissions impact of land use change is generally non-trivial. In addition to land use change and indirect land use change being one of the most uncertain components in greenhouse gas emissions estimation of biofuels (Plevin *et al.*, 2010), the availability of biomass resources and the methods used to obtain biomass feedstocks play important roles in the sustainability of biofuels. Hence, second- to fourth-generation biofuels and biochemicals rely on using non-food biomass to avoid many of the issues associated with direct and indirect land use change. Non-food biomass, which includes lignocellulosic biomass and waste biomass, typically has zero land use change emissions, especially for residues and wastes. Additionally, using non-food biomass resources such as agricultural residues, wood wastes and municipal wastes avoids indirect land use change emissions and the competition of biofuel with food. However, the utilisation of non-food biomass for drop-in biofuel may come with other consequential indirect emissions, which may arise from diverting these materials from existing streams (Ou *et al.*, 2022). These consequential emissions may vary significantly across different supply chains and can be positive or negative, depending on competing applications, such as diverting food waste from landfilling or anaerobic digestion. Therefore, understanding the key consequential emissions impacts of using biomass in biofuel applications is crucial for realising the benefits of biofuels and other biomass-related technologies.

2.4.3.2 Physical, economic and system expansion

Furthermore, whether attributional or consequential life cycle assessment methods are used, emissions are allocated to co-products when they exist in a product or process life cycle. Allocation methods are utilised to share the emission impacts of a process when it generates multiple outputs (co-products). Generally, the three primary types of allocation methods are physical, economic and system expansion. Physical allocation is based on sharing emission impacts among co-products using physical parameters, such as mass, energy, or volume. Economic allocation shares emission impacts among co-products using their relative market value or price. While system expansion employs a consequential life cycle assessment approach to allocate emissions to co-products by expanding the system boundaries to consider the impacts of the co-products on the entire system (the global environment). Because physical and economic allocations can be highly subjective, as they depend on factors such as product yield, mass, and price, which can change significantly over time, geography and technology. Additionally, physical and economic parameters, such as energy, mass, and price, may not be directly available for certain co-products in a process. System expansion is typically recommended for allocating emissions to co-products over physical and economic allocations in many standards, including ISO 14 040 and 140 44 and the EU Product Environmental Footprint (ISO, 2006b, 2006a; European Commission, 2018). Nevertheless, the emissions from synthetic fuels and chemicals can vary significantly depending on the allocation method (Jong *et al.*, 2017; Kolosz *et al.*, 2020).

2.4.4 Time horizons: Conventional and prospective life cycle assessments

By time horizons, life cycle assessments can be classified into conventional and prospective life cycle assessments. Conventional life cycle assessments analyse the environmental impacts of a product or process based on existing technologies and practices, while prospective life cycle assessments analyse

the potential future environmental impacts of technologies and practices, considering the changes that may occur over time. Conventional life cycle assessments offer insight into the environmental impacts of a product or process using current technologies, and are particularly important for regulatory and compliance purposes, such as meeting emission limits set by the EU's RED and the UK's RTFO. On the other hand, prospective life cycle assessments are crucial for evaluating emissions performance for both emerging and existing technologies over time, especially those whose design and operational factors may change significantly over time. Prospective life cycle assessments can be utilised to reduce the emissions of products or processes over time, or where the mass and energy balance and emission factors are not widely known or anticipated to change significantly over time.

Generally, the emissions estimates for prospective life cycle assessments are often aimed to be lower than those of conventional life cycle assessments, due to the drive for emission reductions and other process improvements. These targets or reductions in emissions could be driven by many factors, including market forces (e.g., cost of raw material and consumer preferences), organisation goals and regulatory requirements (e.g., (European Union, 2019; CARB, 2020)). Although sometimes, emissions reductions are not achieved in all emissions impact categories for a product or process. For example, Zuiderveen et al. reported reductions in environmental impacts, such as greenhouse gas emissions and fossil depletion, of benzene, toluene and xylene from 2020 to 2050 and an increase in other environmental impacts, such as land occupation and water consumption (Zuiderveen *et al.*, 2024).

2.4.5 The functional unit and system boundary

The functional unit in life cycle assessment is the basis for assessing the quantity of a product or process over a specified boundary condition. The functional units used in assessing fuels and chemicals include kg (and its multiples) and MJ (and its multiples) (Hsu, 2012; Jong *et al.*, 2017; Concawe and Aramco, 2024). The functional unit chosen can significantly change the system boundary and the resolution of the results, e.g., the functional unit of MJ and MJ.km in transport fuel applications. Hence, the functional unit should be chosen carefully in order to address the needs of an assessment.

2.4.6 Life cycle assessment studies of synthetic fuels and chemicals

Currently, many life cycle assessment analyses have been done on the life cycle impacts of synthetic fuels and chemicals (Jong *et al.*, 2017; Vienescu *et al.*, 2018; Kolosz *et al.*, 2020; Concawe and Aramco, 2024), however, these studies are heavily focused on the global warming potential of fuels, neglecting other sustainability factors such as abiotic depletion and human toxicity potential. The global warming potential of fuels and chemicals enables easy comparison of fuels and chemicals with conventional petroleum fuels. The greenhouse gas emissions of fuels and chemicals from various sources are estimated to be as low as -122 gCO_2e per MJ to estimates exceeding 100 gCO_2e per MJ. This significant variation in emissions is due to factors such as feedstock types and associated land use change impacts, fuel and chemical processing techniques, product types, transformations for transport and storage, transportation modes and distances, and the form of fuel and dispensing method at the point of delivery to the user, and energy sources (Table 2.3). Also, the emissions may differ by life cycle assessment methodology, such as including or excluding embodied emissions from infrastructures (e.g., production equipment and transport vehicles), allocation methods employed to attribute impacts across multiple product outputs, and system boundary definitions. However, generally, when feedstock sources, especially biomass and electricity, are obtained sustainably with marginal emissions factors, the greenhouse gas emissions are usually significantly lower than those of petroleum fuels and chemicals, and in some cases, can even be negative in value. It is important to note that current policies in the EU and UK require that renewable fuels in transport applications achieve at least 65% greenhouse gas emissions savings (or 70% if they are of non-biological origins)

relative to fossil fuels (European Union, 2023a; DfT, 2024a). Additionally, the embodied emissions associated with biofuels and biochemicals may be significant (Concawe and Aramco, 2024), especially when international supply chains are involved. Hence, it is important to understand the impact of these factors on greenhouse gas emissions of synthetic fuels and chemicals supply chains.

Table 2.3: Summary of key life cycle assessment studies on synthetic fuels and chemicals.

Source	Techniques	LCA type	Metrics assessed	Greenhouse gas emissions (gCO_2e/MJ for fuel or tCO_2e/CO_2 captured for CO_2)	Product	Other comments
(Bennion *et al.*, 2015)	▪ Fuel path: HTL and pyrolysis of microalgae with hydroprocessing ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 MJ of diesel ▪ Allocation method: Energy	Attributional	GWP	-11.4 and 210	Advanced biofuels (biodiesel)	▪ Fuel emissions for HTL and pyrolysis routes, respectively ▪ HTL had lower fuel emissions ▪ Major GHG emissions driver: Drying of microalgae feedstock
(Vienescu *et al.*, 2018)	▪ Fuel path: Pyrolysis of corn stover and oil upgrading using various approaches ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 kg of biofuel ▪ Allocation method: Energy	Attributional	GWP	53.3−142.9	Advanced biofuels	▪ Fuel emissions of bio-oil hydroprocessing were the best, in comparison to other upgrading approaches ▪ Major GHG emissions driver: Electricity for energy demand
(Snowden-Swan and Male, 2012)	▪ Fuel path: Pyrolysis and hydroprocessing of woody biomass using various energy sources ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 MJ of gasoline ▪ Allocation method: Energy	Attributional	GWP	31.5−36.8	Advanced biofuels (bio-gasoline)	▪ Fuel emissions from biomass power are lower than grid power ▪ Major GHG emissions driver: Power and natural gas usage
(Ou *et al.*, 2022)	▪ Fuel path: HTL and hydroprocessing of swine manure ▪ Boundaries: Well-to-Wheels ▪ FU: 1 MJ of liquid fuels ▪ Allocation method: Energy	Consequential	GWP	-33.3	Advanced biofuels	▪ Major GHG emissions driver: Avoided emissions from the current treatment method and fuel production stage
(Peters, Iribarren and Dufour, 2015)	▪ Fuel path: Pyrolysis and hydroprocessing of hybrid poplar ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 MJ of liquid fuels ▪ Allocation method: Energy and mass	Attributional	GWP, ADP, eutrophication potential (EP), acidification potential (AP)	39	Advanced biofuels	▪ Major GHG emissions driver: Electricity consumption, especially from biomass dryer

Source	Techniques	LCA type	Metrics assessed	Greenhouse gas emissions (gCO_2e/MJ for fuel or tCO_2e/CO_2 captured for CO_2)	Product	Other comments
(de Jong *et al.*, 2017)	▪ Fuel path: Jet fuel from various feedstocks via six fuel conversion technologies, including Hydroprocessed Esters and Fatty Acids, FTS, HTL, pyrolysis, Alcohol-to-Jet ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 MJ of jet fuel ▪ Allocation method: Energy and system expansion (displacement) methods	Attributional	GWP	-3–40	Advanced biofuels	▪ Thermochemical routes had the lowest fuel emissions. Emissions of gasification lower than HTL and HTL lower than pyrolysis processes ▪ Major GHG emissions driver: Feed cultivation and co-credit in the gasification route, while H_2 use in HTL and pyrolysis
(Hsu, 2012)	▪ Fuel path: Pyrolysis and hydroprocessing of forest residues ▪ Boundaries: Well-to-Wheels ▪ FU: 1 km of travel by a light-duty passenger vehicle ▪ Allocation method: Energy	Attributional	GWP	25–39	Advanced biofuels	▪ Fuel emissions from biomass-derived electricity lower ▪ Major GHG emissions driver: Fast pyrolysis stage
(Frank *et al.*, 2013)	▪ Fuel path: HTL and hydroprocessing of algae ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 MMBTU of diesel ▪ Allocation method: Energy	Attributional	GWP	29.4	Advanced biofuels (biodiesel)	▪ Major GHG emissions driver: H_2 upgrading
(Tews *et al.*, 2014)	▪ Fuel path: HTL and pyrolysis of woody feedstocks with hydroprocessing ▪ Boundaries: Well-to-Wheels ▪ FU: 1 MJ of liquid fuels ▪ Allocation method: Energy	Attributional	GWP	27–34	Advanced biofuels	▪ Fuel via HTL had lower emissions than pyrolysis ▪ Major GHG emissions driver: Fuel production stage

Source	Techniques	LCA type	Metrics assessed	Greenhouse gas emissions (gCO_2e/MJ for fuel or tCO_2e/CO_2 captured for CO_2)	Product	Other comments
(Masoumi and Dalai, 2021)	▪ Fuel path: HTL of algae with hydroprocessing, using biochar energy source ▪ Boundaries: Well-to-Wheels ▪ FU: 1 kg of fuel ▪ Allocation method: Energy	Attributional	GWP	-5.9–-1.1	Advanced biofuels	▪ Fuel emissions from the use of char for energy in HTL are lower than its use in the fuel catalysis ▪ Major GHG emissions driver: Methanol used as reactive organic co-solvent in HTL
(Tsalidis *et al.*, 2017)	▪ Fuel path: Gasification with FTS of torrefied wood pellets, wood pellets and straw ▪ Boundaries: Well-to-Wheels ▪ FU: 1 km of distance travelled by a vehicle ▪ Allocation method: Energy	Attributional	GWP, EP, particulate matter potential, AP	15.6–17.2	Advanced biofuels (biodiesel)	▪ Fuel emissions from torrefied wood pellets are lowest, followed by wood pellets and then straw ▪ Major GHG emissions driver: Gasification and gas cleaning
(Fernanda Rojas Michaga *et al.*, 2022)	▪ Fuel path: Gasification of forest residues with FTS and CCS ▪ Boundaries: Well-to-Wheels ▪ FU: 1 MJ of jet fuel ▪ Allocation method: Energy and system expansion (displacement) methods	Attributional	GWP	-127.1–15.6	Advanced biofuels	▪ Fuel production with CCS and allocation by system expansion methods had the lowest emissions ▪ Major GHG emissions driver: CCS and wood chips processes
(Sun *et al.*, 2021)	▪ Fuel path: Fermentation to ethanol, pyrolysis to bio-oil, and gasification to jet fuel using corn stover ▪ Boundaries: Well-to-Wheels ▪ FU: 1 GJ biofuel consumed ▪ Allocation method: Energy and system expansion	Attributional	GWP, AP, EP, HTP and ozone layer depletion potential	19.9	Advanced biofuels	▪ Fuel emissions from fermentation were slightly lower than gasification, while pyrolysis had the highest emissions ▪ Major GHG emissions driver: Bio-oil upgrading in pyrolysis and fuel synthesis and refining in gasification

Source	Techniques	LCA type	Metrics assessed	Greenhouse gas emissions (gCO_2e/MJ for fuel or tCO_2e/CO_2 captured for CO_2)	Product	Other comments
(Deutz and Bardow, 2021)	▪ Direct air capture: Solid sorbent capture ▪ FU: 1 kg CO_2 captured from the air ▪ Energy source: Wind, Solar and grid electricity ▪ System boundary: Cradle-to-grave (synthetic fuel production and permanent storage)	Attributional	Multiple, including GWP, EP and ozone layer depletion potential	0.01−1	Chemical (CO_2)	Limited assessment of electricity emissions factors was made, especially for renewables, which could vary significantly by location factors. Changes in other input materials and energy emission factors, such as zeolite sorbents, not been assessed.
(McQueen *et al.*, 2020)	▪ Direct air capture: Solid sorbent capture ▪ FU: Not stated ▪ Energy source: Natural gas, waste heat from geothermal, or slip steam from nuclear ▪ System boundary: Cradle-to-grave (permanent storage)	Attributional	GWP	0.29−0.65	Chemical (CO_2)	▪ Limited process modelling parameters assessed: No modelling of the impacts of sorbent properties. ▪ No sorbent costing and emissions assessments. ▪ Geospatial location is limited to the US only
(Terlouw *et al.*, 2021)	▪ Direct air capture: Solid sorbent capture ▪ FU: 1 t CO_2 removed from the air ▪ Energy source: Electricity from the grid and PV installation, as well as heat from a waste heat source, solar-thermal heat collector and heat pumps ▪ System boundary: Cradle-to-grave (permanent storage)	Attributional	Multiple, including GWP, EP and ozone layer depletion potential	0.03−0.91	Chemical (CO_2)	Limited assessment of electricity emissions factors was conducted, especially for renewables, which can vary significantly due to location factors. Changes in other input materials and energy emission factors, such as sorbents, not been assessed.

Source	Techniques	LCA type	Metrics assessed	Greenhouse gas emissions (gCO_2e/MJ for fuel or tCO_2e/CO_2 captured for CO_2)	Product	Other comments
(de Jonge *et al.*, 2019)	▪ Direct air capture: Liquid sorbent capture ▪ FU: Not stated ▪ Energy source: Electricity from different sources, including natural gas combined cycle power plant ▪ System boundary: Cradle-to-grave (permanent storage)	Attributional	GWP	0.10−0.90	Chemical (CO_2)	Limited scenarios considered in this work, e.g., limited range of energy sources, sorbents, location and temporal factors
(Madhu *et al.*, 2021)	▪ Direct air capture: Solid and liquid sorbents capture ▪ FU: 1 t CO_2 captured ▪ Energy source: Grid electricity mix, and low-carbon electricity ▪ System boundary: Cradle-to-grave (permanent storage)	Attributional	Multiple, including GWP, water depletion and land occupation	0.12−0.60	Chemical (CO_2)	Limited scenarios considered in this work, e.g., limited range of energy sources, sorbents, location and temporal factors
(Wulf and Zapp, 2018)	▪ Fuel path: H_2 via water electrolysis, transported as LH2, dibenzyltoluene, methylcyclohexane and novel organic carrier ▪ Boundaries: Well-to-Wheels ▪ FU: 1 kg H_2 consumed	Attributional	Multiple, including GWP, EP and ozone layer depletion potential	17–50	Electro-fuels (e-H_2)	▪ Did not assess renewable electricity location factors and other key location factors ▪ No clear data on the methodology used
(Di Lullo *et al.*, 2022)	▪ Fuel path: H_2 via water electrolysis and H_2 and methane mixtures, transported as CH2, natural gas and H_2 mixtures, NH_3, and dibenzyltoluene ▪ Boundaries: Well-to-Wheels ▪ FU: Not clearly stated	Attributional	GWP	4–93	Electro-fuels (e-H_2)	▪ Did not assess renewable electricity location factors and other key location factors ▪ Emissions estimated without embodied emissions

Source	Techniques	LCA type	Metrics assessed	Greenhouse gas emissions (gCO_2e/MJ for fuel or tCO_2e/CO_2 captured for CO_2)	Product	Other comments
(BEIS, E4tech and LBST, 2021)	▪ Fuel path: H_2 via different sources, including electrolysis, biomass and fossil fuels with carbon capture ▪ Boundaries: Well-to-Wheels ▪ FU: 1 MJ H_2	Attributional / consequential	GWP	0–100	Electro-fuels (e-H_2)	▪ No clear methodology given for the assessment of renewable electricity location factors and other key location factors. Only short product delivery distance assessed (up to 350 km) ▪ Emissions estimated without embodied emissions
(Concawe and Aramco, 2024)	▪ Fuel path: e-H_2, e methane, e-methanol, e-NH_3, e-gasoline, OME_x, e-diesel and e-kerosene ▪ Boundaries: Different, including Well-to-Tank and Cradle-to-Gate ▪ FU: 1 MJ electro-fuel	Attributional	GWP	0–22	Electro-fuels	▪ Boundary of the assessment limited to the dispensing station ▪ Limited details on the hourly resolutions of renewable electricity ▪ H_2 losses in the plant were not accounted for
Key: FU for functional unit, PV for photovoltaics, FTS for Fischer-Tropsch synthesis, GHG for greenhouse gas, HTL for hydrothermal liquefaction, CCS for carbon capture and storage, CH2 for compressed H_2, FT-liquid for Fischer-Tropsch liquids and OME_x for polyoxymethylene dimethyl ethers.						

2.5 Centralised and decentralised production and reconversion approaches

The production of a product from raw materials through various processes into the final usable form can be done in a single location, as in the case of centralised production, or in multiple locations where one form of key processing occurs at a different location, as in the case of decentralised production. Figure 2.6 shows centralised and decentralised production approaches for biofuels produced via hydrothermal liquefaction. On the other hand, the reconversion of a product into its final usable form can be done at the import or distribution location, or it could even be inherent to the production of the product at the production location, as in the case of centralised reconversion. Additionally, it can be done at the retail and end-user locations, as in the case of decentralised reconversion.

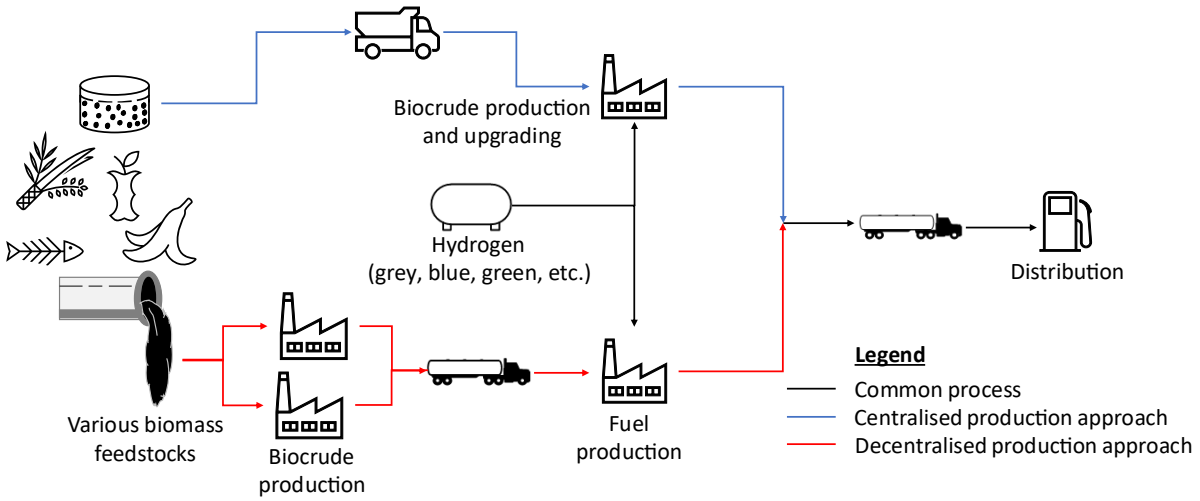

Figure 2.6: Centralised and decentralised production approaches for synthetic biofuels and biochemicals from hydrothermal liquefaction of biomass.

Generally, a centralised production or reconversion approach can be chosen when there is a large availability of raw materials or demand for products in one location, or when other factors, such as supply chain constraints, technical expertise, and regulatory standards, strongly influence design, operations, and plant configurations. This approach traditionally offers a significant advantage in production costs due to the economies of scale, as large-scale plants are often used in centralised fuel production or reconversion. Additionally, it provides significant opportunities for extensive heat integration, resulting in potential reductions in energy costs, as energy is recovered from the system.

However, under certain conditions, decentralised production and reconversion approaches could offer some cost and emissions benefits, especially in transportation costs and emissions, as reported in the literature. For example, the use of decentralised fuel production approaches in converting low bulk density or high moisture content biomass feedstocks, such as straw and sewage sludge, was reported to offer better fuel production price benefits than centralised production approaches (Snowden-Swan *et al.*, 2017). Hence, smaller plant scales are often employed in a decentralised production approach to meet local demand, transforming low-density and high-moisture-content feedstocks into high-energy-density intermediates, such as biocrude, which can be transported at lower cost to a centralised facility for further processing into final products. Additionally, a smaller plant scale could be utilised for products where one of the raw materials is located in another location in smaller quantities. For example, bio-CO_2 from a bioethanol plant can be used to produce synthetic fuels and chemicals by utilising H_2 from another location, especially since H_2 is readily available in the general market. However, decentralised production and reconversion approaches leave little

allowance for heat integration due to the nature of the segmented operations. Another key barrier to decentralised production and reconversion approaches is the loss of economies of scale from larger, centralised production facilities. This may lead to higher design and product costs.

Despite the proposed benefits of centralised and decentralised production and reconversion approaches, there have been very limited investigations into the impacts of centralised and decentralised operations on the costs and environmental emissions of synthetic fuels and chemicals. Currently, it is unclear how centralised and decentralised production and reconversion approaches may impact the cost and environmental emissions of synthetic fuels and chemicals. This is due to the different nature of the activities involved in the supply chains of synthetic fuels and chemicals. For example, a traditional H_2 production approach has generally relied on a centralised production scheme, with H_2 produced from natural gas and consumed within the same location without the need for complex distribution infrastructures (IEA, 2023d). Hence, there is a limited experience of international H_2 trade globally. However, emerging supply chains can be complex as they require transboundary supply chains, certainly involving multimodal transportations, with current considerations including a range of different H_2 carriers that may necessitate conversion/reconversion steps. H_2 reconversion can occur at import terminals or distribution centres in a centralised approach, or at fuel dispensing stations or on-board vehicles in a decentralised approach. The energy consumption, cost and environmental emissions of some production and reconversion configurations at distinct locations – production plants, import terminals, distribution centres, fuel dispensing stations or vehicles – may vary significantly depending on the point of production and reconversion due to design and operational factors (e.g., plant design, process integration and energy source). Hence, it is crucial to comprehend the implications of adopting various production and reconversion approaches on the overall cost and life cycle environmental impacts of synthetic fuels and chemicals.

2.6 Energy policies

Currently, there are no emission limits for synthetic fuels and chemicals in domestic or industrial applications; however, several policies, such as (DfT, 2024a, 2024b), (European Union, 2023a, 2023c, 2023b) and (CARB, 2020), govern their use in the transport sector. Generally, transport fuel policies on emission limits can be relatively static (e.g., EU (IEA, 2023) and the UK RTFO (DfT, 2024a)), dynamic over different purposes, time or locations (e.g., the UK RTFO (DfT, 2024a) vs SAF mandate (DfT, 2024c) and California Low Carbon Fuel Standard (CARB, 2020)) and in other cases, no emission limits (e.g., domestic heating and industrial use of H_2). Furthermore, these different policies can vary in key factors, such as the definition of fuels, emission limits for fuels, and the availability (volume fraction) of low-carbon fuels in transport fuels. These differences could be a significant issue, especially in international supply chains and if emission limits differ by fuel classification. Hence, transport fuel policies may need to be broad, consistent with other policies, and mutually acceptable by respective jurisdictions worldwide to enable their success. A key requirement would be the need for mutual acceptance and recognition of supply chain certificates by respective jurisdictions worldwide.

Amongst the transport policy issues is the difference in definitions. Currently, some policy definitions (e.g., UK RTFO (DfT, 2024a, 2024b)) require the energy content of renewable fuels of non-biological origins (RFNBOs) to come from 100% renewable energy of non-biological origin, while others (e.g., EU (European Union, 2023a, 2023c, 2023b)) do not offer any strict definition of the renewable energy fraction. Consequently, UK RTFO (DfT, 2024a, 2024b) gives rise to other fuel classifications such as partial RFNBOs, partial renewable fuels of biological origin (RFBOs), etc. Partial RFNBOs are defined by the UK RTFO (DfT, 2024a, 2024b) to be fuels that have 1–99% of their energy content from renewable energy of non-biological origin. Other similar definitions follow partial non-RFNBO, partial RFBO, etc. These different definitions of e-fuel could be an issue, especially in international supply chains and if

emission limits differ by fuel classification. Additionally, a strict definition of 100% renewable energy of non-biological origin for e-fuel poses a significant challenge to operations and net zero targets, especially during plant start-ups and recovery from process disruptions, as well as mitigating the issue of electricity congestion that has seen around 3% of renewable electricity curtailment globally (IEA, 2023e; Novan and Wang, 2024). E-fuels, which can function as chemicals for long-term energy storage, could be used to mitigate renewable electricity curtailment issues by using electricity that would otherwise be curtailed. In the UK alone, renewable curtailment of 3.5 TWh in 2022 had a financial impact of £750 million, and this is projected to grow to £3.5 billion by 2030 (Drax, 2022; Sani, 2023). However, there is a possibility that the energy for their production also coming from other electricity sources from the grid in the event of any uncertainty in operations (e.g., balancing the electricity sent to the grid vs the one actually used due to transmission losses, etc.). Hence, the EU (European Union, 2018, 2023a, 2023b) definitions and approaches are considered more operationally friendly because they accommodate current solutions for operational issues; however, they also have their drawbacks.

Amongst the key transport fuel regulators, the EU regulations (European Union, 2018, 2023a, 2023c) require that RFNBOs achieve a minimum 70% reduction in greenhouse gas emissions compared to the fossil fuel benchmark of 94 gCO_2e/MJ. This means that the life cycle greenhouse gas emissions of an RFNBO-qualified fuel must not exceed 28.2 gCO_2e/MJ. Similarly, the UK RTFO (DfT, 2024a, 2024b) requires RFNBOs to achieve a minimum 65% reduction in greenhouse gas emissions, equivalent to a maximum emission threshold of 32.9 gCO_2e/MJ. In contrast, the UK SAF (Sustainable Aviation Fuel) mandate allows a higher emission limit of 53.4 gCO2e/MJ, representing a 40% reduction compared to conventional jet fuel, for RFNBOs used as SAFs (DfT, 2024c). Hence, it is essential to develop policies that address both specific and general needs to tackle the diverse range of challenges that may exist.

In summary, for the successful deployment of low-carbon fuels, it is advisable to have consistency in the definitions of low-carbon fuels and chemicals amongst different jurisdictions. Additionally, there would be a need for mutual acceptance and recognition of supply chain certificates for H_2 and its derivatives by respective jurisdictions globally, consistent with the COP28 declaration of intent in 2023 (Hydrogen Council, 2023). Using LCA-based, asset-based certification, radio frequency identification (RFID), a database of approvals, amongst others, could help in tracking and managing LCFs' emissions and fraud (European Union, 2023b). Furthermore, given the low success rate of prior low-carbon technologies and policies (Belaïd, 2022; Sokołowski and Heffron, 2022; Odenweller and Ueckerdt, 2025), it is advisable that regulations allow a broad range of solutions to narrow the implementation gap of low-carbon solutions. For a successful energy policy, it is crucial that it is based on an assessment of resource availability, technology designs and operations, environmental, costs and social impacts. This will help avoid issues such as unmet targets, delay or cancellation of policies, fraud, slowdown of technological innovation and social inequalities (Belaïd, 2022; Sokołowski and Heffron, 2022; Odenweller and Ueckerdt, 2025; The White House, 2025).

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3 Extended review and analysis of dry and wet biomass-to-liquids technologies

This chapter contributes to the overall thesis aim of assessing low-carbon fuel and chemical technologies by critically reviewing and analysing biomass-to-liquids supply chains, including the availability of non-food biomass (with the UK as a case study), the production of drop-in biofuels from biomass via thermochemical routes, the impacts of production approaches (e.g., hydrogen sources, centralised and decentralised production approaches), the estimation of fuel production volumes, and life cycle greenhouse gas emission impacts of drop-in biofuels (with the UK as a case study).

The paper presents both an extensive review of biomass resources and advanced biofuel supply chains from technical, economic and life cycle assessments perspectives, as well as original research that estimates the advanced biofuel production volumes and greenhouse gas emissions reductions that could be achieved in the UK. The availability of non-food biomass resources in the UK was estimated to range from 167–205 Mtpa (wet) [839–1033 PJ per year], as more than 50% of these volumes are from high moisture content feedstocks such as biogenic municipal waste and sewage sludge. Other biomass feedstocks that are produced in significant quantities include straw and wood waste. Also, it was estimated that the total UK drop-in fuel manufacturing potential ranged from 269–563 PJ per year. When used to displace fossil fuels in road transportation, this could lead to a total GHG reduction of 18.8–64.7% (18.7–64.4 $MtCO_2e$ per year) relative to UK's 2021 road transport emissions.

The work was published in the Sustainable Production and Consumption journal in June 2024. The published work is titled "A review of techno-economic analyses and life cycle greenhouse gas emissions of biomass-to-hydrocarbon "drop-in" fuels" and is presented as Chapter 3 here. The supplementary information for the work, published alongside the paper, is reprinted in Appendix A1.

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Review Article

A review of techno-economic analyses and life cycle greenhouse gas emissions of biomass-to-hydrocarbon "drop-in" fuels

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ABSTRACT

Synthetic "drop-in" fuels are compatible with existing fuel and vehicle infrastructures and, when produced sustainably, they could play an important role in mitigating the emissions of greenhouse gases (GHG) from transportation, especially in the hard-to-decarbonise sectors like freight and aviation. However, there is a need to understand the availability of biomass resources for drop-in fuel applications and the potential challenges associated with using these feedstocks including the supply chain issues. Hence, this paper offers a critical review of non-food biomass and drop-in fuel production including the biomass availability in the UK, the production of drop-in fuels from biomass feedstocks via thermochemical routes, estimated fuel production prices and volumes, and life cycle GHG impacts. The paper explores several fuel production factors, including energy and hydrogen requirements, as well as supply-chain considerations, which were used to estimate the drop-in fuel potential in the UK economy. We estimate the availability of non-food biomass resources in the UK to be in the range of 167–205 Mtpa (wet) [839–1033 PJ per year], as more than 50 % of these volumes are from high moisture content feedstocks such as biogenic municipal waste and sewage sludge. Other biomass feedstocks that are produced in significant quantities include straw and wood waste. Also, it is estimated that the total UK drop-in fuel manufacturing potential is in the range of 269–563 PJ per year. When used to displace fossil fuels in road transportation, this could lead to a total GHG reduction of 18.7–64.4 Mt. CO_2eq per year which is 18.8–64.7 % relative to the UK's overall road transport emissions from all fuels in 2021.

1. Introduction

One of the greatest challenges of the 21st century is the global transition to a low-carbon, sustainable energy system. Current energy systems are heavily dependent on emissions-intensive energy sources, resulting in the accumulation of greenhouse gas (GHG) emissions in the atmosphere and contributing to the changes in the global climate. According to the IEA (IEA, 2022c), about 36 gigatonnes of carbon dioxide (CO_2) were emitted in 2021 from combustion sources and industrial processes, and this was over 10 times more than the emissions at the start of the 20th century. About a third of the emissions in 2021 were from the transportation sector, where fossil fuels currently supply about 95 % of transport energy demand (Climate Watch, n.d.). However, concerns over energy security and environmental sustainability have led to a growing interest in the use of alternative technologies in the transport sector. Despite the strong interest in renewable energy such as

Abbreviations: AD, Anaerobic digestion; ADP, Abiotic depletion; AP, Acidification potential; BMW, Biogenic municipal waste; BTL, Biomass to liquids; CCS, Carbon capture and storage; CO_2, Carbon dioxide; EfW, Energy-from-waste; EP, Eutrophication potential; FTS, Fischer-Tropsch synthesis; GGE, Gasoline gallon equivalent; GHG, Greenhouse gas; GWP, Global warming potential; HTL, Hydrothermal liquefaction; HTP, Human toxicity potential; ICEVs, Internal combustion engine vehicles; iLUC, Indirect land use change; LCA, Life cycle assessment; LHV, Low heating value; LUC, Land use change; MFSP, Minimum fuel selling price; MSW, Municipal solid wastes; MTG, Methanol-To-Gasoline; RED, Renewable Energy Directive; SCWG, Supercritical water gasification; SI, Supplementary Information; SMR, Steam methane reforming; TEA, Techno-economics analysis; TIGAS, Topsoe Integrated Gasoline Synthesis; USD, United States dollar.

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2352-5509/© 2024 The Authors. Published by Elsevier Ltd on behalf of Institution of Chemical Engineers. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

biofuels, biofuels contribute only about 4 % of the UK and global transport fuel consumption volumes by energy in 2021, respectively (IEA, 2022a; DESNZ, 2023b). This contribution is significantly lower than the targets of roughly 15 % by 2030 set by numerous government mandates, such as the EU Renewable Energy Directive (RED II) (European Commission, 2019).

Conventional biofuels, often called first-generation biofuels such as bioethanol and biodiesel, which are used currently are limited in application due to concerns over their competition with food production, environmental impacts and compatibility limits with existing engines. The food vs fuel debate has strongly intensified since the global food crisis of 2008, which was partly attributed to first-generation biofuels (European Commission, 2011). Conventional biofuels are typically produced from food-based biomass through the fermentation of starch and sugar and the transesterification or hydrogenation of fats and oils. Also, the utilisation of biomass feedstocks for these biofuels can lead to considerable land and environmental impacts when biofuel crops displace the production of food or natural habitation. The land use change (LUC) and indirect land use change (iLUC) associated with using forests, food crops and grasslands can be significant (Searchinger et al., 2008; Plevin et al., 2010). According to Searchinger et al. (Searchinger et al., 2008), when accounting for the impact of LUC in corn cultivation, the GHG emissions of corn-based ethanol could double over 30 years instead of achieving the 20 % saving initially estimated without LUC. Although other studies have published a smaller estimate for the LUC effect of corn ethanol, the GHG consequence of LUC is generally non-trivial. Despite LUC and iLUC being the most uncertain components in the GHG emissions estimation of biofuels (Plevin et al., 2010), the availability and way in which biomass feedstocks are obtained play important roles in the sustainability of biofuels. As a result, current government documents such as the UK Biomass Strategy developed by DESNZ (DESNZ, 2023a) require that emissions associated with LUC and iLUC are accounted for in biomass applications. The strategy also required biofuels to have at least 60–65 % emissions savings relative to a fossil fuel comparator of 94 gCO_2eq/MJ in energy and transport applications. Additionally, bioethanol and biodiesel (transesterified) can only be used with petroleum fuel in blends up to a certain percentage in current engines without costly engine modifications. These limitations not only impact the production of first-generation biofuels but also their utilisation, and therefore, the development of alternative fuels such as renewable hydrocarbon fuels is considered a key innovation for addressing these issues.

Renewable hydrocarbon liquid fuels, such as renewable gasoline and renewable diesel, are designed as drop-in solutions so that they can be used as direct replacements for petroleum fuels, thus allowing for a broader application of renewable fuels in transportation. Drop-in fuels are chemically identical to petroleum gasoline, diesel, or jet fuel, and can be used in engines without the need for blending with petroleum fuels or costly engine modifications. Drop-in fuels are typically produced from second and third-generation biomass feedstocks such as agricultural waste (Anex et al., 2010) and algae (Jones et al., 2014). They can also be produced from waste CO_2 (d'Amore et al., 2023). Drop-in fuel production allows the utilisation of non-food biomass resources and can improve the sustainability of biofuels by addressing issues such as LUC, iLUC and the availability of biomass resources. Non-food biomass which is lignocellulosic biomass or food waste typically has LUCs of zero, especially for residues and wastes. Additionally, using non-food biomass resources such as agricultural residues, wood wastes and municipal wastes avoids iLUC and the competition of biofuel with food. However, the utilisation of non-food biomass for drop-in biofuel applications may come with other consequential indirect emissions which may arise from diverting these materials from existing streams (Ou et al., 2022; Lilonfe et al., 2024). These consequential emissions may be positive or negative depending on the foregone applications, for example, the diverting of food waste from landfilling or anaerobic digestion (AD). Furthermore, the availability of non-food biomass is generally substantial across many regions as almost every society generates wastes from biomass feedstocks such as food and forestry. Lignocellulosic biomass feedstocks are available on a renewable basis (Ho et al., 2011).

In 2019, the UK became the first major economy to pass a net zero emissions law which has legally binding climate targets across its economy (BEIS and Skidmore, 2019). As a result, there is a strong compelling drive towards mitigating GHG emissions by increasing the uptake of biofuels in the transport sector, particularly in hard-to-decarbonise areas. Consequently, many recent publications such as the Royal Society (Royal Society, 2023) and Geissler et al. (Geissler et al., 2024) estimated the potential volumes of biomass and drop-in fuels that can be produced in the UK and US, respectively. These studies estimated the prices, life cycle GHG emissions, potential volume availability and GHG emissions of drop-in fuel. However, they did not estimate the potential emissions savings of using drop-in fuels and the consequences of diverting biomass feedstocks from existing applications. Competing applications can have a significant impact on drop-in fuel production, both in terms of GHG emissions and cost. Hence, understanding the potential implications of diverting these feedstocks from the existing supply chain and corresponding GHG emissions savings from biofuels is particularly important in the sustainability of drop-in biofuels.

Therefore, in this report, we reviewed the availability of non-food biomass feedstocks and their existing applications across the UK market. Also, we reviewed thermochemical drop-in biofuel production technologies, their techno-economics and life cycle GHG assessments. Additionally, we assessed the potential volumes and GHG emissions impacts of using drop-in biofuels in road transport applications in a manner not captured in previous publications, by evaluating key features such as biomass supply chains, hydrogen demand, fuel potential, and attributional and consequential GHG emissions associated with these drop-in biofuels.

2. Methodology

The methodology used in the paper is divided into two parts: (1) The methods used for the critical literature review where the existing key literature on biomass and drop-in biofuel production including supply chain and techno-economics were analysed and: (2) The approaches that were used for estimating the potential drop-in volumes and GHG emissions impacts in the UK.

The methodology used for the literature review was focused on non-food biomass resources, drop-in fuel production, biomass and biofuel policies, and techno-economic and life cycle assessments of drop-in fuels. Therefore, search strings having these keywords were used to search for publicly available information in various databases including ScienceDirect, government websites, and reputable sources such as IEA, NREL, WRAP and NNFCC. Key materials retrieved and critically analysed included peer-reviewed publications, policies, regulations, theses, books, reports, and websites.

The estimation of the availability of UK non-food biomass feedstocks was done using two scenarios – the 100 % feedstock and the competing cases. For the 100 % feedstock case which estimates the whole availability of biomass, the estimation of the potential volumes of biomass available in the UK was done by reviewing existing literature. Also, in accounting for biomass availability in the competing use case, volumes of biomass from existing competing applications were used in estimating the availability of the biomass feedstocks. The impacts of existing biomass utilisation technologies, such as cost and environmental impacts, were used in determining the availability of the biomass feedstocks in the competing case. Additionally, due to the diverse range of biomass feedstocks, a case-by-case approach was also applied in some instances, see Sections 3.1.1 to 3.1.8 for details on specific methodologies.

The approach used for estimating the potential drop-in volumes and GHG emissions impacts in the UK was based on the material and energy balance data of pilots, demonstrations or experimental units of various

drop-in fuel production technologies published in the literature. The GHG emissions estimates were based on well-to-wheel emissions data from important peer-reviewed literature such as those which provided detailed life cycle assessment (LCA) analysis. Where a significant variation in data exists for a parameter as reported by various authors, any or both of these approaches were adopted (a) Prioritisation of demonstration, pilot, and regional data (b) Use of averages of the most represented range in the literature. Also, because the UK biomass strategy required that biofuels should have at least 65 % emissions savings relative to a fossil fuel comparator of 94 gCO_2eq/MJ in transport applications, this criterion was prioritised in the selection of the fuel conversion routes. Furthermore, the UK Biomass Strategy 2023 considers mostly emissions directly associated with biomass processing or use, which may not represent other potential impacts that may arise from diverting biomass resources from existing applications. The indirect emissions it considers are only the iLUCs. Therefore, both attributional and consequential GHG emission impacts of using these biomass resources for drop-in fuel applications were evaluated. Consequential LCA analyses the direct and indirect emissions associated with the fuel. Direct emissions could include LUC, crop cultivation, fuel conversion, etc. Indirect emissions from the diversion of feedstocks for fuel production could include iLUC, foregone energy benefits, foregone fertiliser benefits, avoided landfill emissions, etc. Consequential emissions help in evaluating the potential impacts including iLUC that may arise from the diversion of the feedstocks in fuel production.

3. Findings and discussions

3.1. Non-food biomass feedstocks in the UK

The availability, distribution and characteristics of biomass resources are key in the production of biofuels. While biomass feedstocks are widely considered sustainable, they can be limited in availability (e.g., forest resources in the UK), and these could have considerable impacts on the environmental and economic benefits of biofuels, as well as biofuels' production volumes. In this section, the volumes and distribution, properties and competing applications of UK-origin, non-food biomass feedstocks, which can be obtained from agricultural residues, straw and other non-food biomass, are evaluated by reviewing existing literature.

3.1.1. Municipal solid waste (biogenic fraction)

Municipal solid waste (MSW) is comprised of wastes from households and other waste of similar nature and composition such as packaging waste, construction and demolition waste and commercial and industrial waste. As seen from Table 1, 34.6 Mtpa (wet) of biogenic municipal waste (BMW) is generated annually in the UK. E4tech (E4tech, 2017) and Royal Society (Royal Society, 2023) reported that 40.2 Mtpa and 40 Mtpa of BMW are generated in the UK, respectively. These are slightly higher than the estimate here. However, both publications failed to highlight the basis of their estimation, although the E4tech estimate was based on 2015 UK BMW generation rates.

The competing uses for BMW are strong, with many projects using or considering using BMW for energy or other purposes, see Supplementary Information (SI) Section 1.1 for more details on current BMW uses. However, a volume of 6.1 Mtpa of BMW was sent to landfill in the UK in 2020 (Defra, 2022b), see Fig. 1 for details. Excluding 1.9 Mtpa of food waste landfilled as part of BMW and including 1.8 Mtpa of BMW used in energy-from-waste (EfWs), the minimum availability of BMW in the competing case is estimated as 6.0 Mtpa. The generation outlook of BMW will likely remain constant over the next few years unless significant changes in production or consumer behaviour are initiated, as the generation rates of households and commercial & industrial sources have remained stable since 2015, see SI Section 1.1 for more details. Based on the capacity data on EfWs plants from Tolvik (Tolvik, 2022) and NNFCC (NNFCC, 2021), no BMW will be landfilled in 2030, as all BMWs are used majorly in energy applications.

BMW is suitable for bioenergy production via different pathways, both biochemical and thermochemical methods, due to its moisture content of roughly 50 % on average. Utilising BMW in thermochemical processes like gasification or hydrothermal liquefaction (HTL) may require pre-treatment before conversion to fuel. The lower heating value (LHV) of the biogenic component of MSW on a dry basis is estimated to be in the range of 13.1–17.5 MJ/kg (Moora et al., 2017; Fetene, 2021). The GHG emissions from current BMW usage are in the range of 0 kg of CO_2eq/t MSW for recycling to nearly 400 kg of CO_2eq/t MSW released from landfills (Nordahl et al., 2020). Energy and composting applications of BMWs have associated emissions which depend on the conversion method used. Hence, consequential emissions may be suitable for evaluating and comparing the emissions of potential biomass applications with existing ones. Additionally, gate fees are charged at EfW plants. The gate fee charged for processing BMW at EfW plants is around £90 to £95, while a fee of £111 to £116 is charged at landfills (WRAP, 2021). Gates fees can serve as a good source of attraction and benefits for drop-in fuels, making drop-in fuel production more competitive.

3.1.2. Straw

Straw is an agricultural waste whose cultivation in the UK is mainly derived from wheat, barley, oil seed rape and oats (Defra, 2019). Straw production in the UK is in the range of 11–12 Mtpa (NNFCC, 2014;

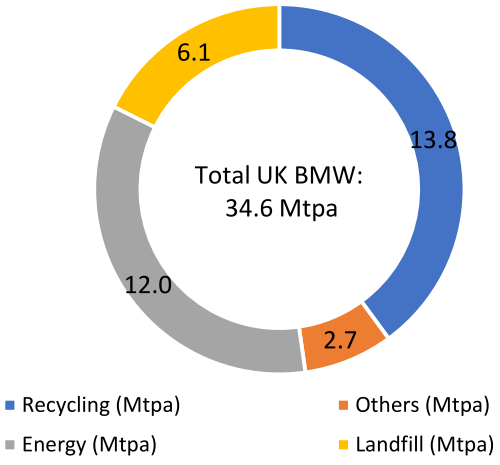

Fig. 1. UK BMW generation with competing uses in 2021.

Table 1
BMW streams in the UK.

Waste stream	Household waste stream, wet (Mtpa)	Commercial waste stream, wet (Mtpa)	References
Food waste	5.1	4.9	(Facchini et al., 2018; WRAP, 2019c, 2019b, 2020b; Jeswani et al., 2021; Defra, 2022b)
Garden & others	5.4	0.6	
Paper & cardboard	4.9	8.7	
Wood waste	1.0	4.0	
Total	**16.4**	**18.2**	

Defra, 2019). These volumes do not consider the straw uncollected during baling, which is up to 50 % of the total straw grown (total potential production). The amount of uncollected straw is highly driven by the markets, if the prices are uneconomic, straws are usually ploughed back into the soil (NNFCC, 2014; Defra, 2019; Tolvik, 2019). However, not all straws can be collected without significant iLUCs as some amount of straw is used to improve soil structure and nutrient status. Straw production in the UK is a regional market, with its main supply from the east of England (NNFCC, 2014).

Straw produced in the UK is typically used for animal bedding, animal feed, and power generation, as shown in Fig. 2. Assuming volumes of straw available in surplus and in power stations can be used for drop-in fuel production, the volume of straw available in the case of the competing application can be estimated as 2.9–3.6 Mtpa. Both the use of straw in power stations and drop-in fuel are in energy applications. Based on the data by Defra (Defra, 2019) and NNFCC (NNFCC, 2014), the total demand for and supply of straw is expected to remain stable up to 2030.

One of the key properties of straw is its low bulk density. The density of baled straw is in the range of 110–200 kg/m^3 while that of loose or chopped straw is 20–80 kg/m^3 (Satlewal et al., 2018). The low density of straw, even after balling, attracts a cost to the transportation of straw from farms. Straw has a moisture content of about 50 %, which reduces to less than 15 % after natural drying on fields (van Nguyen et al., 2016). The fixed carbon of straw is 11–19.5 % of dry mass, while volatiles is 35.0–72.4 % of dry mass (Montero et al., 2016; Satlewal et al., 2018). The LHV of straw is 14.3–15.6 MJ/kg on a dry basis (Teagasc, 2010; Bradna et al., 2016; Xia et al., 2019). Current bioenergy applications of straw in Europe are reported to have emissions varying from 16 to 55.8 g CO_2eq per MJ of electricity, based on a net electrical efficiency of 29 % (Giuntoli et al., 2013; Welfle et al., 2017). The cost of straw is reported in the range of £40–75 per tonne, depending on seasons and regions across the UK (AHDB, n.d.; Lewis Business Media, 2022).

3.1.3. Manure

Animal manure, made up mostly of animal faeces, is generated as a by-product of animal rearing including cattle, pigs, and poultry (NNFCC, 2019). The UK manure generation rates are estimated at 72 Mtpa to 90 Mtpa (Defra, 2009, 2011; Smith and Williams, 2016). The distribution of UK manure by sources is cattle (80 %), pigs (7 %), horses (5 %), poultry (5 %) and others (2 %), based on Smith and William (Smith and Williams, 2016).

Currently, almost all the manure produced is applied to agricultural land annually in the UK, with only a small amount used for AD, as shown in Fig. 3. Using manure for drop-in fuels instead of agriculture may attract significant emissions savings, up to -33.0 g CO_2eq/MJ fuel (-390

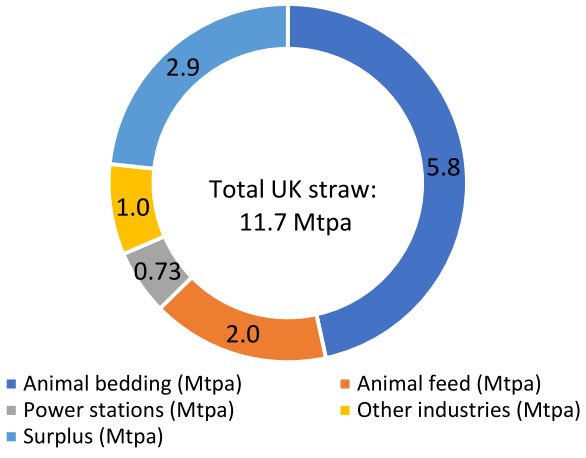

Fig. 2. UK straw production (Defra, 2019).

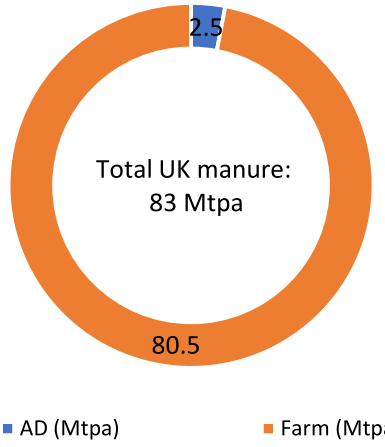

Fig. 3. UK manure availability in 2021 (NNFCC, 2021).

kg CO_2eq per dry tonne manure) as reported by Ou et al. (Ou et al., 2022) when consequential emissions are accounted for. However, a key challenge to accessing manure is its very low distribution. Hence, it can be assumed that 0–87.5 Mtpa of manure (excludes those used in AD) can be available in the competing case. Based on Defra's (Defra, 2022a) publication in 2022, there is no significant change in animal farming activities and policies recently that could impact animal faeces generation presently and in the future. Therefore, the total generation and utilisation outlook of animal manure is expected to remain flattened over the next few years, up to 2030.

Manure is a very high moisture content feedstock, containing up to 96 % moisture (NNFCC, 2019), which makes it challenging for energy applications such as combustion and gasification. However, these have made it very suitable for wet biomass application processes like AD and HTL. Animal manure has a significantly high amount of volatiles and a low fixed carbon content on a dry basis, typically in the range of 62–74 % and 33–45 %, respectively (Cao et al., 2016; Tushar et al., 2016; Moghaddam et al., 2021). The LHV of animal manure on a dry basis is 14.4–16.8 MJ/kg, based on data from Sahu (Dávalos et al., 2002; Sahu et al., 2016). The GHG emissions for manure's land application stage range from 164 to 335 kg CO_2eq per dry tonne of manure, assuming a 10 % average manure moisture content (Aguirre-Villegas and Larson, 2017). Manure has a low-cost value and is estimated to have a value of up to £17 per tonne, based on the fertiliser replacement value of the nutrients it can contain (Alli Grundy, 2022).

3.1.4. Wood waste

According to Environmental Agency "wood, which is not virgin timber (that is, wood that has been used for any purpose) and associated residues such as off-cuts, shavings chippings and sawdust, either treated or not treated, is waste" (Environmental Agency, 2017). In 2019, wood waste generation was 5.0 Mtpa (Tolvik, 2019). Currently, the use of wood waste in the UK is significant, with only a small fraction left over as surplus, as shown in Fig. 4. Since both EfWs and drop-in fuel are energy applications, it can be assumed that the volume of wood waste available in the competing case is between 2.9 and 3.7 Mtpa. Wood waste outlook is expected to remain flattened over the next few years (Tolvik, 2019).

Wood waste has an average moisture content of 20 % and an LHV of 18.5–21.0 MJ/kg on a dry basis (Forestry Commission, n.d.; Huhtinen, 2005; Akhator et al., 2017). The GHG emissions of bioenergy (combined heat and power) from wood waste vary significantly depending on the grade of wood, ranging from 53.8 to 200 kg CO_2eq per MWh (14.9–55.6 g CO_2eq per MJ) for grade A and B wood waste and from 600.0 to 814.2 kg CO_2eq per MWh (166.7–226.2 g CO_2eq per MJ) for grade C and D. Grades C and D wood waste contains chemicals such as urea formaldehyde and urea melamine resin which contribute to their high GHG

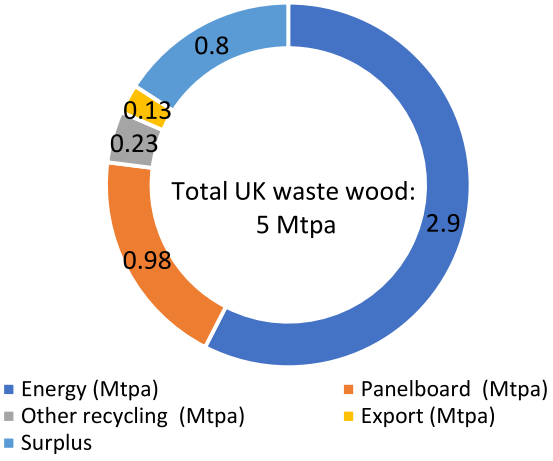

Fig. 4. UK waste wood availability and use (Tolvik, 2019; Defra, 2021).

emissions (Röder and Thornley, 2018). Also, the cost of wood waste is dependent on the grade of the wood waste, often attracting negative prices due to its waste disposal requirement. High-grade wood waste – which is clean and non-hazardous wood, majorly grade A to C wood waste such as softwood and process off-cuts from the manufacture of virgin/sawn timber – is reported to cost between -£5 to £20 in 2021 (letsrecycle.com, 2021b). Low-grade wood waste which includes treated wood costs between -£55 to -£5, as its disposal may be subject to hazardous waste regulations (letsrecycle.com, 2021b). In drop-in fuel application, using biomass, especially grade C and D of wood waste which contain chemicals, may cause additional operational complexity such as the increased risk of corrosion, catalyst deactivation and product contamination. Therefore, additional measures, for example, the use of corrosion-resistant alloys like nickel alloys, may be required to manage the varying nature of the feedstocks (Lee et al., 2016; Boukis and Stoll, 2021).

3.1.5. Sewage sludge

Sewage sludge is a by-product produced from the treatment of wastewater released from various sources, including homes, industries, medical facilities, street runoff and businesses. It has a significant amount of water compared to solids such as organics. Based on data by Nuamah et al. (Nuamah et al., 2012) and Ofwat (Ofwat, 2015), sewage sludge production in the UK was estimated at 1.4–1.5 Mtpa (dry), which is equivalent to 28–30 Mtpa (wet).

Sewage sludge disposal or recycling is typically done through spreading on agricultural land and incineration, as shown see Fig. 5. Several factors can impact sludge application on land (e.g., safety and cost implications). As sewage sludge can contain toxic elements (such as chromium) which are only safe if they're below set limits (Defra, 2018), sludge application on land can lead to the contamination of water and the transmission of pathogens via spreading sites or contaminated groundwater, drinking water wells, amongst others (Reilly, 2001). Furthermore, the cost implication of treating raw sewage is significantly high as it can cost up to £200 per dry tonne of sludge, only to be discharged almost free of cost (£1–2 per dry tonne) (Katsou, 2019). Therefore, using alternative treatment methods (e.g., HTL) can be key for optimum sewage sludge management. In HTL, digested sludge – which has been stripped of biogas and has not passed through high energy-consuming drying processes – can be used for drop-in fuel production. The forgone benefits such as fertiliser credits for using sewage sludge for drop-in fuel were estimated at 22.9 g CO_2eq per MJ (Lilonfe et al., 2024). The overall attributional and consequential GHG emissions of using sewage sludge for HTL in the UK were reported as 0–36 g CO_2eq per MJ and 59 g CO_2eq per MJ, respectively (Royal Society, 2023; Lilonfe et al., 2024). Hence, the competing case assumes all of sewage sludge can be available for drop-in fuel production.

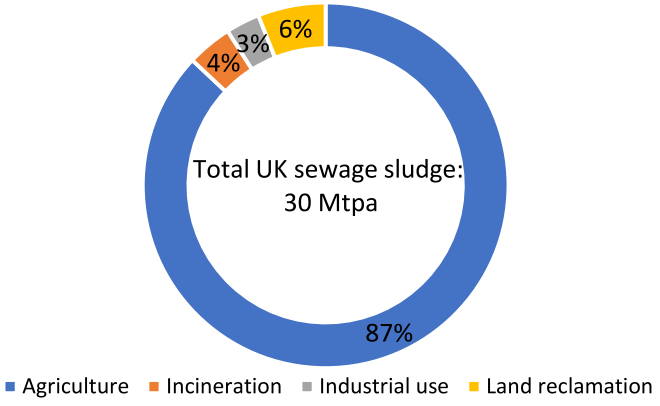

Fig. 5. UK sewage sludge generation and utilisation (Biosolids Assurance Scheme, n.d.).

Raw sewage sludge has a very high moisture content, with moisture content ranging from 84 to 96 % (Zhang et al., 2010; Chen et al., 2013; Marrone et al., 2018). On a dry basis, the average LHV of sewage sludge is 12–15 MJ/kg (Nuamah et al., 2012; Ostojski, 2018). Dry sewage sludge is often disposed of at almost free of cost, attracting selling prices between £1 to £2 per dry tonne (Katsou, 2019). Typical GHG emissions associated with the application of dry sludge on land can be assumed to be zero since almost all methane would have been stripped off from sewage sludge during its treatment in industrial AD and aeration plants.

3.1.6. Food waste

United Nations definition refers to food waste as food and related inedible portions removed from the human food supply chain sectors (United Nations, 2023). Based on the analyses by WRAP (WRAP, 2019a, 2020b), the total food waste generation in the UK is estimated at 11.1 Mtpa. Jeswani et al. (Jeswani et al., 2021) estimated UK food waste generation at 13.1 Mtpa, which is very close to the numbers by WRAP. Food waste generation in the UK is expected to continue to decrease, following the trend from 2007 and food conversation programs, which aim to reduce food waste by 50 % in 2030 compared to 2007 levels.

The competing use of food waste is high, with applications in areas such as biogas production, composting and recycling, see food waste SI Section 1.2 for details. However, a significant portion of food waste ends up in landfills. The volumes of food waste landfilled as part of BMW in 2020 can be estimated as 1.9 million tonnes, based on data from Defra for the fraction of food waste in MSW (Defra, 2017) and the volumes of MSW sent to landfills (Defra, 2022b). Drop-in fuel production from food waste which is landfilled in the UK can produce GHG emissions of -21.5 g CO_2eq per MJ by avoiding landfill. When the fuel production from food waste competes with existing applications like AD and composting, it is estimated to lead to indirect emissions of 22.8 g CO_2eq per MJ as food waste is diverted from existing applications (Lilonfe et al., 2024). The overall attributional and consequential GHG emissions of using food waste for drop-in fuel via HTL in the UK were reported as 33.7 g CO_2eq per MJ and 35.0 g CO_2eq per MJ, respectively (Lilonfe et al., 2024). Hence, considering existing energy and digestates applications of food waste, the volume of food waste available for drop-in fuel in the competing case can be estimated at 2–6 Mtpa.

Food waste has a very high moisture content, which ranges from 48 to 95 % (Amuzu-Sefordzi et al., 2014; Selvam et al., 2021). The LHV of food waste on a dry basis is 16.8–22.9 MJ/kg (Kadlimatti et al., 2019; Chae et al., 2020; Selvam et al., 2021). Like BMW, the GHG emissions from food waste usage are in the range of 0 kg of CO_2eq/t MSW for recycling to nearly 400 kg of CO_2eq/t MSW released from landfills (Nordahl et al., 2020). These emissions rates are dependent on the food waste management method used such as incineration, landfilling and composting. Food waste has a significantly high fraction of volatiles and

a low fraction of fixed carbon, about 61–62 % and 6–23 %, respectively (Cao et al., 2016; Tushar et al., 2016; Moghaddam et al., 2021). The cost of food waste in AD is estimated to range from -£15 to £15 in 2021, according to letsrecycle.com (letsrecycle.com, 2021a). WRAP reported a similar average gate fee of £0 per tonne for food waste processing in AD plants (WRAP, 2022).

3.1.7. Digestates

Digestate, a by-product produced from AD, is a slurry waste consisting of fibre and slurry. It is rich in nutrients which makes it to be applied as fertiliser (NNFCC, 2016). The fibre contains a higher content of solids, making it more suitable for transportation, however, separation is not done on all AD sites (WRAP, 2020a). There was a total of 15.5 million tonnes of feedstock which were digested in 642 AD plants in the UK in 2021 (NNFCC, 2021). Using an average digestate yield of 92.5 %, an estimated 14.2 Mtpa of digestates were produced in the UK in 2021. There has been a significant increase in the number of AD sites, from 85 in 2013 to 642 in 2021. The number of AD plants is expected to continue to increase with the development of new sites.

Almost all the digestates produced in the UK are applied to soils, as shown in Fig. 6. WRAP (WRAP, 2020a) reported that 1.3 % of feedstocks are being removed during and after anaerobic digestion due to factors such as gross contamination and feedstock outside the input specification. Feedstocks including digestates from food waste can be contaminated by plastics, thereby, rendering their application on land inadequate (WRAP, 2020a). Digestates can find applications in drop-in fuel production due to their high moisture content. However, diverting digestates feedstocks from existing applications such as fertiliser and other energy recovery into drop-in production in the UK can produce consequential emissions of 24 CO_2eq per MJ (Lilonfe et al., 2024). The overall attributional and consequential GHG emissions of using digestates for drop-in fuel via HTL in the UK were reported as 0–36 g CO_2eq per MJ and 59 g CO_2eq per MJ, respectively (Royal Society, 2023; Lilonfe et al., 2024). Hence, in the competing case, it was taken that digestates can find applications in both fertiliser and drop-in fuel applications.

Digestate is a very high level of moisture waste, containing water in the range of 90–95 wt%. The LHV of digestates on a dry basis is 14.3–18.4 MJ/kg (Cao et al., 2019; Jurczyk et al., 2021; Taufer et al., 2021). Like dry sludge, typical GHG emissions associated with the application of digestates on land can be assumed to be zero since almost all methane would have been stripped off from digestates during AD treatment. Digestates have a high fraction of volatiles and low fixed carbon, about 79.8–85.1 % and 14.9–21.6 %, respectively (Cao et al., 2019; Jurczyk et al., 2021). The cost of digestates is reported by WRAP to be in the range of -£8 to £5 (WRAP, 2020a).

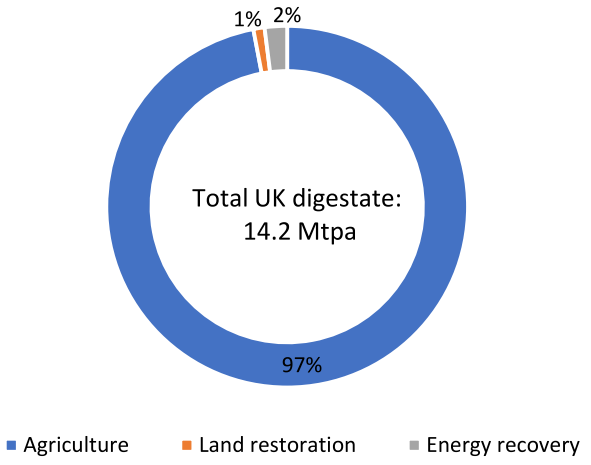

Fig. 6. UK digestates generation and utilisation (NNFCC, 2016).

3.1.8. Other feedstocks

Other biomass feedstocks produced small or in insufficient quantities in the UK, such as forest residues, miscanthus, short rotation coppice and crude glycerine, can be found in Table 2. Additional details on these feedstocks can be found in the SI. It is worthwhile to note that virgin wood which is produced in significant quantities in the UK is not sufficient to meet the UK national demand. The UK is strongly a net importer of virgin wood resources and imported a total of 20.6 Mt. of wood in 2020 (Forestry Commission, 2021).

3.1.9. Total volume of UK-origin non-food feedstocks

Table 2 summarises the UK-origin biomass feedstock availability. The total volume of UK-origin non-food biomass can be estimated as 839–1033 PJ per year (167–205 Mtpa) in 2021. This is significantly higher than the volumes published by DESNZ (DESNZ, 2023a) of 370 PJ per year for 2025 but agrees with the range of the volumes published by Supergen Bioenergy (Welfle et al., 2020) of 1014–2138 PJ per year for 2025. The volume reported by DESNZ (DESNZ, 2023a) is conservative and may likely represent the volume of biomass available after competing use. For example, in the breakdown of DESNZ (DESNZ, 2023a) volumes, the component of residual biogenic waste is 60 PJ per year. In this report, the total available potential volume of BMW is 330.4–382 PJ per year, with a minimum of 57.3 PJ per year available after competing use. The volumes presented by Supergen Bioenergy (Welfle et al., 2020) are for 2025 scenarios. Also, they considered some biomass resources that were not included in this report such as food crops and algae. This report considers only non-food biomass feedstocks that are of UK origin. Currently, algae production is negligible, but in the future, it may form a significant source of biomass in the UK.

3.2. Overview of drop-in fuel production

Drop-in fuels can be produced from non-food biomass feedstocks through two major routes, which can be classified into thermochemical and biochemical methods. The thermochemical methods usually involve a combination of thermal and chemical processes, such as gasification with Fischer–Tropsch synthesis (FTS) and pyrolysis with upgrading. Thermochemical routes often referred to as biomass to liquids (BTL), are fast and energy-intensive, occurring at moderate to high temperatures, see Fig. 7 and Table 3. Biochemical routes utilise microbes through processes such as AD and fermentation to break down biomass feedstocks into intermediates, which can be chemically converted to renewable hydrocarbons. Thermochemical methods have many advantages in fuel production over biochemical methods, such as (i) Fast reaction rate and plant start-up time, due to the short process completion time ranging from seconds to minutes, unlike biochemical methods which are relatively slow and often lead to the process plants having a very long start-up and plant stabilisation time of up to several weeks (Bridgwater, Meier and Radlein, 1999); (ii) Ability to handle a wide variety of feedstocks and a sudden change in feed composition without a significant process upset; (iii) Higher fuel conversion rates. However, unlike biochemical processes, thermochemical methods are usually characterised by (i) Higher energy demand due to the energy intensity of the processes, (ii) Undesirable tar and char formations which contribute to catalyst poisoning and corrosion, and (iii) Slag and salt depositions which can cause low heat transfer and corrosion (Kruse and Faquir, 2007; Kruse, 2008; Yakaboylu et al., 2015).

Energy consumption and integration of thermochemical processes can play an important role in fuel production yield and production price. Thermochemical processes with lower external thermal energy and lower external hydrogen demand would generally produce a lower product yield per biomass feed since some of the biomass feed and intermediaries would be consumed within the processes for hydrogen and heat generations. This can be seen from Fig. 7, which shows drop-in fuel production processes with higher energy consumption had higher product yield compared to processes with lower energy consumption.

Table 2
UK non-food biomass feedstocks availability.

Feedstock	Moisture content (%)	LHV on dry basis (MJ/kg)	Production, Mtpa (wet)	Competing case, Mtpa	Potential access for new competing uses	
					In 2021	In 2030 vs 2022
BMW	42–55	13.1–17.5	34.6–40 (19.6–24.6[a])	6–11	Good	Decreases
Straw	15	15–18.6	11–12	2.9–3.6	Good	Stable
Animal manure	78.5	14.4–16.8	72–90 (69.5–87.5[b])	0–87.5[b]	Good	Stable
Forest residues	50	15.8–21.4	2.7–4.1	~2.2	Good	Slight increase
Wood waste	20	18.5–21.0	4.5–5	0.8–3.7	Low	Decreases
Virgin wood	52	15.8–21.4	10.8	~0	Low	Stable
Sludge waste	95	12–15	28.2–30	28.2–30	Good	Stable
Food waste	58–95	16.8–22.9	11.1–13.1 (6.2–8.2[c])	2–6[c]	Good	Decreases
Digestates	90–95	14.3–19.6	14.2	0–14.2	Good	Increases
Miscanthus	16	17	0.08–0.13	~0	Low	Stable
Short rotation coppice	20	16.5–19	0.03–0.05	~0	Low	Stable
UCO	0	37	0.25–0.40	~0	Low	Stable
Black and brown liquor	82–85	9.0–13	0.28	~0	Low	Stable
Tallow	0	37.0–38.4	0.08–0.12	~0	Low	Stable
Crude glycerine	5–15	14.0–20	0.03	~0	Low	Stable

[a] Volumes of BMW excludes 10 Mt. MSW food waste and 5 Mtpa wood waste volumes to avoid double counting. See Sections 3.1.1 to 3.1.8 for details.
[b] Assumed volume of manure excludes 2.5 Mtpa used in AD to avoid double counting.
[c] Volume of food waste used in AD is removed from the volume of food waste available to avoid double counting.

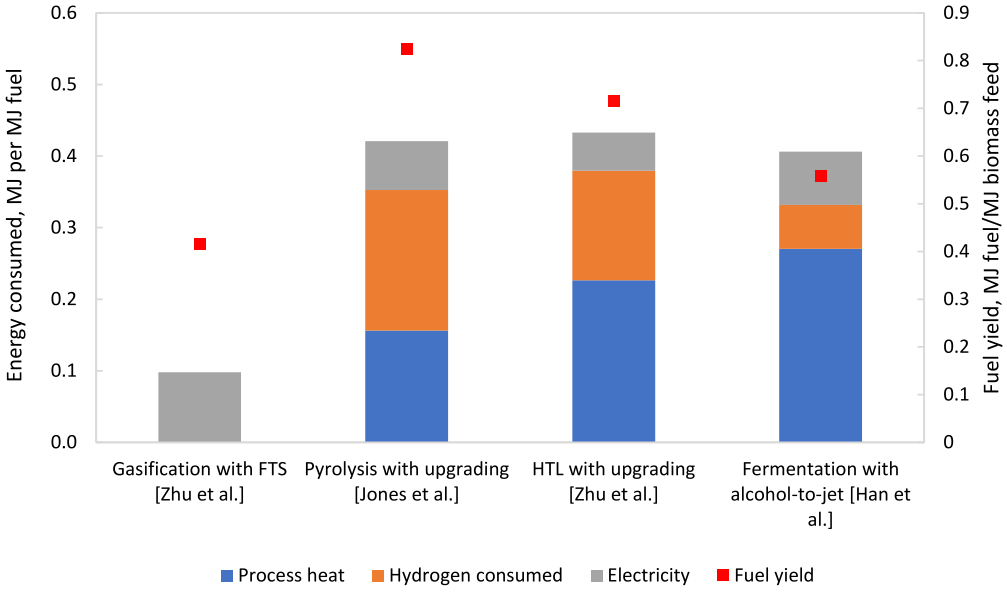

Fig. 7. Energy consumption of some thermochemical drop-in fuel production processes in comparison to biochemical-based processes, based on data reported by Zhu et al. (Zhu et al., 2011, 2014), Jones et al. (Jones et al., 2009), and Han et al. (Han et al., 2017). Process heat in these studies was supplied by natural gas, however, other low-carbon sources like biomass or green electricity can also be used for heating.

Table 3
Summary of key drop-in fuels thermochemical processing routes.

Process	Feed suitability	Conditions		Yield	Unit	Ref.
		Pressure	Temp.			
Gasification	Dry	Low	600–1300 °C	3–8.3 wt%(25–48.5 wt%)	H_2 (syngas)/kg dry feed	(Naik et al., 2010; Moghadam et al., 2014; Jaganathan et al., 2019)
Pyrolysis	Dry	Low	350–1000 °C	70–75 wt%	Bio-oil[a]/kg dry feed	(Bridgwater et al., 1999; Canabarro et al., 2013)
Supercritical water gasification (SCWG)[b]	Wet	22–35 MPa	350–800 °C	0.2–6 wt%	H_2/kg dry feed[c]	(Basu and Mettanant, 2009; Okolie et al., 2019; Yang et al., 2020)
HTL[a]	Wet	5–40 MPa	200–400 °C	20–80 wt%	Biocrude[b]/kg dry feed	(Zhang, 2016; Yang et al., 2020; Mishra et al., 2022)

[a] Bio-oil and biocrude which have similar properties to crude oil have energy contents of 13–18 MJ/kg and 16–19 MJ/kg, respectively.
[b] The operating boundaries of SCWG and HTL are different with SCWG using water at a supercritical state in contrast to the HTL operating with water at a sub-critical state. See Sections 3.2.3 and 3.2.4 for details.
[c] Methane is another valuable product produced in comparable quantity, 2–16 wt% CH_4/kg dry feed.

For biochemical processes like fermentation, the limitation is often driven by the reaction stoichiometry and subsequent biofuel upgrading pathway. As the energy demand of thermochemical processes can exceed 0.30 MJ/MJ of fuel produced, the energy penalty of thermochemical processes will maintain a very high influence on the fuel production yield and price. Therefore, heat integration can be critical to the success of drop-in fuel production. Heat integration of pyrolysis processes by Yang et al. (Yang et al., 2018) claimed up to 70 % reduction in energy consumption can be achieved in microwave-assisted pyrolysis. Also, Pedersen et al. (Pedersen et al., 2018) analysis showed similar benefits on energy demand following the heat integration of hydrothermal liquefaction of lignocellulosic biomass, as heating and cooling demand reductions of 55.2 % and 89.6 % respectively were achieved upon heat integration. Consequently, the impact of energy savings can have a significant reduction in the fuel production price, as more than a 20 % reduction in fuel production price was achieved by Yang et al. (Yang et al., 2018) in comparison to prices in the absence of heat integration.

This review considers key thermochemical methods for drop-in fuels from biomass, which can be sub-classified into four major pathways: gasification pathway, supercritical gasification pathway, pyrolysis pathway and HTL pathway. Table 3 shows some of the characteristics of the thermochemical drop-in fuel production methods.

3.2.1. Gasification

Gasification is a process which produces a gas mixture through the partial oxidation of carbon-based materials in the presence of oxidizing agents such as air, oxygen, and steam at high temperatures. The main product of gasification is synthesis gas, also known as syngas, which mainly consists of CO and H_2. The hydrogen gas yield is in the range of 30–83 (485) g H_2 (syngas)/kg feed, see Table 3. Gasification processes can be catalytic and non-catalytic. Catalytic gasification typically requires lower temperatures of around 900 °C compared to non-catalytic which requires as high as 1300 °C (Naik et al., 2010). Also, gasification is typically applied to low moisture content feedstocks due to the high energy requirements of drying higher moisture content feedstocks.

Drop-in fuel production through the gasification route involves the use of two or more key processes alongside, where the syngas from gasification is further upgraded into the final product. Processes used to upgrade syngas include FTS (Larson, Jin and Celik, 2009), Methanol-To-Gasoline (MTG) (Jones and Zhu, 2009), Topsoe Integrated Gasoline Synthesis (TIGAS) (Dimitriou, Goldingay and Bridgwater, 2018). As shown in Fig. 8, which summarises some of the various gasification pathways for drop-in fuel production, various liquid fuel products such as gasoline and diesel can be produced through this pathway.

3.2.2. Pyrolysis

Pyrolysis is a high-temperature process which decomposes carbon-based materials into smaller units in an oxygen-free environment, as shown in Table 3. Depending on the heating rate and temperature of the process, pyrolysis can be divided into fast and slow pyrolysis. Fast pyrolysis, which is usually employed in BTL, combines rapid heating of biomass, high temperature and short residence time of fewer than 2 s (Bridgwater et al., 1999). The high heating rate employed in fast pyrolysis is characterised by high heat transfer, making the use of fluidised bed reactors widely applicable in fast pyrolysis (Wang et al., 2005; Zhang et al., 2011). The product distribution is liquid (70–75 wt%), gas (10–15 wt%) and char (10–15 wt%). The liquid product often referred to as bio-oil is a highly viscous and complex mixture consisting of many organic compounds such as benzene, phenols and aldehydes (Mourant et al., 2013; Aysu and Küçük, 2014). It has a typical mass density and LHV of 1200–1300 kg/m^3 and 13–18 MJ/kg, respectively (Ringer et al., 2006). Like gasification, pyrolysis is suitable for low moisture content biomass feedstocks, due to the high energy demand associated with the drying of wet feedstocks before thermal degradation.

The production of drop-in fuels using the pyrolysis route is usually achieved through a combination of different processes, such as pyrolysis with upgrading (Anex et al., 2010) or pyrolysis with bio-oil gasification and upgrading (Li et al., 2015), where the bio-oil produced in pyrolysis is converted into liquid hydrocarbon fuels. Also, bio-oil can be co-processed (up to 20 %, by weight) with petroleum-intermediate feedstocks such as vacuum gas oil in existing refineries without triggering major plant modifications (Bhatt et al., 2020). Fig. 9 shows a schematic of the various drop-in fuel production pathways from the pyrolysis route.

3.2.3. Supercritical water gasification

Supercritical water gasification (SCWG) is a moderate temperature process which produces a fuel gas through the conversion of high moisture content biomass at high pressures. SCWG takes place in the presence of water, above its critical pressure of 221 bar and temperature of 374.29 °C, where the distinction of water between liquid and vapour phases does not exist (Heidenreich et al., 2016; Moghaddam et al., 2021). The water, by acting both as a reactant and catalyst, decomposes biomass feedstocks into a fuel gas which is mainly H_2 and CH_4. The hydrogen gas yield in SCWG is in the range of 1–30 mol H_2/kg dry feedstock (Basu and Mettanant, 2009; Okolie et al., 2019; Yang et al., 2020). In SCWG, biomass with a high moisture content that can exceed 90 wt% such as cattle manure and sewage sludge can be converted into drop-in fuels without employing the energy-consuming pre-treatment process of drying, which is required for processes such as gasification and pyrolysis (Heidenreich et al., 2016; Boukis et al., 2017). About 2.3 MJ/kg at atmospheric conditions is required to evaporate water in biomass feedstocks (Datt, 2011), and this can lead to negative net energy production in cases where the energy produced is less than the energy used for drying the biomass. Hence, SCWG is most suitable for high moisture-content feedstocks.

Like gasification, drop-in fuel production methods based on SCWG can employ processes such as SCWG with FTS (Campanario and Gutiérrez Ortiz, 2017), methanol synthesis with MTG, and gasification with TIGAS (Dimitriou et al., 2018). Fig. 10 shows a summary of the drop-in fuel pathways using SCWG.

3.2.4. Hydrothermal liquefaction

HTL is a process in which biomass is converted into a high-energy-density liquid product using pressurized hot water at sub-critical conditions (see Table 3). Typically, HTL is employed at high pressures of 5–40 MPa, moderate temperatures of 250–350 °C, and a short reactor residence time of 5–90 min. Like SCWG, HTL allows for the use of very high moisture feedstocks without the need for the energy-intensive

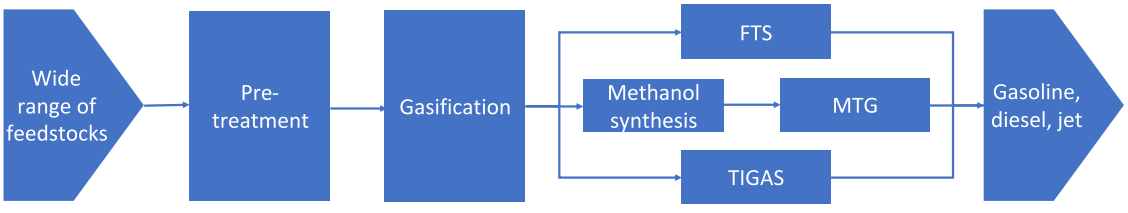

Fig. 8. Drop-in fuel production pathways via gasification pathway.

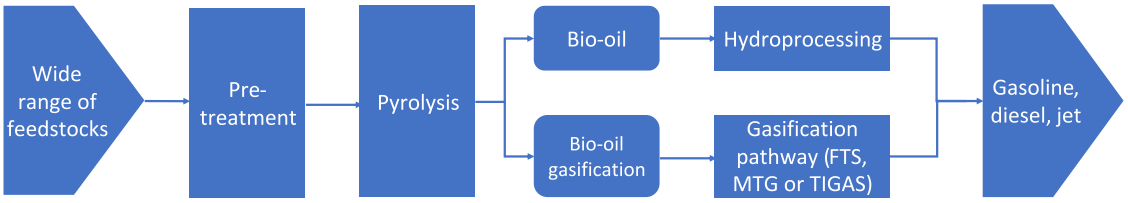

Fig. 9. Drop-in fuel production pathways via pyrolysis pathway.

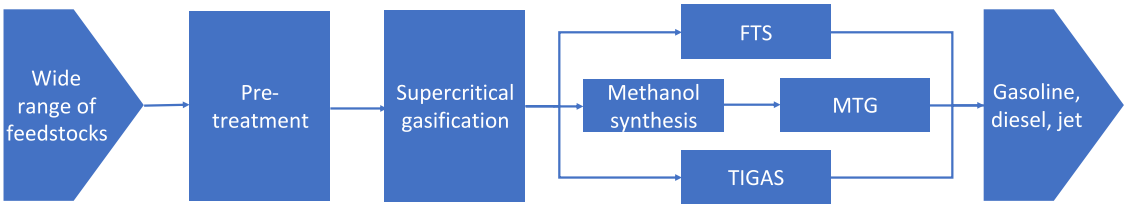

Fig. 10. Drop-in fuel production pathways via SCWG pathway.

process of drying. The liquid product, often referred to as biocrude, has a yield typically in the range of 20–80 wt% biocrude per dry mass of feed (Li et al., 2013; Mishra et al., 2022). Biocrude produced from HTL typically has a high mass density in the range of 910–1120 kg/m^3, which is similar to that of pyrolysis bio-oil. However, biocrude heating value of 30–40 MJ/kg is significantly better than those of pyrolysis bio-oil of 16–19 MJ/kg (Ringer et al., 2006; Yang et al., 2020). Like crude oil, the chemical composition of biocrude is complex, consisting of a mixture of many organic compounds ranging from fatty acids (myristic acid, palmitic acid, stearic acid, and oleic acid) to oxygenates (esters, ketones, alcohols, furans) (Yang et al., 2020).

Like pyrolysis, biocrude produced from HTL can be converted into drop-in fuel using hydroprocessing at dedicated refineries or by co-processing with petroleum in conventional refineries (Snowden-Swan et al., 2017; Bhatt et al., 2020). Co-processing of biocrude with petroleum intermediates in conventional refineries may be limited by technical requirements due to some unsuitable physio-chemical properties of biocrude like high nitrogen content. Also, biocrude can be gasified into syngas, where renewable hydrocarbon fuels can be obtained by further processing the syngas, although this process is not commonly practised mainly due to the high quality of biocrude and lower yield of gasification, see Fig. 11.

3.3. Hydrogen sources

In addition to thermal energy consumption, hydrogen is a key input in the thermochemical processes. The consumption of hydrogen is dependent on the drop-in fuel production routes, with pyrolysis bio-oil upgrading and HTL biocrude upgrading requiring 3.9–5.8 kg of hydrogen per 100 kg biocrude or bio-oil (Jones et al., 2014; Bennion et al., 2015; Jiang et al., 2019). Gasification routes may not directly consume hydrogen, as hydrogen is a key product in syngas, however, a water-gas-shift reaction is often used to improve the yield of hydrogen prior to fuel production using FTS. Hydrogen can be produced in situ or externally and imported into the plant for hydroprocessing. Generally, the production of hydrogen in situ in fuel production processes can cause serious impacts on fuel product yield and subsequently, the production price, especially when the biomass feeds are used in situ as sources of hydrogen. Based on Jones et al. (Jones et al., 2009), the use of biomass or bio-oil instead of natural gas for hydrogen production led to a 35 % reduction in the fuel product yield, as shown in Fig. 12. Also, approximately one-third of the biomass feedstock would be required for hydrogen generation in wood pyrolysis and upgrading, based on the 100 % renewable feedstock basis. Currently, other low-carbon sources of hydrogen are gaining market attention, such as green hydrogen produced from water electrolysis using renewables. This can improve the sustainability of drop-in fuel production.

The sensitivity analysis performed by many authors (Jones et al., 2014; Pedersen et al., 2018; Yang et al., 2018) indicated that the production price of drop-in fuels is highly dependent on the cost of

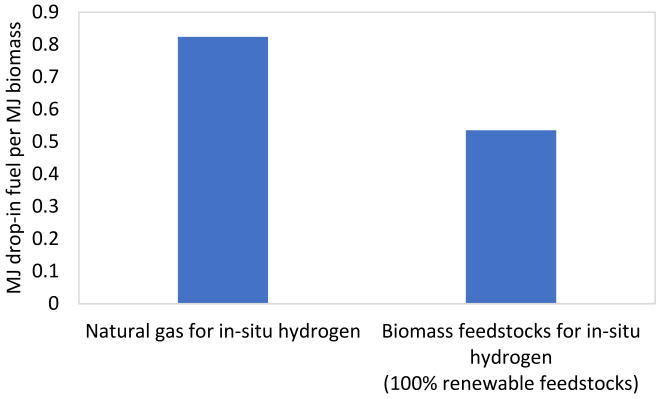

Fig. 12. Drop-in fuel product yield for different hydrogen sources in bio-oil upgrading facilities. Data from Jones et al. (Jones et al., 2009).

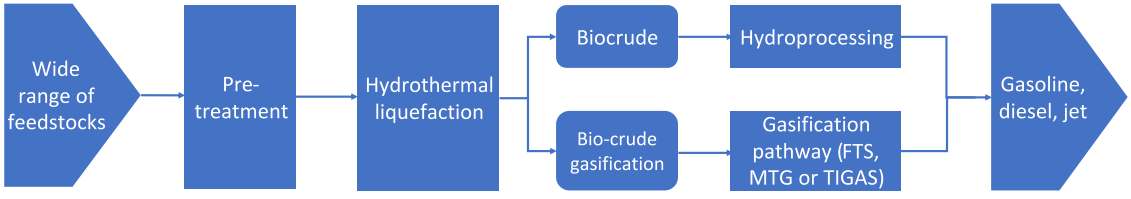

Fig. 11. Drop-in fuel production pathways via HTL pathway.

Table 4
Hydrogen sources, their cost, and emissions factors.

Hydrogen source	Cost, $/kg		Emissions factors, g CO_2eq/MJ (LHV)		References
	2020	2050	2020	2050	
Natural Gas SMR (no carbon capture and storage [CCS])	0.7–1.6	–	83.6	82.0	(BEIS, E4tech and LBST, 2021; IEA, 2022b)
Natural Gas SMR with CCS	1.2–2.1	1.2–2.1	21.4	19.2	(BEIS, E4tech and LBST, 2021; IEA, 2022b)
Coal (no CCS)	1.9–2.5	–	203.3–229.2	203.3–229.2*	(Valente et al., 2021; IEA, 2022b)
Coal with CCS	2.1–2.6	2.2–2.5	64.2	64.2*	(Valente et al., 2021; IEA, 2022b)
Low-carbon electricity	3.2–7.7	1.3–3.3	0.1	0.1	(BEIS, E4tech and LBST, 2021; IEA, 2022b)

* Assumed negligible changed in emissions due to the fossil nature, similar to natural gas SMR.

hydrogen sources. Hydrogen from different sources has different prices and associated GHG emissions factors (see Table 4), and this may impact both the fuel prices and GHG emissions of the fuel since both fuel economics and GHG emissions are highly dependent on the material and energy inputs. Lilonfe et al. (Lilonfe et al., 2024) analysis of drop-in fuel showed that an additional fuel production cost of up to £5.40 per GJ can obtained from the use of low-carbon hydrogen. However, the GHG emissions benefits of using low-carbon hydrogen are better, with up to 40 % reduction in emissions relative to the corresponding grey hydrogen scenarios.

3.4. Production approaches: Centralised vs decentralised

The production of a product can be done in a single location as in the case of centralised production or in multiple locations where one form of processing occurs at a different location as in the case of decentralised production, see Fig. 13. A centralised production approach for drop-in fuels is achieved when both the feedstock conversion to intermediate products (such as syngas) and the conversion of the intermediates to drop-in fuels are done in a single facility. This approach traditionally offers a significant advantage in production cost because of the economy of scale, as often large plant scales are used in centralised fuel production. Also, it offers great opportunities for extensive heat integration and consequently potential reduction in energy cost, since off-gases produced from feedstock pre-treatment and conversion to intermediates can be used in the fuel conversion stage and vice-versa. However, the use of decentralised approaches in fuel production from biomass feedstocks has been suggested by some authors to offer better benefits in fuel production prices, especially in the reduction of biomass feedstocks transportation cost, which is typically significant due to the low bulk density and high moisture content of some biomass feedstocks such as straw and sewage sludge. Smaller plant scales are often used in a decentralised approach to meet the local demand and transformation of low-density and high moisture-content feedstocks into high-energy-density intermediates such as biocrude and syngas (Snowden-Swan et al., 2017). As a result, decentralised approaches are also suggested to offer better GHG emissions associated with the transportation of feedstocks, intermediates, and products. However, decentralised approaches leave little allowance for heat integration due to the nature of the segmented operations. Another key barrier in decentralised approaches is losing the economy of scale from the larger, centralised facility.

Despite the proposed benefits of centralised and decentralised approaches in drop-in fuel production prices and GHG emissions, not many extensive investigations have been made on the impacts of centralised and decentralised operations on fuel production cost. A study by Lilonfe et al. (Lilonfe et al., 2024) showed that the use of either a centralised or decentralised operation for optimising fuel production price is highly dependent on the availability and distribution of feedstocks in a location, as both the economy of scale and feedstock transportation plays a significant role in fuel economics. Based on the study, for biomass feedstocks with high moisture content, low availability and distribution, a centralised approach is more economical as the benefits of economy of scale outweigh the high feedstock transportation costs. However, above certain local availability and distribution of the feedstocks, 6000 kg/h of dry feed for wet biomass, the decentralised approach performs better than the centralised approach as the impact of transporting wet feedstocks becomes more dominant in the overall economics. Furthermore, the difference in GHG emissions from using a centralised versus decentralised approach in fuel production is negligible, as the emissions associated with the transportation of feedstocks make up only a small portion of the fuel's total GHG emissions.

3.5. Economic analysis

Drop-in fuels from biomass have attracted significant attention in recent years due to their environmental benefits and easy integration

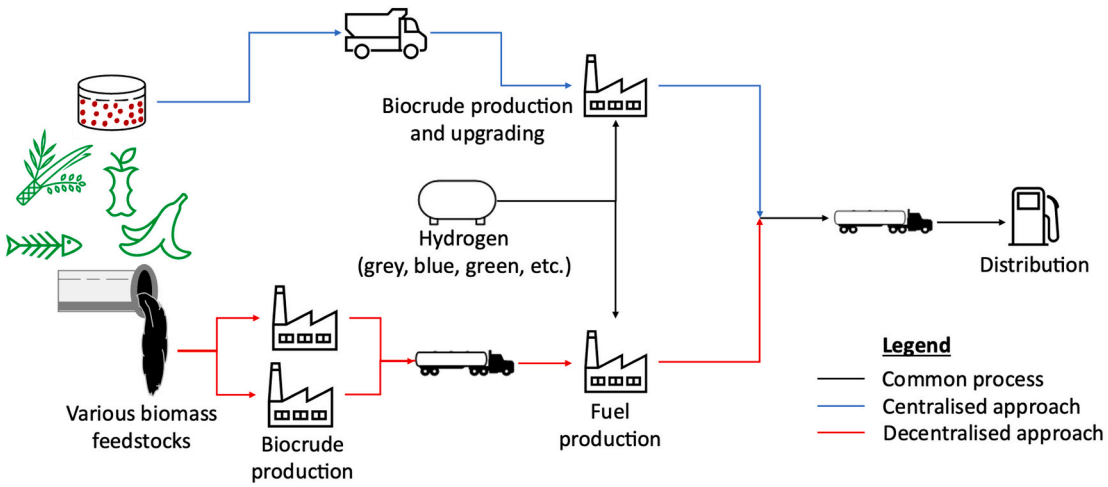

Fig. 13. Centralised and decentralised fuel production approaches in drop-in fuel production via HTL.

into existing vehicle engines and fuel supply chains. TEA is a tool for analysing the economic performance of industrial plants, processes, or products (Zimmermann et al., 2020). It is widely used in the estimation of the capital cost, operating cost, revenue, and product cost of drop-in fuels, based on technical and financial input parameters. These technical and economic data are particularly important and provide preliminary insights to inform plant design, construction, and operations of successful drop-in fuel plants. Numerous studies have been published on the TEA of BTL using various fuel production approaches, see Table 5. These studies reported minimum product prices for drop-in fuels in the range of $0.60–3.88 per gasoline litre equivalent (GLE) [$17.14–110.82 per GJ] when adjusted to the 2021 USD. Chemical engineering plant cost indices and 2021 exchange rate of £1 to $1.3496 were used where necessary, to adjust for changes in the original results, due to inflation and currency differences from the original analysis. The range of drop-in fuel prices, which are dependent on many factors, reflects the 2021 average price of conventional diesel fuels of $1.22 per GLE ($38.57 per GJ), based on 2021 wholesale prices of diesel published by RAC (RAC, n. d.). These fuel prices are highly impacted by factors such as the fuel conversion route, feedstock cost, transportation cost, tax rate, total capital investment, internal rate of return (IRR), product yield, plant scale, and hydrogen source. The optimal integration of these factors into the TEA is critical for the profitability and competitiveness of BTL.

Table 5
Summary of some important TEA studies on drop-in fuels via thermochemical processing routes.

Source	Technique	Product	Plant type	Capital cost (million USD_{2021})	MFSP (USD_{2021} per GLE)
(Michailos et al., 2017)	▪ Feed input of 2200 t/d cane bagasse ▪ Gasification with FTS	Drop-in fuels	No data	40–46	0.61
	▪ Feed input of 2200 t/d cane bagasse ▪ Fast pyrolysis with upgrading	Drop-in fuels	No data	33–50	0.66
(Li et al., 2015)	▪ Feed input of 2000 t/d biomass/bio-oil ▪ Fast pyrolysis, bio-oil gasification and FTS	Drop-in fuels	nth	685	1.66
(Zhu and Valkenburg, 2011)	▪ Feed input of 2200 t/d wood chips ▪ Gasification with FTS ▪ Different gasifier heating scenarios considered	Drop-in fuels	nth	525–711	1.42–1.64
	▪ Feed input of 2200 t/d wood chips ▪ Gasification, methanol conversion and MTG ▪ Different gasifier heating scenarios considered	Gasoline, LPG	nth	476–660	1.08–1.37
	▪ Feed input of 2200 t/d wood chips ▪ Fast pyrolysis with upgrading ▪ Different gasifier heating scenarios considered	Drop-in fuels	nth	439	0.84
(Swanson et al., 2010)	▪ Feed input of 2000 t/d corn stover ▪ Gasification with FTS	Drop-in fuels	nth	725–870	1.56–1.72
	▪ Two scenarios were considered- low and high temperature gasification, ▪ Nth and first-of-its-kind plant	Drop-in fuels	first-of-a-kind	1594–2029	2.74–2.93
(Carrasco et al., 2017)	▪ Feed input of 2000 t/d forest residues ▪ Fast pyrolysis with upgrading ▪ Laboratory demonstration and TEA of liquid fuels from forest residue via pyrolysis	Drop-in fuels	first-of-a-kind	584	1.85
(Tanzer et al., 2019)	▪ Feed input of 500 t/d various agricultural residues ▪ Gasification with FTS	Drop-in fuels	first-of-a-kind	281–358	1.90–3.88
	▪ Feed input of 500 t/d various agricultural residues ▪ Fast pyrolysis with upgrading	Drop-in fuels	first-of-a-kind	224–332	1.61–3.35
	▪ Feed input of 500 t/d various agricultural residues ▪ HTL with upgrading	Drop-in fuels	first-of-a-kind	268–370	1.50–4.27
(Dimitriou et al., 2018)	▪ Feed input of 2000 t/d woody biomass ▪ Gasification with FTS ▪ Various BTL pathways	Drop-in fuels	No data	678–703	0.82–0.84
	▪ Feed input of 2000 t/d woody biomass ▪ Gasification, methanol conversion and MTG ▪ Various BTL pathways	Drop-in fuels	No data	841–895	1.08–1.19
	▪ Feed input of 2000 t/d woody biomass ▪ Gasification, TIGAS ▪ Various BTL pathways	Drop-in fuels	No data	661–711	0.90–0.92
(Rahbari et al., 2019)	▪ Feed input of 16,000 t/y algae ▪ SCWG with FTS ▪ Solar-driven SCWG-reforming and FTS	Drop-in fuels	nth	172	2.69
(Campanario and Gutiérrez Ortiz, 2017)	▪ Feed input of 60 t/h bio-oil aqueous phase ▪ SCWG with FTS	Drop-in fuels	No data	85–189	1.08
(Zhu et al., 2014)	▪ Feed input of 2000 t/d woody biomass ▪ HTL with upgrading	Drop-in fuels	first-of-a-kind	742	1.60
	▪ Nth and first-of-its-kind plant	Drop-in fuels	nth	678	0.90
(Pedersen et al., 2018)	▪ Feed input of 1000 t/d organic matter ▪ HTL with upgrading ▪ Heat integration of model using pinch analysis	Drop-in fuels	No data	303	0.90–1.23
(Tews et al., 2014)	▪ Feed input of 2000 t/d forest residue ▪ HTL with upgrading ▪ Comparative studies of fast pyrolysis and HTL	Drop-in fuels	nth	323	0.60
(Jones et al., 2014)	▪ Feed input of 1349 t/d algae ▪ HTL with upgrading	Diesel	nth	608	1.40

3.6. Life cycle assessment

Currently, many LCA studies have been done on the life cycle impacts of drop-in fuels (De Jong et al., 2017; Vienescu et al., 2018; Kolosz et al., 2020), however, these studies are heavily focused on the global warming potential (GWP) of fuels, neglecting other sustainability factors such as abiotic depletion (ADP) and human toxicity potential (HTP). GWP of fuels enables easy comparison of drop-in fuels with conventional petroleum fuels. The GHG emissions of drop-in fuels from various sources are estimated to be in the range of -122 and 98 g CO_2eq per MJ, in which the upper band is as high as those of fossil fuels (94 CO_2eq/MJ-UK and EU RED II reference numbers). The large variation is due to factors such as feedstocks and associated land use change impacts, fuel processing techniques, allocation methods employed to attribute impacts across multiple product outputs, system boundary definitions, and energy sources (Fig. 14 and Table 6). However, generally, when biomass sources are obtained sustainably with no or marginal LUC and iLUC impacts, the GHG emissions are usually significantly lower than those of petroleum fuels and, in some cases, can even be negative in value. It is important to note that current policies in the EU and UK require that advanced renewable fuels achieve at least 65 % GHG savings (or 70 % if it is renewable fuels of non-biological origins) relative to fossil fuels (DESNZ, 2023a). Fig. 14 presents the summary of various approaches adopted by researchers in LCA analysis of drop-in fuels from thermochemical pathways. Fuels produced via gasification typically have the lowest GHG emissions, followed by those produced via HTL and then pyrolysis, due to the different material and energy demands of the processes.

3.7. Demonstration, pilot and commercial plants

Several BTL plants are in their commercial, pilot or demonstration stages. These plants typically utilise dry feedstocks for drop-in fuel production, as shown in Table 7.

3.8. Estimating potential UK drop-in fuel and GHG emissions volumes from available feedstocks

As summarised previously in Table 2, the key available feedstocks in the UK are BMW, straw, animal manure, forest residues, wood waste, sludge waste, food waste, and digestates. A total of 156–195 Mtpa (745–939 PJ per year) of UK-origin biomass are produced from non-food crops, excluding virgin wood as the UK is a net importer of wood biomass. In this analysis, two scenarios were used to estimate the potential of drop-in fuel in the UK, namely: the 100 % feedstock case and the competing case. The 100 % feedstock case is a theoretical scenario that assumes that all the non-food biomass in the UK can be utilised in drop-in fuel production, except those already used in biofuel applications like UCO. The competing case considers the existing competition that may exist with the use of the feedstocks such as the potential cost and GHG emissions implications amongst the competing alternatives.

In estimating the fuel and GHG emissions potential, it is worthwhile to note that the use of either a centralised or decentralised approach in processing biomass feedstocks produces the same fuel volumes since the supply chain losses for both approaches were assumed to be zero. Also, the use of a centralised or decentralised approach offers a negligible difference in GHG emission, however, the fuel production prices from these approaches can vary significantly (Lilonfe et al., 2024).

The product yields of drop-in fuels from the available biomass feedstocks are shown in Table 8. These biomass feedstocks can be readily processed using various fuel production methods discussed in Section 3.2. The yield of drop-in fuels from these production methods varies by biomass and by the fuel production methods. The availability and distribution of the feedstocks, moisture content, and product yield are used to determine what processing techniques are suitable for the feedstocks. Generally, gasification and pyrolysis are more suitable for low moisture content feedstocks like straw, while HTL and SCWG are more suitable for high moisture content feedstock like manure. Also, priority was given to methods of producing fuels such as those through bio-oils or biocrude synthesis and upgrading, which typically have higher product yields compared to gasification with FTS. The biofuel production methods that are suitable for these feedstocks are evaluated in Table 9.

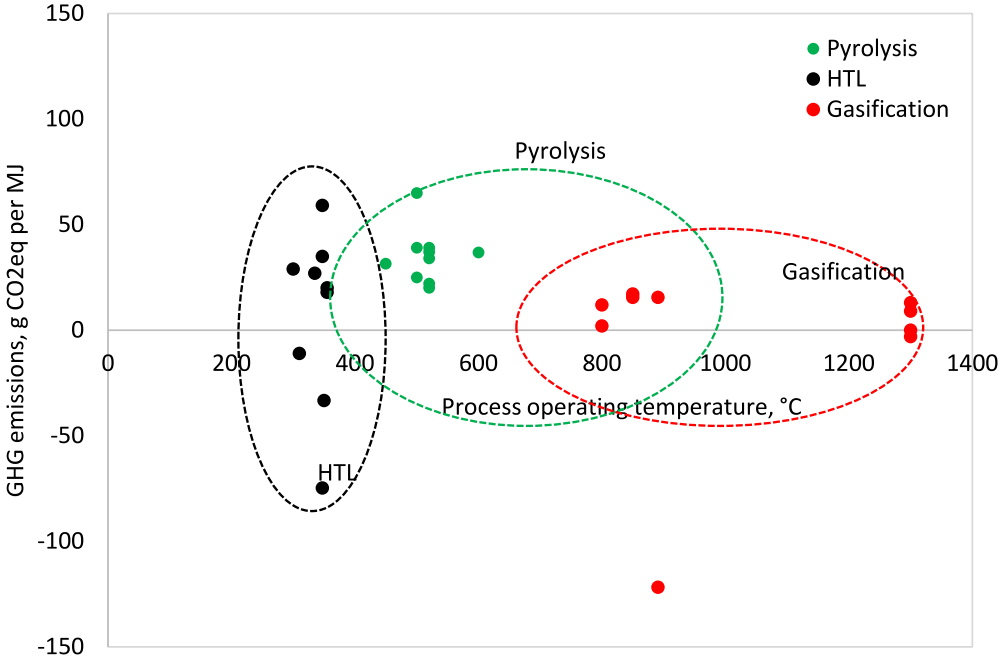

Fig. 14. The GHG emissions of drop-in fuels from key thermochemical processes. Negative net GHG emissions can be achieved incorporating CCS in the fuel production processes or avoiding severe consequential emissions sources.

Table 6
Summary of key LCA analysis on thermochemical fuel production routes.

Source	Techniques	LCA type	Metrics assessed	GHG Emissions (g CO_2eq/MJ)	Product	Other comments
(Bennion et al., 2015)	▪ Fuel path: HTL and pyrolysis of microalgae with hydroprocessing ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 MJ of diesel ▪ Allocation method: Energy	Attributional	GWP	-11.4 and 210	Diesel	▪ Fuel emissions for HTL and pyrolysis routes respectively ▪ HTL had lower fuel emissions ▪ Major GHG emissions driver: Drying of microalgae feedstock
(Vienescu et al., 2018)	▪ Fuel path: Pyrolysis of corn stover and oil upgrading using various approach ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 kg of biofuel ▪ Allocation method: Energy	Attributional	GWP	53.3 – 142.9	Liquid fuels	▪ Fuel emissions of bio-oil hydro-processing were the best, in comparison to other upgrading approaches ▪ Major GHG emissions driver: Electricity for energy demand
(Snowden-Swan and Male, 2012)	▪ Fuel path: Pyrolysis and hydroprocessing of woody biomass using various energy sources ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 MJ of gasoline ▪ Allocation method: Energy	Attributional	GWP	31.5 – 36.8	Gasoline	▪ Fuel emissions from biomass power are lower than grid power ▪ Major GHG emissions driver: Power and natural gas usage
(Ou et al., 2022)	▪ Fuel path: HTL and hydroprocessing of swine manure ▪ Boundaries: Well-to-Wheels ▪ FU: 1 MJ of liquid fuels ▪ Allocation method: Energy	Consequential	GWP	-33.3	Liquid fuels	▪ Major GHG emissions driver: Avoided emissions from the current treatment method and fuel production stage
(Peters et al., 2015)	▪ Fuel path: Pyrolysis and hydroprocessing of hybrid poplar ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 MJ of liquid fuels ▪ Allocation method: Energy and mass	Attributional	GWP, ADP, eutrophication potential (EP), acidification potential (AP)	39	Gasoline, diesel	▪ Major GHG emissions driver: Electricity consumption, especially from biomass dryer
(de Jong et al., 2017b)	▪ Fuel path: Jet fuel from various feedstocks via six fuel conversion technologies including Hydroprocessed Esters and Fatty Acids, FTS, HTL, pyrolysis, Alcohol-to-Jet ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 MJ of jet fuel ▪ Allocation method: Energy and system expansion (displacement) methods	Attributional	GWP	-3 – 40	Jet fuel	▪ Thermochemical routes had the lowest fuel emissions. Emissions of gasification lower than HTL and HTL lower than pyrolysis processes ▪ Major GHG emissions driver: Feed cultivation and co-credit in the gasification route, while hydrogen use in HTL and pyrolysis
(Hsu, 2012)	▪ Fuel path: Pyrolysis and hydroprocessing of forest residues ▪ Boundaries: Well-to-Wheels ▪ FU: 1 km of travel by a light-duty passenger vehicle ▪ Allocation method: Energy	Attributional	GWP	25 – 39	Gasoline, diesel	▪ Fuel emissions from biomass-derived electricity lower ▪ Major GHG emissions driver: Fast pyrolysis stage
(Frank et al., 2013)	▪ Fuel path: HTL and hydroprocessing of algae ▪ Boundaries: Well-to-Wheels analysis ▪ FU: 1 MMBTU of diesel ▪ Allocation method: Energy	Attributional	GWP	29.4	Diesel	▪ Major GHG emissions driver: Hydrogen consumption in oil upgrading
(Tews et al., 2014)	▪ Fuel path: HTL and pyrolysis of woody feedstocks with hydroprocessing ▪ Boundaries: Well-to-Wheels ▪ FU: 1 MJ of liquid fuels ▪ Allocation method: Energy	Attributional	GWP	27 – 34	Gasoline, diesel	▪ Fuel via HTL had lower emissions than pyrolysis ▪ Major GHG emissions driver: Fuel production stage
(Masoumi and Dalai, 2021)	▪ Fuel path: HTL of algae with hydroprocessing, using biochar energy source ▪ Boundaries: Well-to-Wheels ▪ FU: 1 kg of fuel ▪ Allocation method: Energy	Attributional	GWP	-5.9 – -1.1	Liquid fuels	▪ Fuel emissions from the use of char for energy in HTL are lower than its use in the fuel catalysis ▪ Major GHG emissions driver: Methanol used as reactive organic co-solvent in HTL

(*continued on next page*)

Table 6 (*continued*)

Source	Techniques	LCA type	Metrics assessed	GHG Emissions (g CO_2eq/MJ)	Product	Other comments
(Tsalidis et al., 2017)	▪ Fuel path: Gasification with FTS of torrefied wood pellets, wood pellets and straw ▪ Boundaries: Well-to-Wheels ▪ FU: 1 km of distance travelled by a vehicle ▪ Allocation method: Energy	Attributional	GWP, EP, particulate matter potential, AP	15.6 – 17.2	Diesel	▪ Fuel emissions from torrefied wood pellets are lowest, followed by wood pellets and then straw ▪ Major GHG emissions driver: Gasification and gas cleaning
(Fernanda Rojas Michaga et al., 2022)	▪ Fuel path: Gasification of forest residues with FTS and CCS ▪ Boundaries: Well-to-Wheels ▪ FU: 1 MJ of jet fuel ▪ Allocation method: Energy and system expansion (displacement) methods	Attributional	GWP	-127.1 – 15.6		▪ Fuel production with CCS and allocation by system expansion methods had the lowest emissions ▪ Major GHG emissions driver: CCS and wood chips processes
(Sun et al., 2021)	▪ Fuel path: Fermentation to ethanol, pyrolysis to bio-oil, and gasification to jet fuel using corn stover ▪ Boundaries: Well-to-Wheels ▪ FU: 1 GJ biofuel consumed ▪ Allocation method: Energy and system expansion	Attributional	GWP, AP, EP, HTP and ozone layer depletion potential	19.9	Jet fuel	▪ Fuel emissions from fermentation were slightly lower than gasification, while pyrolysis had the highest emissions ▪ Major GHG emissions driver: Bio-oil upgrading in pyrolysis and fuel synthesis and refining in gasification

Table 7
List of some BTL plants.

Project, Location	Product	Key processes	Operation status	Type	Ref.
Sierra Biofuels Plant, USA	▪ Feed: MSW ▪ Capacity: 175,000 t/y of MSW ▪ Product: Drop-in fuels	Gasification, FTS	2022	Commercial	(Fulcrum BioEnergy, n.d.)
The COMSYN, Finland	▪ Feed: Various biomass ▪ Capacity: 800 t/y of biomass ▪ Product: Drop-in fuels	Gasification, FTS	2017	Demonstr. unit	(COMSYN, n.d.)
BTG Bioliquids, Netherlands	▪ Feed: Various biomass ▪ Capacity: 24,000 t/y of bio-oil ▪ Product: Bio-oil	Pyrolysis	2015	Commercial	(*Empyro Hengelo, NL, n.d.*)
TRI PDU, USA	▪ Feed: Various biomass ▪ Capacity: 4 t/y of biomass ▪ Product: Drop-in fuels	Gasification, FTS	2020	Demonstr. unit	(TRI, n.d.)

The potential GHG emissions associated with fuel production from the UK-origin biomass feedstocks, which are available in scalable quantities as shown in Table 9, were calculated using the emission factors in Table 10. Some of the wet biomass feedstocks like food waste may have GHG emissions of 35 gCO_2eq/MJ, producing emissions reductions of 63 % relative to a fossil fuel comparator of 94 gCO_2eq/MJ, which is just slightly missing the target mark of 65 % GHG emissions reduction relative to fossil fuel set by DESNZ (DESNZ, 2023a). Since the GHG emissions rates have some degree of uncertainties with the limited number of references available for these feedstocks, these numbers were nevertheless used in estimating the GHG emissions of fuel here. The fuel's GHG emissions from these feedstocks can be reduced by changing the supply chain or fuel production process. For example, by replacing the process heat supply from natural gas and grey hydrogen for hydroprocessing with renewables (Lilonfe et al., 2024). Using waste biomass feedstocks can have other additional impacts beyond GHG emissions as highlighted in Sections 3.1.1 to 3.1.7. Also, it is worthwhile for biofuel policies relating to the application of waste biomass feedstocks to consider the consequential impacts of utilising waste biomass feedstocks. Table 9 provides both attributional and consequential GHG emissions impacts of the non-food biomass feedstocks considered in this analysis.

3.9. Drop-in fuel volumes

There is a significant potential for the production of drop-in fuel from UK-origin biomass feedstocks. The volumes of drop-in liquid fuels, which can be produced from UK-origin feedstocks are estimated to be 563 PJ per year and 269 PJ per year, for the 100 % feedstocks and competing case scenarios, respectively, as shown in Fig. 15. Most of the potential fuel volumes originate from wet feedstocks, such as BMW, animal manure, food wastes and sludge wastes, which can provide more than 75 % of the total drop-in fuel potential. These wet feedstocks are produced by human activity in cities and due to agricultural practices across the different regions of the UK, and their utilisation for fuel production would not compete with food crops. Manure, which is the most available resource in the UK, produces the highest fuel volumes compared to the other feedstocks. Comparing these potential volumes with 2021 UK road transport fuel consumption, these volumes are 38.2 % and 18.3 % of the 2021 road transport fuel volume consumption, based on 100 % feedstocks and competing cases, respectively. DESNZ (DESNZ, 2023b) reported the UK road transport fuel consumption volumes of 1473 PJ (1557 PJ by gross heating value, equivalent to 42,094 million L) in 2021. This shows there is a significant potential for drop-in fuels production from non-food biomass feedstocks to meet a significant portion of the current UK demand for transport fuels. The target for renewable fuel volume in transport fuel consumption in 2030 is at least

Table 8
Product yield of various drop-in fuels production routes.

Feedstock	Gasification (MJ/dry kg feed)	Pyrolysis (MJ/dry kg feed)	HTL (MJ/dry kg feed)	Comment/reference
BMW	–	–	13.7	(Snowden-Swan et al., 2017; Chen et al., 2020; Lilonfe et al., 2024)
Straw	6.0–8.1 (8.1*)	–	–	(Larson et al., 2009; Anex et al., 2010)
Animal manure	–	–	11.9	(Snowden-Swan et al., 2017, 2020)
Forest residues	4.8–8.8	6.35–13.9	8.5–13.9 (13.9*)	(Jones et al., 2009; Zhu et al., 2011, 2014; Snowden-Swan and Male, 2012; Dimitriou, 2013; Tews et al., 2014)
Wood	4.8–8.8	6.35–13.9 (13.9*)	8.5–13.9	(Jones et al., 2009; Zhu et al., 2011, 2014; Snowden-Swan and Male, 2012; Dimitriou, 2013; Tews et al., 2014)
Sludge waste	–	–	11.3	(Snowden-Swan et al., 2017; Lilonfe et al., 2024)
Food waste	–	–	13.7	(Snowden-Swan et al., 2017; Chen et al., 2020; Lilonfe et al., 2024)
Digestates	–	–	12.9	(Snowden-Swan et al., 2017; Lilonfe et al., 2024)

* Value used in this analysis to estimate drop-in fuel potential.

14 %, based on RED II (European Commission, 2019). Our initial estimates indicate that, purely from a UK feedstock availability perspective, this can potentially be achieved using non-food biomass feedstocks.

3.10. Total drop-in fuel GHG emissions

There is a significant emissions reduction from the use of these non-biomass feedstocks in the UK. Based on attributional and consequential GHG emissions factors evaluation, GHG emissions savings of 39.2 and 64.4 Mt. CO_2eq per year can be achieved by using 563 PJ per year of these drop-in fuels in the 100 % feedstock cases, respectively, relative to fossil fuels. These emissions savings are equivalent to 39.4 % and 64.7 % of the UK's 2021 road transport GHG emissions of 99.5 Mt. CO_2eq (Tiseo, 2024), respectively. Also, in the competing cases, GHG emissions savings of 18.7 and 29.8 Mt. CO_2eq per year can be achieved by using 269 PJ per year of drop-in fuels, respectively. These emissions savings are equivalent to 18.8 % and 29.9 % of the UK's 2021 road transport GHG emissions. The various emissions associated with fuel produced from the biomass feedstocks and the use of conventional diesel to meet the remaining demand of UK 2021 road transport fuel consumption are shown in Fig. 16. While these drop-in fuels can supply up to 38.2 % of current UK road transport fuel demand, in addition to the current 4 % being supplied by first-generation biofuels, there is a need for supplementary fuels such as synthetic electro-fuels to balance the total fuel demand. In the future, alternative vehicle technologies such as electric vehicles may reduce the overall liquid fuel demand in the transportation sector, thereby, making it potentially possible to meet the UK transport fuel demand sustainably from biomass feedstocks.

3.11. Hydrogen demand

The demand for hydrogen is significant and critical for drop-in fuel applications. Total hydrogen demand from the production of drop-in fuels from UK non-food biomass is estimated at 38.5–75.6 PJ per year, which is roughly 13 % of the drop-in fuel production potential energy volumes, see Table 11.

4. Conclusion

Concerns over climate change, energy security, food price inflations, and forestry degradations have led to rising interest in the developments and use of advanced generation fuels, particularly for the hard-to-abate freight and aviation transport sectors. Sustainable drop-in fuels can be produced from a variety of sources, including second to fourth-generation biomass feedstocks, which leverage waste and residual biomass products with potentially lower environmental impacts. Thermochemical methods of producing these advanced biofuels such as gasification with FTS and pyrolysis with upgrading, can be integrated into existing refineries. Thermochemical methods enable the use of a wide variety of biomass feedstocks ranging from agricultural residues to high moisture content wastes like food wastes. The performance indicators of thermochemical processes, such as product yield and price,

Table 9
Selection of feedstocks and processing techniques.

Feedstock	Availability, Mtpa (wet)	Competing case, Mtpa	MC (%)	Suitable for			Available in scalable quantities	Selected for drop-in biofuel
				Gasification	Pyrolysis	HTL		
BMW	19.6–24.6	6.0–11	50	✓	✓	✓	✓	✓
Straw	11–12	2.9–3.6	15	✓	✓	×	✓	✓
Animal manure	69.5–87.5	0–87.5	79	×	×	✓	✓	✓
Forest residues	2.7–4.1	~2.2	50	✓	✓	✓	✓	✓
Wood waste	4.5–5	0.8–3.7	20	✓	✓	×	✓	✓
Virgin wood*	10.8	~0	52	✓	✓	✓	×	×
Sludge waste	28.2–30	28.2–30	95	×	×	✓	✓	✓
Food waste	6.2–8.2	2–6	75	×	×	✓	✓	✓
Digestates	14.2	0–14.2	90	×	×	✓	✓	✓
Miscanthus*	0.08–0.13	~0	16	✓	✓	✓	×	×
Short rotation coppice*	0.03–0.05	~0	20	✓	✓	✓	×	×
Imported forestry*	20.6	0	25	✓	✓	✓	×	×
UCO*	0.25–0.40	~0	0	–	–	–	×	×
Black and brown liquor*	0.28	~0	84	×	×	✓	×	×
Tallow*	0.08–0.12	~0	0	–	–	–	×	×
Crude glycerine*	0.03	~0	10	–	–	–	×	×

MC: Moisture content
* Biomass resource is not considered in drop-in biofuel applications due to its availability issues or existing biofuel application.

Table 10
Attributional, consequential GHG emissions and hydrogen demand factors used for the UK-origin feedstocks considered. GHG emission factors in g CO_2eq/MJ and hydrogen demand in MJ/MJ fuel.

Feedstock	Gasification		Pyrolysis		HTL		Selected route	External hydrogen demand	Reference
	Attributional	Consequential	Attributional	Consequential	Attributional	Consequential			
BMW	No data	No data	No data	No data	34	-69	HTL	0.15	(Lilonfe et al., 2024)
Straw	4	4*	25	25*	No data	No data	Gasification	0	(de Jong et al., 2017b; Tsalidis et al., 2017; Tanzer et al., 2019)
Animal manure	No data	No data	No data	No data	24	-33	HTL	0.15	(Ou et al., 2022; Royal Society, 2023; Lilonfe et al., 2024)
Forest residues	3	3*	31	31*	19	19*	HTL	0.15	(Snowden-Swan and Male, 2012; de Jong et al., 2017b; Tanzer et al., 2019)
Wood waste	3	3*	31	31*	19	19*	Pyrolysis	0.20	(Snowden-Swan and Male, 2012; de Jong et al., 2017b; Tanzer et al., 2019)
Sludge waste	No data	No data	No data	No data	18	59	HTL	0.15	(Royal Society, 2023; Lilonfe et al., 2024)
Food waste	No data	No data	No data	No data	34	35	HTL	0.15	(Royal Society, 2023; Lilonfe et al., 2024)
Digestates	No data	No data	No data	No data	18	60	HTL	0.15	(Royal Society, 2023; Lilonfe et al., 2024)

* For any selected fuel conversion route, consequential emission factor is used for attributional emission factor when no literature data is found on attributional emission, and vice-versa.

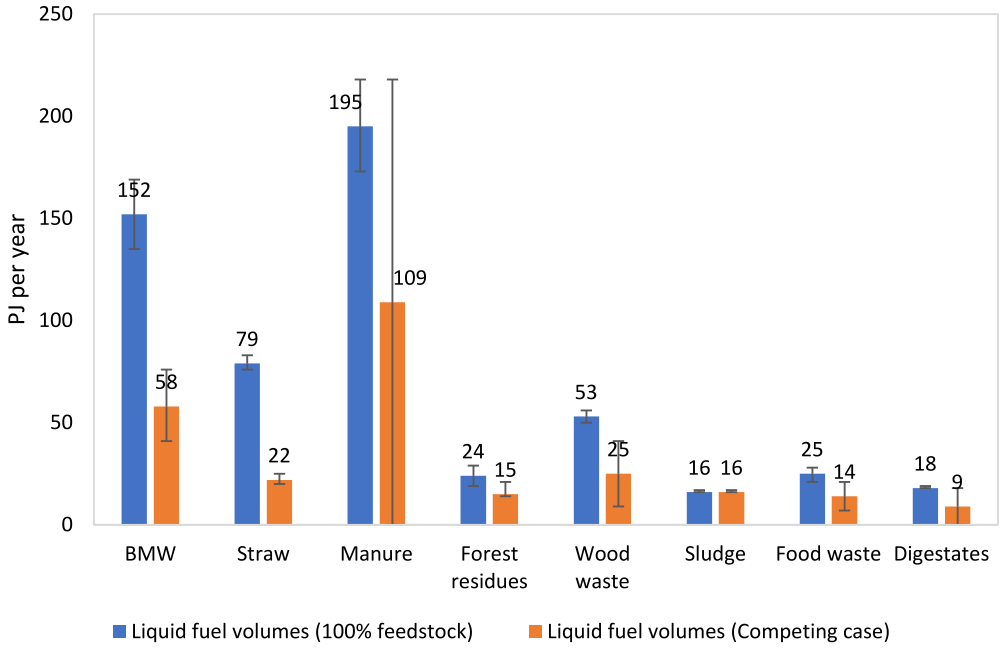

Fig. 15. UK potential liquid fuel supply. Error bars represent minimum and maximum fuel availability based on biomass resource availability range.

are highly dependent on energy and material consumption, as well as other process operation factors, such as production approach. Hence, several operational considerations, such as heat integration, hydrogen sources, and centralised and decentralised operations, are key to the profitability of thermochemical routes. Our review of the literature found the prices of drop-in fuels in the range of $0.60–3.88 per GLE [$17.14–110.82 per GJ]. The lower range of these prices showed that in some cases drop-in fuels can be competitive with the wholesale price of petroleum diesel of $1.22 per GLE ($38.57 per GJ).

Also, our review of LCA studies on drop-in fuels highlights the low-carbon potential of the pathways, and when produced sustainably, the GHG emissions of drop-in fuels can be much lower than those of petroleum fuels. The emissions from these fuels are in the range of -122 and 98 g CO_2eq per MJ. However, several key factors could impact the GHG emissions of these fuels, including the types of renewable feedstocks and energy sources, LUC and iLUC, LCA methodologies and foregone emissions.

The availability of feedstocks is an important factor for the successful operation of any process or production plant. Biomass is available in various regions in the UK, however, the availability is limited. The production of non-food UK-origin biomass feedstocks is estimated at 167–205 Mtpa (wet) [839–1033 PJ per year]. High moisture content feedstocks such as manure and sewage sludge, accounted for 140–173 Mtpa [523–650 PJ per year]. Other biomass feedstocks which are also

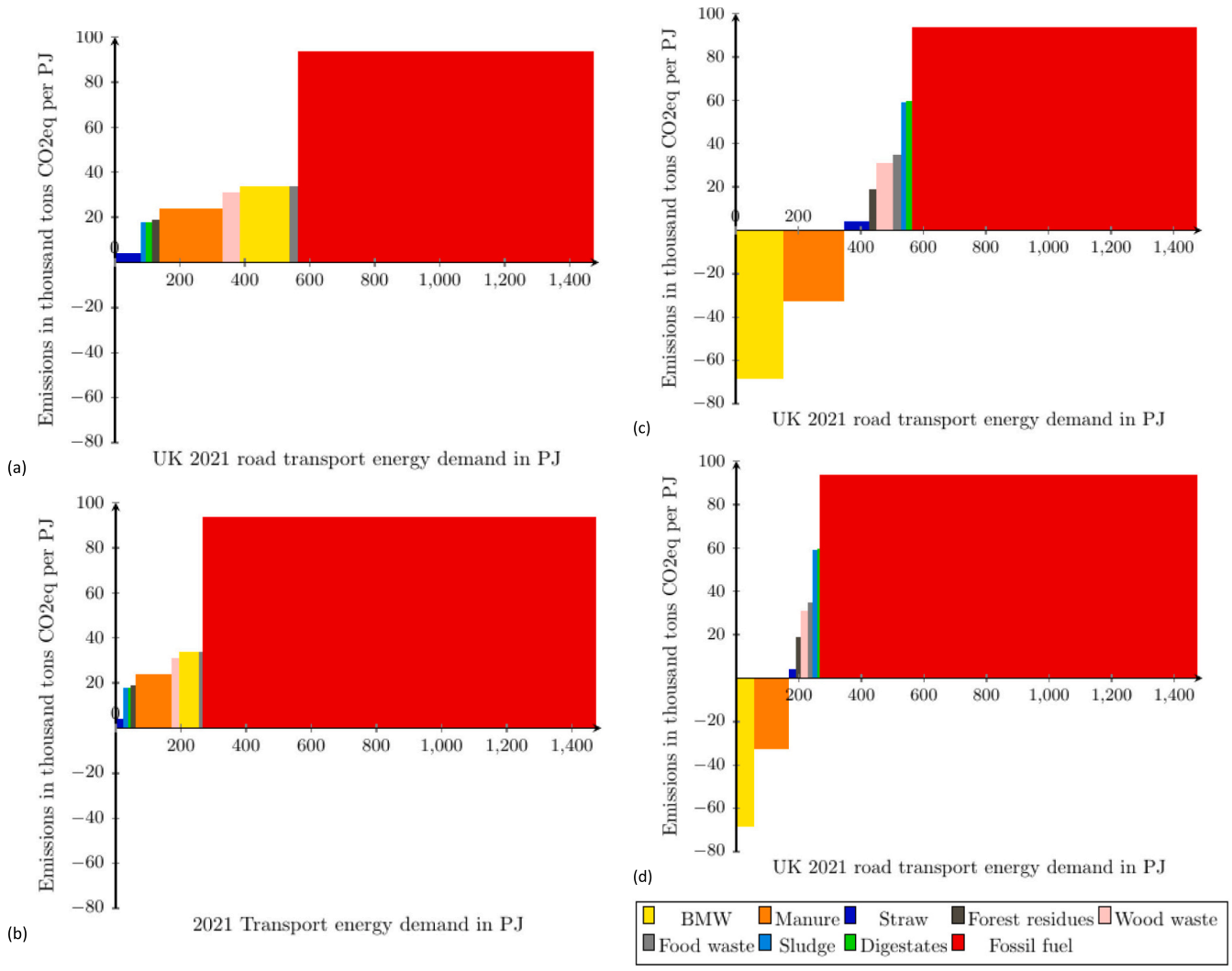

Fig. 16. a–d: Total GHG emissions associated with liquid fuel utilisation under (a) 100 % feedstocks utilisation, attributional (b) Competing case, attributional (c) 100 % feedstocks utilisation, consequential and (d) Competing case, consequential GHG emissions.

Table 11
Total UK drop-in fuel estimated potential production volumes and emissions.

	Fuel potential		Attributional emissions, Mt CO_2eq/year	Consequential emissions, Mt CO_2eq/ year	Hydrogen demand, PJ/year
	PJ/year	Millions L/year			
100 % feedstocks	563	16,076	13.7	-11.5	75.6
Competing case	269	7700	6.7	-4.4	38.5

produced in significant quantities include wood and straw. These feedstocks are subject to many competing uses such as bioenergy generation in biomass plants, panelboard, fertiliser applications and AD. However, wet feedstocks like BMW, food wastes, digestates are in excess, even after deducting for other competing uses, and are often disposed of without energy recovery.

Furthermore, it is estimated that a total of up to 563 PJ per year and up to 269 PJ per year can be produced from UK-origin biomass feedstocks, based on the 100 % feedstocks and competing cases, respectively. This fuel supply is dominated by fuel production from wet feedstocks such as manure and sewage sludge, which make up the majority of UK non-food biomass resources. Producing fuel from these waste resources could provide an alternative method for waste management, thus, partly addressing the challenges accompanying current waste management systems.

The total GHG emissions savings from the use of non-food biomass feedstocks as drop-in fuels in ICEVs can significantly reduce the UK transport sector's GHG emissions. Our initial estimate indicates that the emissions savings from the use of drop-in fuels in the UK could reach up to 64.7 % of the UK's total road transport GHG emissions in 2021. Thus, there is strong potential for the application of BTL in the UK.

Importantly, this study highlights the potential of sustainable drop-in fuels in general as an option for GHG mitigation for the UK's transport sector. More broadly, based on the insights of this review, we would recommend that policymakers also consider encouraging rapid developments and uptake of a wide range of advanced, low-carbon fuels as a complementary strategy to decarbonise the global transport sectors. LCA, and other comprehensive techno-environmental assessment tools, should be used to guide policy decisions towards achieving a decarbonised transport future.

CRediT authorship contribution statement

Sylvanus Lilonfe: Writing – review & editing, Writing – original draft, Visualization, Software, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Ben Davies:** Writing – review & editing, Supervision, Conceptualization. **Amir F.N. Abdul-Manan:** Writing – review & editing, Funding acquisition. **Ioanna Dimitriou:** Writing – review & editing, Supervision, Conceptualization. **Jon McKechnie:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

Jon McKechnie reports financial support was provided by Saudi Aramco Technologies Company. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

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4 Research methodologies

This chapter summarises the general methodology employed in the study because of the diverse nature of the study, which covered the technical, economic and life cycle assessments of different technologies (biomass-to-liquids, direct air capture and power-to-X). The different nature of these technologies typically requires various assessment methods, e.g., minimum selling price of biofuel vs levelized cost of CO_2 and attributional vs consequential life cycle assessment, in which their implementation in a project could vary significantly due to factors such as technology, raw materials and products, policies, and alternative applications in the case of consequential emissions. Additionally, the inventory, mass and energy balance and emissions factors data (e.g., raw material consumption and electricity emission factors) comprise an extensive collection of information, which also significantly varies by technology, geography, and time horizon. These datasets could encompass hundreds of thousands of unique data points, as over thirty thousand supply chain scenarios were evaluated in this work – making it impractical to present all the specific details here. Hence, only key methodologies and the rationale behind the methodologies used in the thesis were presented here. Table 4.1 summarises the contribution of each chapter and the key specific methodologies taken in the study. Furthermore, specific details on the study, including methodologies, are presented in Chapters 3 and 5–8, and they have been published in peer-reviewed publications.

Table 4.1: Summary of key methodologies taken in this study

Study case	Publication title	Key methodologies
Chapter 3 (Dry and wet biomass-to-liquids assessment)	A review of techno-economic analyses and life cycle greenhouse gas emissions of biomass-to-hydrocarbon “drop-in” fuels	▪ Critically review biomass-to-liquids technologies and offer insights in a manner not found in previous literature, by evaluating key features such as biomass supply chains, H_2 demand, fuel potential, and attributional and consequential emissions associated with biomass-to-liquids ▪ Developed novel methods for assessing both attributional and consequential greenhouse gas emission impacts of dry and wet biomass-to-liquids
Chapter 5 (Wet biomass-to-liquids assessment)	Comparative techno-economic and life cycle analyses of synthetic “drop-in” fuel production from UK wet biomass	▪ Developed novel methods for assessing both attributional and consequential greenhouse gas emission impacts of wet biomass-to-liquids ▪ Performed the first integrated techno-economic and life cycle assessments of wet biomass feedstocks in the UK ▪ Assessed the impacts of production approaches, including centralised and decentralised production and H_2 sources (green, blue and grey), in a manner not carried out in prior studies
Chapter 6 (Direct air capture assessment)	Technical, economic and lifecycle greenhouse gas emissions analyses of solid sorbent direct air capture technologies	▪ Created an innovative integrated manufacturing, techno-economic and life cycle assessment methodology ▪ For the first time, the kinetics of adsorption, other key sorbent characteristics and direct air capture have been directly linked using an integrated methodology, providing insights into how various technical factors affect costs and net CO_2 removals in direct air capture processes.

Study case	Publication title	Key methodologies
		▪ Developed methodologies for cradle-to-grave and cradle-to-gate cost and emissions assessments. ▪ Charted development routes for sorbent technologies towards commercialisation ▪ Evaluated a breadth of system options, including energy sources, sorbents, markets, system boundaries, and time to provide global relevance of results
Chapter 7 (Power-to-gases assessment)	Life cycle greenhouse gas implications of low-carbon gaseous fuel supply chains from technological, geospatial, and temporal perspectives	▪ Created innovative and integrated methodologies for H_2 production, transportation, storage and life cycle assessment. ▪ Developed novel methodologies for assessing the transport and delivery of H_2 using its physical states (compressed or liquified H_2) and its carriers (ammonia, methanol, and methylcyclohexane) via ships, pipelines, rail and trucks. ▪ Developed novel methodologies for assessing the use of key centralised and decentralised approaches in gaseous low-carbon fuel supply chains. ▪ Developed methodologies for analysing a set of H_2-related supply chain options over global locations. ▪ Developed novel methodologies for assessing overall emissions with and without the embodied emissions from infrastructures. ▪ Developed methodologies for assessing the dynamic impacts of gaseous low-carbon fuel emissions.
Chapter 8 (Power-to-liquids assessment)	Life cycle assessment of global liquid electro-fuels and chemicals supply chains from technological, geospatial, and temporal perspectives	▪ Created innovative and integrated methodologies for liquid electro-fuels' life cycle assessment. ▪ Developed novel methodologies for assessing the use of centralised and decentralised approaches in liquid electro-fuels supply chains. ▪ Developed methodologies for analysing a set of liquid electro-fuels supply chain options over global locations. ▪ Developed novel methodologies for assessing overall emissions with and without the embodied emissions from infrastructures. ▪ Developed methodologies for assessing the dynamic impacts of liquid electro-fuels emissions.

The methodology used in the published papers is divided into two parts: (1) The methods used for the critical literature review where the key literature on biomass-to-liquids, direct air capture, power-to-X and blue fuels technical, cost and life cycle assessments were analysed and (2) The approaches that were used for assessing the potential fuel volumes, cost and environmental impacts.

The methods for obtaining data in the literature in the publications were based on publicly available data in various databases, including ScienceDirect, government websites, and reputable sources such as IEA and NREL. Where there is a significant variation in data for a parameter as reported by different literature, any or both of these approaches were adopted (a) Prioritisation of commercial plant data

over demonstration and experimental plant data and (b) Use of averages of the most represented range in the literature. In some cases, especially in prospective analysis (e.g., direct air capture using wind energy in 2050), data from established sources (e.g., IEA and NREL) and process modelling were prioritised over data from existing commercial, demonstration and experimental plants. This is done to account for anticipated technological development over time. A further sensitivity and uncertainty analysis was performed to assess the impacts of changes in assumptions taken in the research work.

The approaches for estimating the potential fuel volumes, costs, and environmental impacts were based on material and energy balance data from commercial, demonstration and experimental plants published in the literature. Generally, techno-economic and life cycle assessment results can be significantly affected by Technology Readiness Level, as well as techno-economic and life cycle assessment methodologies (Green, 2007; Feng and Rangaiah, 2011; AACE International, 2020; Rodgers, 2024). Table 4.2 shows the Technology Readiness Level of the key technologies assessed in this work. Hence, sensitivity analysis is performed to understand the impact of changes on key parameters and methods. Both lightweight and heavyweight assessment methodologies were used in this study, depending on the scenarios, including the aim of the research, technological advancement and data availability, as presented in Table 4.4. As noted in Section 4.1, both lightweight and heavyweight assessment methodologies can be used to assess the technical, economic and emissions performances of a technology. Lightweight assessment methodologies are very important when there are existing literature with mass and energy balance data, and negligible changes to these data are anticipated with variations in design and operations. While heavyweight assessment methodologies are very useful when there is no or little mass and energy balance data, especially when there is a high uncertainty in these data due to design and operational factors. Furthermore, sensitivity and uncertainty analysis is performed where applicable to determine the impact of changes in methodologies and parameters arising from the literature and the analysis approaches adopted.

Table 4.2: Technology Readiness Level of key low-carbon technologies assessed in this work

Technology	**Technology Readiness Level**	**Reference**
Hydrothermal liquefaction	6–8	(IEA Bioenergy, no date; Licella, no date; Wijeyekoon *et al.*, 2020; European Union, 2021)
Pyrolysis	8–9	(IEA Bioenergy, no date; AECOM & Fichtner Consulting Engineers, 2021)
Gasification	8–9	(Fulcrum BioEnergy, no date; IEA Bioenergy, no date; AECOM & Fichtner Consulting Engineers, 2021)
Electrolysis (for H_2)	5–9	Table 2.1
Methanation	8–9	(European Energy, no date; Concawe and Aramco, 2024; Sterner *et al.*, 2024)
Solid sorbent direct air capture	6–9	(Climeworks, no date; An *et al.*, 2023)
Methanol-to-gasoline	6–9	(ExxonMobil, no date; Breuer *et al.*, 2022; Concawe and Aramco, 2024)
Methanol-to-kerosene	5–8	(ExxonMobil, no date; Breuer *et al.*, 2022; Concawe and Aramco, 2024)
Fischer-Trosch synthesis	6–9	(Concawe and Aramco, 2024; Paulsen *et al.*, 2024)

4.1 Techno-economic and life cycle assessment methodologies

The methodologies for techno-economic and life cycle assessments can be classified into heavyweight and lightweight assessment methodologies. Heavyweight assessment methodologies utilise rigorous or first principles approaches, such as process modelling for mass and energy balance, equipment costing and emissions models, to determine technical, economic and life cycle environmental impacts, such as capital investment cost, product price and greenhouse gas emissions, see Figure 4.1 for details. On the other hand, lightweight assessment methodologies utilise mass and energy balance data from previous work, such as previous process modelling or demonstration plants, to determine technical, economic and life cycle environmental impacts, such as capital investment cost, product price and greenhouse gas emissions. The differences, advantages and disadvantages of heavyweight and lightweight techno-economic and life cycle assessment methodologies are summarised in Table 4.3.

Table 4.3: Types of techno-economic and life cycle assessment methodologies.

Heavyweight assessment methodologies	**Lightweight assessment methodologies**
They are more complex and detailed, involving process modelling from first principles, often performed by using process modelling tools, to determine mass and energy balance data	They are simpler and less detailed as mass and energy balance data are obtained from previous work, e.g., process modelling from heavyweight assessments, pilot plants or experimental rigs
They can be used to generate original technical data for pilot and commercial plants	They can be used to generate some technical data for pilot and commercial plants
They typically provide more specific data on technology (designs and operations) scenarios, including dynamic operations, because of their robust and first principles nature	They provide data faster and are vital for easily assessing several to thousands of technology scenarios, since changes in some data may not significantly affect plant design and operations
Note: In this research, both heavyweight and lightweight assessments methodologies were used depending on the scenarios, aim of the research, and data availability, as shown in Table 4.4.	

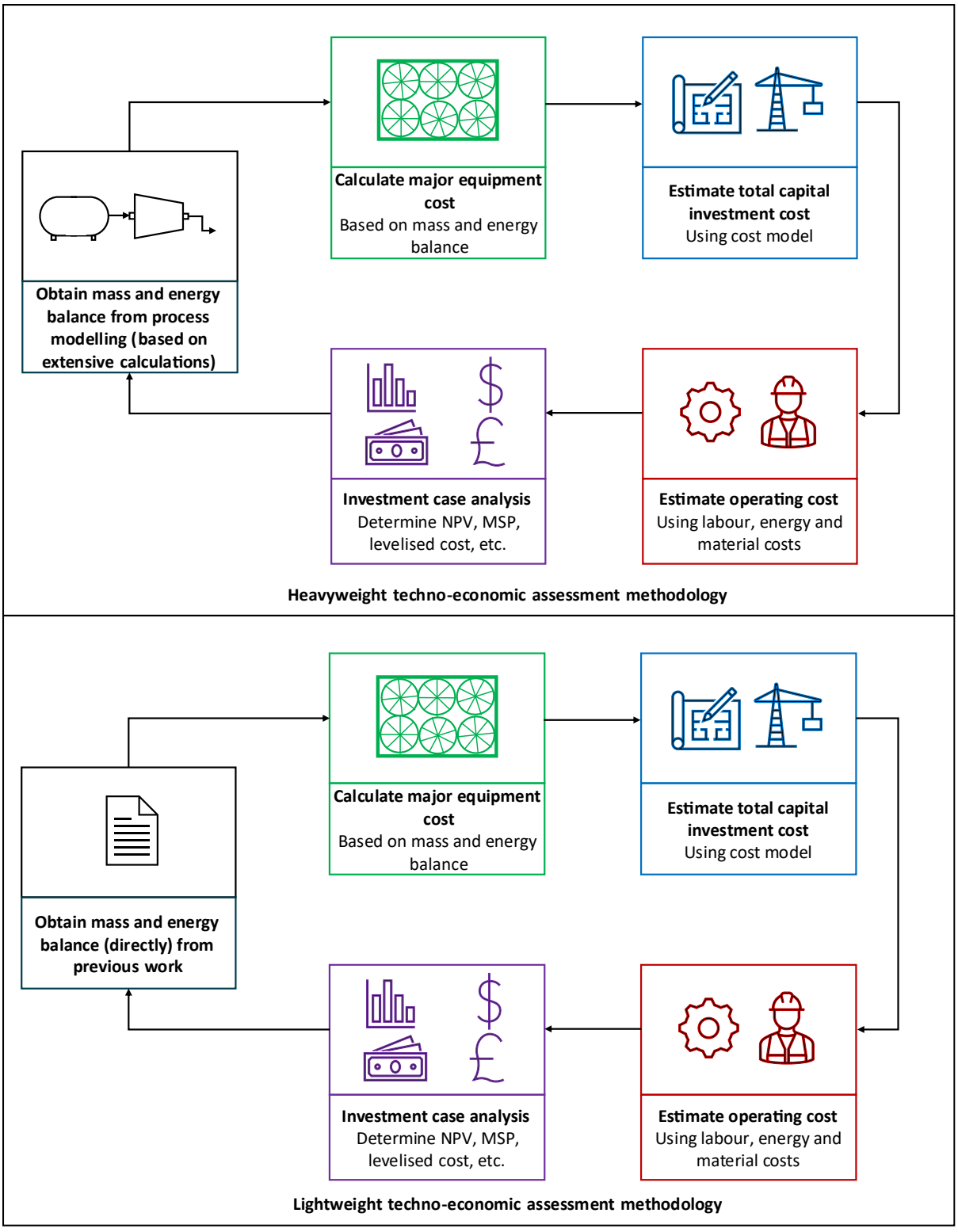

Figure 4.1: Flow diagram of techno-economic assessment methodologies.

4.2 Selection of lightweight and heavyweight assessment methodologies

The bases for the selection of lightweight and heavyweight assessment methodologies in the different assessments in this study are shown in Table 4.4.

Table 4.4: Basis for the selection of lightweight and heavyweight assessment methodologies.

Study case	**Assessment approach**	**Justification**
Chapter 3 (Dry and wet biomass-to-liquids assessment)	Lightweight assessment	▪ Some of the technologies are developed (in commercialisation), while others are under development. However, there is no anticipated significant uncertainty in the process model and mass and energy balances up to 2050, especially regarding key parameters such as product yield and energy demand, given current technology development. ▪ Assessed different production approaches from different feedstocks, including gasification, supercritical gasification, pyrolysis and hydrothermal liquefaction, making it ineffective to perform process modelling within the project scope, especially with the presence of important reference models in the literature, e.g. NREL and PNNL (Snowden-Swan *et al.*, 2017). ▪ Assessed different biomass feedstocks, including dry biomass (e.g., straw and wood) and wet biomass (e.g., food waste and sewage sludge).
Chapter 5 (Wet biomass-to-liquids assessment)	Lightweight assessment	▪ Technology is under development, with key challenges around operations due to high operating pressure. However, there is no anticipated significant uncertainty in the process model and mass and energy balances up to 2050, especially regarding key parameters such as product yield and energy demand, given current technology development. ▪ Assessed different production approaches from different feedstocks, including centralised and decentralised production approaches, making it ineffective to perform process modelling within the project scope, especially with the presence of important reference models in the literature. ▪ Assessed different wet biomass feedstocks, including digestates, food waste and sewage sludge.
Chapter 6 (Direct air capture assessment)	Heavyweight assessment	▪ Technology is developed (in early commercialisation), but mass and energy balance, as well as costs of design and operations, could change significantly with novelty in the carbon capture approach, e.g., changes in sorbent type, adsorption time, energy source and process boundary. ▪ Nature of the technology assessed – solid sorbent direct air capture, assessing new and existing sorbents. ▪ No comprehensive assessment of how technical parameters could reduce capture cost to estimates within \$100/tCO_2 captured while maintaining direct air capture negative emissions benefits. Prior studies rely on learning rate assumptions and statistical models (based on arbitrary parameters), offering little information on the design and operational requirements for low-cost direct air capture.
Chapter 7 (Power-to-gases assessment)	Lightweight assessment	▪ Life cycle greenhouse gas emissions are more sensitive to the emission factors of materials and energy than to mass and energy balance. Hence, a process can be low-carbon or high-carbon depending on the material and energy source, e.g., renewable vs fossil electricity emission factors, even for the same energy demand estimates.

Study case	Assessment approach	Justification
		▪ Over 10,000 supply chain scenarios of gaseous synthetic fuels were assessed, making it ineffective to perform process modelling with the availability of widely acceptable references.
Chapter 8 (Power-to-liquids assessment)	Lightweight assessment	▪ Life cycle greenhouse gas emissions are more sensitive to the emission factors of materials and energy than to mass and energy balance. Hence, a process can be low-carbon or high-carbon depending on the material and energy source, e.g., renewable vs fossil electricity emission factors, even for the same energy demand estimates. ▪ Over 10,000 supply chain scenarios of liquid electro-fuels were assessed, making it ineffective to perform process modelling with the availability of widely acceptable references.

4.3 Technical (mass and energy balance) analysis

In the heavyweight assessment methodology, mass and energy balance data were obtained from process modelling using Aspen HYSYS and Microsoft Excel tools. This methodology was used in Chapter 6 to assess solid sorbent direct air capture technologies. Furthermore, additional details on the specific process modelling and mass and energy balance methodologies can be found in Chapter 6.

In the lightweight assessment methodology, mass and energy balance data were obtained from the literature, which included literature on process models and experimental models, as well as pilot plant and commercial plant data. In this study, a higher preference was given for data from commercial plant models over demonstration plants, process modelling and experimental plants, especially in the assessment of well-developed technologies. However, in some cases, e.g., technologies in the early commercial stage and prospective analysis, the data from assessment by established science-based organisations (e.g., IEA and NREL) were prioritised over first-of-a-kind plants or technologies in active development. This methodology is widely used in research, especially for prospective analysis, where the performance of technologies (e.g., wind turbines) is expected to improve over time. The nth plant approach was also used to model scenarios where no significant improvement in technology performance is expected with time. These methods were employed in Chapters 3 and 5–8. Please see the respective headings for specific information on mass and energy balance data.

4.4 Economic analysis

The key approaches adopted in the economic model for estimating product prices were based on costing methodologies by different authors, including the Association for the Advancement of Cost Engineering (AACE), NREL, the Hand factor method (Towler and Sinnott, 2021) and Seider et al. (Seider *et al.*, 2017). Different approaches were adopted due to the varying nature of the technologies assessed and the project's aims. This is because some methodologies may be more suitable for certain products or markets. For instance, a minimum selling price is often preferred for products directly used by final consumers (e.g., fuels), while a levelized cost is more suitable for products used as intermediates in another plant (e.g., CO_2). Hence, specific details on the economic analysis methods, including capital costs, operating costs and product costs, are presented in Chapters 5 and 6.

Economic analysis of processes and products is often based on the assessment of capital costs, operating costs and investment parameters (such as discount rates and tax). Capital costs in this study were based on estimates of total equipment cost and other project cost components, such as

contingency, Outside Battery Limit (OSBL), and working capital. They were determined based on estimates of total equipment cost obtained using data from process modelling and equipment cost correlation equations and charts from references, like (Seider *et al.*, 2017), or based on estimates obtained using rapid cost estimation methods (lightweight assessment methodology). For rapid cost estimation methods, which are simpler, the capital costs of equipment or plants were obtained by scaling original equipment costs from historical data using a scaling factor (n), as shown in Equation (2.9). Equipment costs from previous years are adjusted to a project economic reference year, where necessary, using the chemical engineering plant cost indices (CEPCI), while future costs are determined using technical analysis, learning rates, and estimates from reputable references (such as NREL). Operating costs, such as fixed costs (e.g., labour costs) and variable costs (e.g., raw material and electricity costs), were calculated using labour cost estimations, market prices for materials and energy, and percentages as reported in the literature. Investment parameters, such as discount rates and taxes, were determined using data from the literature and the product costing approach (minimum selling price or levelised cost). A discount rate of 10% was used in this analysis based on the discount rate for energy projects of 7–10% (DESNZ and BEIS, 2020; Kinchin, 2020; Rodgers, 2024). Details on other investment parameters can be found in Chapters 5 and 6.

Generally, product prices in techno-economic assessment are often determined using the minimum selling price and levelised cost approaches. The minimum selling price, the selling price of a product or process at the plant gate or market that makes the project's net present value (NPV) equal to zero over the plant life, was determined using Equation (2.10). The minimum selling price approach is often used for final products that enter markets, such as fuels and chemicals, and may include downstream costs, such as taxes, product transportation costs and retailers' margins. On the other hand, the levelised cost of a product or process, the discounted lifetime cost of constructing and operating a process plant or producing a product, was determined using Equation (2.11). The levelised cost of a product or process is often used for intermediate industrial products and processes, such as renewable electricity, H_2 and CO_2. The levelised cost does not often account for downstream cost factors, such as retailers' margins, which can be key in determining a project's profitability.

4.5 Life cycle assessment

The life cycle assessment methodologies were based on the standards given by ISO 14 040 and 14 044, which include goal and scope definition, inventory analysis, impact assessment and interpretation (ISO, 2006b, 2006a; H. Scott Matthews, Chris T. Hendrickson and Deanna Matthews, 2014). The goal and scope definition, inventory analysis, impact assessment and interpretation used in the thesis can be found in the publication headings (Chapters 3 and 5–8). Other principles, such as accounting for embodied emissions from infrastructure, were also considered in the assessment, on a case-by-case basis, as found in Chapters 3 and 5–8. The emission factors for materials and energy used were 100-year global warming potentials obtained from the literature, including Ecoinvent (version 3.7.1), IEA, NREL, and DESNZ (Ecoinvent, no date; NREL, 2021; DESNZ and BEIS, 2024). Microsoft Excel-based tools were developed for the respective life cycle assessments. Microsoft Excel was chosen over life cycle assessment software for numerous reasons, including 1) easy integration of different assessment methodologies, such as conventional and prospective life cycle assessments (which require recent and prospective data), emissions with and without embodied emissions and multiple boundary conditions 2) the methodology of the work sometimes integrates life cycle assessment with techno-economic assessment, making the use of life cycle assessment software less suitable and 3) sometimes, life cycle assessments of inventory data are performed and integrated with the main life cycle assessments due to the absence of existing emissions data, especially for novel materials. As with the techno-economic assessment, different approaches were taken based on the scenario, including research aims,

technology advancements and data availability, which differ by products or processes (e.g., biomass-to-liquids, direct air capture and power-to-X technologies). Hence, specific life cycle assessment methodologies were not presented here, but in the assessment headings (Chapters 3 and 5–8). Generally, some of the different life cycle assessment approaches taken in this work include:

(1) Attributional and consequential life cycle assessments methodologies: These were used when the indirect impacts of a technology were not widely known or could significantly impact a technology's overall emissions and regulatory requirements. This is very important for biomass-to-liquids (Chapters 3 and 5), especially where biomass resources have strong competing applications.

(2) Conventional and prospective assessments methodologies: Conventional life cycle assessments analyse the environmental impacts of a product or process based on existing technologies and practices, while prospective life cycle assessments analyse the potential future environmental impacts of technologies and practices, considering the changes that may occur over time. Conventional life cycle assessments offer insight into the environmental impacts of a product or process using current technologies, and are particularly important for regulatory and compliance purposes, such as meeting emission limits set by the EU's RED and the UK's RTFO. On the other hand, prospective life cycle assessments are crucial for evaluating emissions performance over time for both emerging and existing technologies, especially those whose design and operational factors may change significantly over time. Prospective life cycle assessments can be utilised to improve the emissions of products or processes over time, or where the mass and energy balance of supply chains and their emission factors are not widely known or anticipated to change significantly over time. For these reasons, both conventional and prospective life cycle assessments approaches were used in this work; see Chapters 3 and 5–8 for specific details. Additionally, sometimes a hybrid of prospective and conventional life cycle assessments approaches was taken in estimating emissions factors of the future, with the impact of changes in mass and energy balance and emissions factors accounted for as practically as possible. This hybrid approach was employed due to the scope of the work and data availability, particularly when changes in the understudy parameter have no significant impact on the results, as revealed by other studies in the literature or sensitivity analysis conducted here.

(3) Emissions including and excluding embodied emissions: These were used where embodied emissions from infrastructures were not widely known, negligible or anticipated to significantly impact findings in existing literature. Additionally, information can be found in Table 4.1 and Chapters 6–8.

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5 Techno-economic and life cycle assessment of wet biomass-to-liquids technology

This chapter contributes to the overall thesis aim of assessing low-carbon fuel and chemical technologies by examining the technical, economic and life cycle emissions of (wet) biomass-to-liquids supply chains, including the impacts of production approaches (e.g., H_2 sources and centralised and decentralised production approaches) on cost and life cycle greenhouse gas emissions of biofuels.

The paper presents the techno-economic and life cycle evaluation of drop-in biofuels produced via hydrothermal liquefaction of wet biomass feedstocks, with originality in the methodologies of techno-economic and life cycle assessments. In this work, more than 24 novel production approaches were analysed, including 1) The utilisation of various wet biomass feedstocks (digestates, food waste, biodegradable municipal waste, and sewage sludge), which have not been extensively assessed previously; 2) The use of centralised and decentralised approaches in fuel production; 3) The estimation of the impact of feedstock transportation and; 4) The utilisation of various H_2 sources (grey, blue and green). The minimum biofuel selling prices, greenhouse gas emission estimates, and fuel and CO_2 mitigation potentials in the UK from key wet biomass were estimated as a result of these evaluations. It was found that co-processing of different waste feedstocks is an important strategy to minimise fuel selling prices by enabling better economies of scale and feedstock transport, resulting in a fuel price of $19.92–27.40 per GJ. The corresponding GHG emissions from the co-processing case range from 11.4–24.9 $kgCO_2e$ per GJ in 2021, based on the consequential life cycle assessment approach. Furthermore, it was estimated that the utilisation of key UK wet feedstocks could only provide 4.5% of current fuel consumption and reduce emissions by 4.5–5.4 $MtCO_2e$/year, which translates to 3.4–4.0% reductions in the UK's 2021 transport emissions.

The work was published in the Chemical Engineering Journal in January 2024. The published work is titled "Comparative techno-economic and life cycle analyses of synthetic "drop-in" fuel production from UK wet biomass" and is presented as Chapter 4 in this work. The supplementary information for the work, published alongside the paper, is reprinted in Appendix A2.

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Comparative techno-economic and life cycle analyses of synthetic "drop-in" fuel production from UK wet biomass

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ABSTRACT

Renewable synthetic hydrocarbon "drop-in" fuels can help mitigate greenhouse gas emissions from transport, particularly in hard-to-abate sectors like freight and aviation. However, no study has extensively addressed the concerns over biomass availability, cost viability, and CO_2 reduction feasibility that are associated with diverse production configurations and feedstocks. Here, we report detailed techno-economics and life cycle greenhouse gas emission assessments of drop-in fuel productions via hydrothermal liquefaction to assess their economic viabilities, CO_2 mitigation potentials, and prospects for scale-up specifically within the UK context. Our approach integrates key production factors which include regional availability of main feedstocks (digestates, food waste, biodegradable municipal waste, and sewage sludge), plant configurations (centralised vs decentralised) and hydrogen sources (grey, blue, green). We demonstrated the economic trade-off between economy-of-scale and feedstock transport distances in the centralised/decentralised configurations, and also the economic and emissions trade-offs associated with the use of different hydrogen sources. We find that co-processing of different waste feedstocks is an important strategy to minimise fuel selling price by enabling better economy of scale and feedstock transport, resulting in a fuel selling price of £14.76 – 20.30 per GJ. The corresponding greenhouse gas emissions from the co-processing case vary from 11.4 to 24.9 kg CO_2eq per GJ for 2021, based on the consequential life cycle assessment approach. Furthermore, we estimated that the utilisation of key UK wet feedstocks could only provide 4.5 % of current fuel consumptions and reduce emissions by 4.5 – 5.4 Mt CO_2eq/year, which translates to 3.4 – 4.0 % reduction in the UK's 2021 transport emissions.

1. Introduction

Addressing climate change by reducing greenhouse gas (GHG) emissions is one of the most important challenges faced by policymakers and industries globally. In the UK, the modern transport sector is responsible for a quarter of national GHG emissions [1]. Hence, the decarbonisation of transportation systems is considered essential, through strategies such as vehicle electrification and the development of other sustainable technologies. Although current policies across many countries promote vehicle electrification and by 2035 in the UK [2–4], the use of drop-in fuels is strongly recommended in the harder-to-decarbonise areas, such as freight, aviation, and to a lesser extent in the existing light-duty fleet which will be in operation beyond 2035. This is due to the challenges associated with vehicle electrification such as long-distance, aviation and heavy-goods transportation. The EU Renewable Energy Directive (RED) II has set a target of 14 % biofuel consumption in road and rail transport by 2030 [5]. However, currently, biofuels contribute only 5 % of the UK transport fuel consumption volumes [6]. Conventional biofuels such as biodiesel which are currently widely applicable in blended stocks with fossil fuels are limited in applications, due to engine compatibility [7]. In addition, conventional biofuels compete with food crops, and this has strongly intensified the food vs fuel debate, since the global food crisis in 2008 which was partly attributed to first-generation biofuels [8]. Therefore, the use of synthetic

Abbreviations: AD, Anaerobic digestion; BMW, Biogenic municipal solid waste; CO_2, Carbon dioxide; FCI, Fixed capital investment; GLE, Gasoline litre equivalent; GHG, Greenhouse gas; H2, Hydrogen gas; HTL, Hydrothermal liquefaction; LCA, Life cycle assessment; MFSP, Minimum fuel selling price; MSW, Municipal solid wastes; OPEX, Operating expenditure; RED, Renewable Energy Directive; TEA, Techno-economic assessment; USD, United States dollar.

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Table 1
UK wet biomass waste management processes in practical applications in 2021.

Waste feedstocks	Volumes, Mtpa	Key processing and disposal pathways							Based on data by
		Re.	AD	Incinerat.	Composting	Landfill	Land	Others	
Food wastes	11.1 – 13.1	16 %	38 %	13 %	4 %	14 %	7 %	4 %	[9,14–18]
Digestates	14.2[a]	–	n.a	3 %	n.a	2 %	95 %	–	[19,20]
Sewage sludge	30	–	n.a[b]	4 %	–	–	93 %	–	[21]
Landfilled BMW	3.9[c]	–	–	–	–	100 %	–	–	[22]
Manure	83	–	3 %	–	–	–	97 %	–	[19,23]

Key: Re. – recycling; AD – anaerobic digestion; Incinerat. – incineration; n.a – not applicable; BMW – biogenic municipal waste.
[a] Volume of digestates includes food waste treated in AD.
[b] Industrial AD treatment of sewage sludge was not accounted for in AD volumes but as dry sewage sludge in accordance with convention.
[c] Volumes of food wastes and digestates landfilled excluded.

Table 2
The summary of the various fuel production scenarios considered.

Feedstock	Production configuration	Hydrogen source
Digestates Food waste BMW Sewage sludge Co-processing	Centralised Decentralised	Grey hydrogen – steam methane reforming Blue hydrogen – steam methane reforming with carbon capture Green hydrogen – renewable electricity electrolysis

liquid hydrocarbon "drop-in" fuels has been widely considered as a solution to current liquid fuels due to their compatibility with existing vehicle technologies and fuel distribution and storage systems, and non-competition with food crops. As a result, this work assesses the viability of drop-in fuel production from the UK wet waste biomass feedstocks, based on several production approaches, including different plant configurations and hydrogen sources. This study focuses on feedstock availability and utilisation in the UK, but general insights are applicable to other regions.

Biomass resources are generally considered sustainable, however, their utilisation can be limited due to the amount of biomass that can be sustainably removed and replenished. In the UK, the production of "fresh" biomass feedstocks (such as forestry) is limited, but waste biomass materials are generated in significant quantities. These waste biomass materials are often under-utilised or mismanaged, as significant quantities of waste, especially food waste and sewage sludge (SS), often end up on land and water bodies without proper recycling or energy recovery. Currently, 15 % of municipal solid waste (MSW) landfilled is food waste [9]. Landfilling of organic waste produces significant GHG emissions to the environment, with nearly 400 kg of CO_2eq/ton MSW released from landfills [10]. The current treatment method of sewage sludge is costly, about £200 per dry tonne of sludge [11]. Also, the use of dry sludge on land even after conventional treatment is subject to serious environmental and safety concerns like the contamination of water and the transmission of pathogens [12,13]. Hence, providing environmentally clean and cost-effective alternatives such as waste-to-energy could help improve wet biomass waste management. Generally, wastes are often managed by recycling, anaerobic digestion (AD), composting, incineration, land application and landfilling. The current wet waste generation volumes in the UK and the management techniques are shown in Table 1.

One of the processes in which wet waste biomass feedstocks can be managed is through hydrothermal liquefaction (HTL). HTL is a non-conventional way of treating and converting waste into energy in the form of synthetic liquid fuels. In HTL, sub-critical water is used to break down biomass feedstocks into three distinct products- biocrude, gas and char. Usually, combinations of high pressure of 5 – 30 MPa, medium temperature of 250 – 350 °C, and short reactor residence time of 5 – 90 min are employed on a wet biomass feedstock [24]. The use of wet biomass feedstocks in HTL avoids the high energy requirement of drying high moisture content biomass. A wide variety of biomass, such as sludge waste, algae and forest residue have been used in HTL, with some

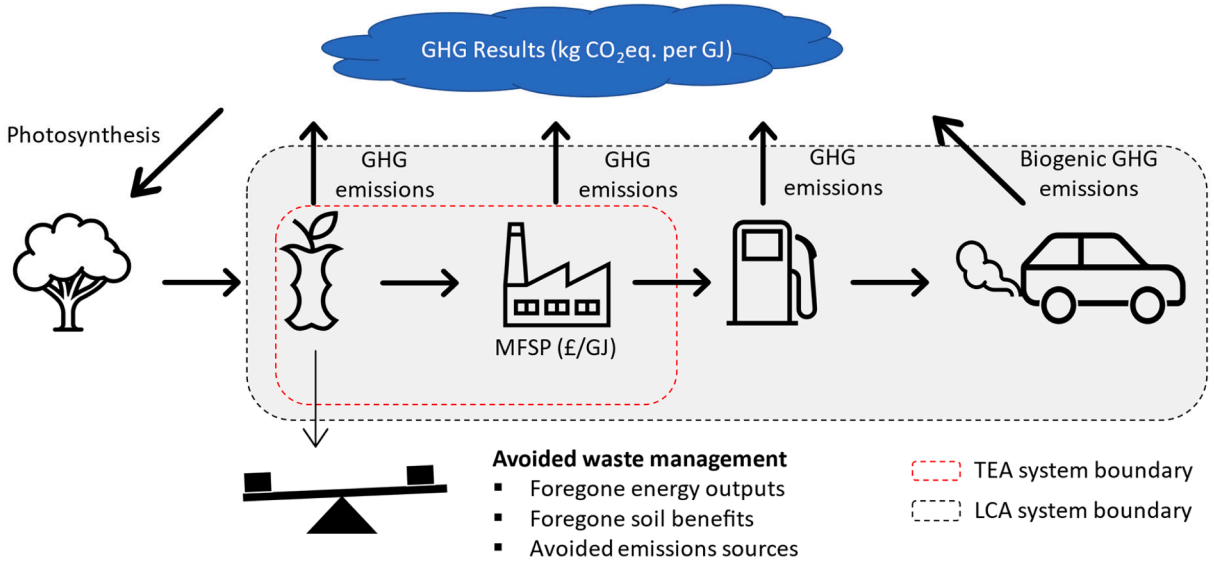


Fig. 1. System boundaries of the study for TEA and LCA.

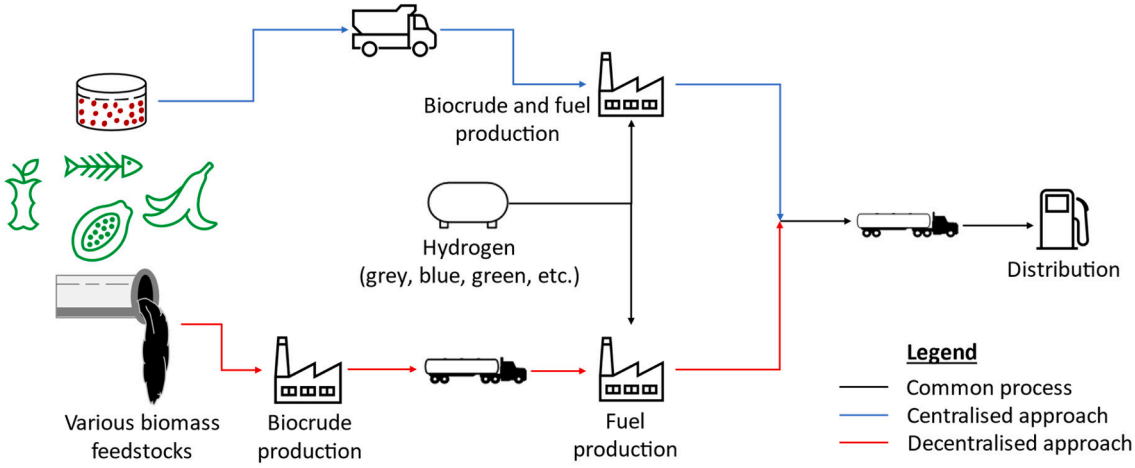


Fig. 2. Summary of HTL drop-in fuel production process.

Table 3
Properties and volumes throughput of waste feedstocks used in this analysis.

Wastes	Volume utilisation, Mtpa	Moisture content (%)	Energy content, dry basis (MJ/kg)	Feed cost (£/wet ton)	Biocrude yield (wt% per dry feed)	References
Digestates	10.7	90	18.0	−8 – 5 (0[a])	37.4	[20,27,58]
Food wastes	6.06	75	19.1	−15 – 15 (0[a])	39.6	[57,59,60]
Landfilled BMW	1.98	50	19.1	−25	39.6	[16,55,59,60]
Sewage sludge	30	95	15.7	−10	32.6	[11,27,61]
Co-processing	20.3	75	17.8	−6.6	37.1	This study

[a] Average value used in this analysis.
Note: (1) Negative feed prices represent the gate fees (excluding landfilled tax) charged by waste treatment plants.
(2) Co-processing case assumes utilisation of feedstocks based on competing use (75% digestates, 46% food waste, 30% BMW and 100% SS), see SI [Section 1.2.1] for additional details.
(3) Energy content on a dry basis obtained from mass and energy balance calculations using an energy efficiency based on Zhu et al. [42].

having moisture content of up to 96 % [25]. The wet treatment of biomass by HTL is reported to provide a significant advantage over other thermochemical processes like gasification and pyrolysis, due to the energy savings associated with the avoidance of drying [26]. Also, drop-in fuel via HTL can easily be integrated into existing infrastructures than other wet biomass technologies like AD [27,28]. However, like other thermochemical processes, it can be affected by issues such as tar formation and catalyst poison [29–32].

HTL technology is yet to be commercialised, as such the technical and economic parameters of the technology are yet to be fully understood with certainty. Previous techno-economic assessment (TEA) studies published employed various design and economic strategies including the location of the HTL biomass-to-liquid plant near the feedstock supply and the decentralisation of HTL of biomass feedstocks subject to a centralised conversion of biocrude to liquid fuels [27,33–39]. A study by Snowden-Swan et al. [27] claimed a high minimum fuel selling price (MFSP) of £30.16 per GJ [£0.96 per gasoline litre equivalent (GLE), 2021 cost basis] when a decentralised production approach was taken, where biocrude is produced at local sites with subsequent biocrude upgrading at a central processing facility. While this study aimed to determine the price of drop-in fuel from a decentralised production approach, the impacts of feedstock transportation over distances and of a centralised processing approach on the price of drop-in fuels were not considered. Transportation and production approaches can have a huge impact on drop-in economics, especially in the case of high moisture content feedstocks, which can lead to significant capital costs as well as transportation costs on the localised plant. As seen in studies by Aierzhati et al. [37], which evaluated the decentralised processing of food waste into biocrude, a high biocrude price with an MFSP of £22.16 per GJ was reported. This price is higher than the prices of drop-in fuels in the range of £13.54 – 19.08 per GJ from centralised approaches, as analysed by some authors such as Tews [40], Pedersen et al. [41] and Zhu et al. [42]. Zhu et al. [42] showed how the MFSP varied with the scale of the plant in a decentralised production operation, as MFSP increased when the scale of the plant at local sites decreased. For plant scale varying from 10 t/d to 2000 t/d, the MFSP varied from £65.24 to £16.00 per GJ, based on 2021 cost adjustment; however, the impact of feedstock transportation costs was not considered. Thus, it is not yet clear how the economy of scale will impact the MFSP of drop-in fuels using decentralised and centralised approaches as most TEA analyses study did not consider extensively the impact of transportation. Also, the availability of biomass feedstocks and where they will come from with regard to fuel production economics and sustainability have not been considered in most published TEAs. However, the sensitivity analysis of various TEA studies has shown that plant size, which can be strongly impacted by feedstock availability, impacts drop-in MFSP [27,33–39]. Additionally, some wet feedstocks like digestates and BMW have not been economically assessed for drop-in fuel production in previous literature. Furthermore, the use of green hydrogen and other hydrogen sources in the upgrading of biocrude to hydrocarbon fuels has not been evaluated in previously published TEA studies. Although current green or blue hydrogen production is negligible, in the future, green and blue hydrogen will likely make up a significant portion of the hydrogen market, and this could have a strong cost impact on fuel production using green hydrogen or other alternatives.

The GHG emissions and other environmental impacts of processes and products are evaluated, reviewed, and improved using life cycle

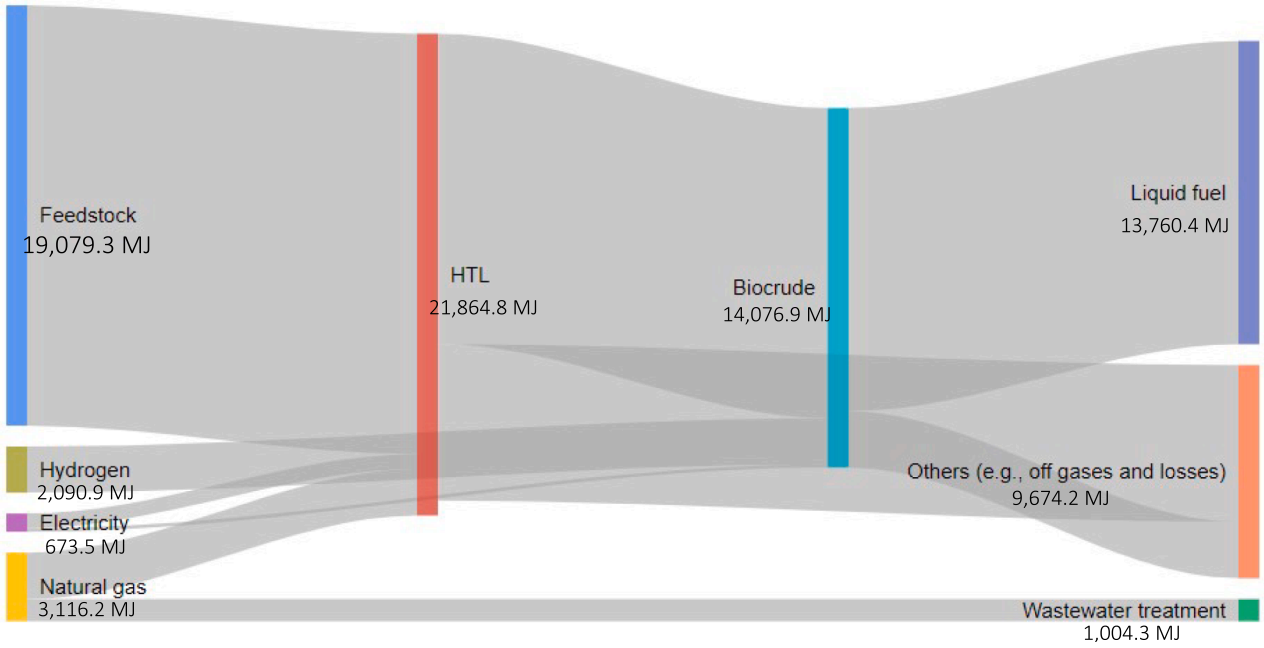


Fig. 3. Sankey diagram of the energy balance of the food waste HTL in drop-in fuel.

assessment (LCA). LCA, which is used to assess environmental impacts associated with new and emerging technologies, enables the comparison of drop-in fuel production approaches as well as drop-in fuels with conventional fuels. The production of drop-in fuels using various approaches, such as feedstock types, centralised vs decentralised production, and hydrogen sources, can have considerable impacts on the overall GHG emissions, as LCA is heavily dependent on energy and material requirements. Bennion et al. [43] revealed variations in the GHG emissions of producing drop-in fuels from microalgae using various production methods, with GHG emissions of −11.4 and 210 g CO_2eq per MJ for fuel production using HTL and pyrolysis, respectively. Many other studies have been published on the LCA of biofuels [44–50], and these analyses estimated the GHG footprint of drop-in biofuels in the range of –122 and 98 g CO_2eq per MJ. The upper band of the emissions numbers from some of the LCA studies are close to those of fossil fuels of 94 CO_2eq/MJ [51], as sustainability factors such as land use change [49] impact fuels' life cycle GHG emissions. Other factors which caused significant variations in the GHG emissions of these drop-in fuels are the fuel processing techniques [43,44,50], emission allocation methods (e.g., mass) [47], system boundaries [46], and LCA methodologies (attributional and consequential) [46,48], amongst others. The impact of different production approaches (centralised and decentralised) and hydrogen sources on GHG emissions have not been explored in current published literature, and so, it is not known to what extent the use of these approaches would affect drop-in fuel's GHG emissions. In addition, despite previous work evaluating the GHG emissions from various feedstocks, the HTL of various available wet feedstocks in the UK which are distributed nationally has received little to no attention, despite wet feedstocks such as food waste, digestates, and SS constituting a significant portion of UK biomass resources.

The development and deployment of drop-in fuels from biomass feedstocks are highly affected by the MFSP, the life cycle GHG emissions and the availability of biomass resources. This work aims to study the variations in factors such as feedstock types, plant configuration (decentralised vs centralised production approach) and hydrogen sources (grey, blue and green) on the cost of producing drop-in fuels. As a result, four wet feedstocks – digestates, food waste, landfilled biodegradable municipal waste (BMW) and SS – which are readily available in the UK are studied. Also, it estimates the amount of drop-in fuels which can be sustainably produced from these UK wet feedstocks. In addition, the GHG emissions associated with producing drop-in fuels, from wet feedstocks and the changes in plant operations, are estimated to determine the impact of diverting and using these feedstocks in drop-in fuel production.

2. Methodology

TEA and LCA methodologies are developed to evaluate drop-in fuel production from wet biomass feedstocks in the UK context under various production configurations (see Table 2). The TEA methodologies developed were based on a review of various important publications in the literature relating to HTL such as those from NREL HTL pilot plant models [27,39,42] and Aierzhati et al. pilot plant models [37]. Therefore, the TEA costing was done in Microsoft Excel to allow for the adoption of cost models related to HTL or other biomass-to-liquids rather than the generic costing model that is available in Aspen Plus or other costing models. Also, the LCA was done in Microsoft Excel with data obtained from various literature including Ecoinvent database. This allows data that is closely associated with the UK market to be considered in the analysis where available. The details of the specific methodology for the TEA and LCA analyses including their drawbacks are presented respectively in this section.

The main scenarios evaluated include the impact of various feedstocks, plant configurations and hydrogen sources. Four wet biomass feedstocks – digestates, food waste, biodegradable municipal waste (BMW) and SS – produced across the UK are considered, in addition to a co-processing scenario where all four feedstocks are processed to fuels at

Table 4
The cost and emission factors of hydrogen sources.

Hydrogen source	Cost ($/kg)	Emissions factor (g CO_2eq/MJ)	References
Grey hydrogen	0.7 – 1.6 (1.15*)	83.6	[65,66]
Blue hydrogen	1.2 – 2.1 (1.65*)	21.4	[65,66]
Green (renewable electricity) hydrogen	3.2 – 7.7 (5.45*)	0.1	[65,66]

* Average cost values, which were used in the base analysis

Table 5
Some key assumptions for the nth plant economic analysis, based on reports by Zhu [42], Snowden-Swan et al. [27], Jones et al. [39] and Aierzhati et al. [37].

Key assumptions	Value
Analysis type	nth
Based year	2021
Discount rate (r)	10 %
Inflation rate	2 %
Plant life	22 years
Income tax rate	35 %
Working capital cost	5 % of FCI
Capital spending	2/4 in 1st year, 1.6/4 in 2nd year, 0.4/4 in 3rd year
Depreciation schedule	10-years linear depreciation
Construction period	2.5 years
Post-construction start-up time	6 months
Plant salvage value	No value
On-stream factor	8000 h

.

Table 6
Cost factors for direct and indirect cost analysis, based on Snowden-Swan et al. [27].

Direct costs	
Component	**% of total installed cost (TIC)**
Buildings	4 %
Site development	10 %
Additional piping	4.5 %
Total direct costs (TDC)	**18.5 %**
Indirect cost	**% of TDC**
Prorated expenses	10 %
Home office & construction fees	20 %
Field expenses	10 %
Project contingency	10 %
Startup and permits	10 %
Total indirect cost	**60 %**
Fixed capital investment (FCI)	**TDC + total indirect cost**
Working capital	**5 % of FCI**
TCI	**FCI + working capital**

the same site. The distribution of the feedstocks across various regions of the UK including East of England, East Midlands, London, North East, North West, N. Ireland, Scotland and Wales, is also considered in the analysis scenarios. Also, scenarios which are based on two production configurations – centralised and decentralised approaches – were evaluated. The centralised approach examines the processing of biomass into biocrude and subsequently into drop-in fuels within one central facility, while the decentralised approach considers the conversion of biomass feedstocks into biocrude at localised locations followed by the upgrading of biocrude into drop-in fuels at a central facility, as shown in Fig. 2. Lastly, scenarios considering different sources of hydrogen – grey, blue and green hydrogen – are also evaluated. Table 2 summarised the various scenarios considered in the analysis.

The key scenarios used to evaluate the various feedstocks are labelled: "Centralised, Grey H2" representing Centralised fuel production using grey hydrogen; "Decentralised, Grey H2" for Decentralised fuel production using grey hydrogen; "Centralised, Blue H2" for Centralised fuel production using blue hydrogen; "Decentralised, Blue H2" for Decentralised fuel production using blue hydrogen; "Centralised, Green H2" for Centralised fuel production using green hydrogen; and "Decentralised, Green H2" for Decentralised fuel production using green hydrogen. See Supplementary Information (SI) Section 1.1 for more details on scenario configurations.

2.1. Flow diagram

The process flow diagram of the fuel product is taken to start from the point of waste generation and ends in the fuel combustion stage. The system boundaries for the TEA and LCA analyses are shown in Fig. 1, see

Table 7
Variable OPEX parameters.

Variable OPEX	Value	Reference
Feedstock, £/wet ton	−25–0	[11,20,55–57]
Feed transportation, £/km/ton waste (2021$)	0.26	[62]
Natural gas, £/100 scf UK prices (2021)	1.16	[67]
Electricity, £/kWh (2021)	0.13	[68]
Solid disposal, £/ton (2021)	16.66	[38]
Quicklime (CaO), £/ton biocrude input (2021$)	103.73	[69]
Process water, £/m^3 (2021)	0.44	[70]
Biocrude catalyst, £/kg feed input (2021)	0.0495	[27,71]
Hydrotreater catalyst, £/gal biocrude input (2021)	0.0087	[27]
Hydrocracking catalyst, £/gal biocrude input (2021)	0.0006	[27]
Cooling tower chemical, £/gal biocrude input (2021)	0.0003	[27]

SI for more details on the individual process stages [Section 1]. A cradle-to-gate TEA approach and well-to-wheel LCA approach were taken for the study, as GHG emissions associated with the infrastructures (process plant and vehicles) were not considered. The mass and energy balances of the fuel's production stages are used in the computation of cost and fuel production rate, while GHG emissions are computed from the key supply chain and fuel production approaches.

2.2. Fuel production

In the fuel production process, which can be divided into biocrude production and upgrading, the feed is converted into biocrude and then subsequently upgraded into liquid fuels, as shown in Fig. 2. Biocrude is assumed to have a moisture content of 4 %, based on the model by Snowden-Swan et al. [27]. The fuel production model was based on the models by Zhu [42] and Snowden-Swan et al. [27]. In the first step, the feedstocks, which are the waste materials, are pumped and preheated in the pre-treatment unit of the plant before further heating in a fired heater using a hot oil system. The heated and pressurized feedstock is then fed to the HTL reactor where the HTL of the feedstock into biocrude is done. Some side products are produced in the HTL reactor which includes aqueous solution, solids and gas. The biocrude yields of the various feedstocks are shown in Table 3. The biocrude produced via HTL can be processed into liquid fuels- renewable gasoline and diesel-through hydroprocessing, in a way similar to that done in conventional petroleum refineries. Hydrogen from various sources can be used to break down the complex organic molecules of the biocrude during hydroprocessing [27,40,42,52]. In addition, sulphur, oxygen, nitrogen and metals are removed from the biocrude through this process. The liquid fuel yield is taken to be 77.9 wt% of biocrude, based on Snowden-Swan et al. [27]. A detailed description of the process model including

Table 8
Fixed OPEX parameters [72].

Fixed OPEX	Rate (£M/yr)	Number, plant size in dry tpa		
		Plant size < 0.5	0.5 < plant size < 5	Plant size > 5
Plant manager/ engineer	0.109	1	1	1
Plant engineer	0.052	0	1	1
Maintenance superv.	0.042	1	1	1
Lab manager	0.041	1	1	1
Shift supervisor	0.036	0	1	1
Lab technician	0.030	0	1	2
Maintenance tech.	0.030	0	1	2
Shift operators/ supervision	0.036	3	3	6
Clerks and secretaries	0.027	1	1	1
Overhead & maintenance	90 % of labour & supervision			
Maintenance capital	3 % of TIC			
Insurance & taxes	0.7 % of FCI			

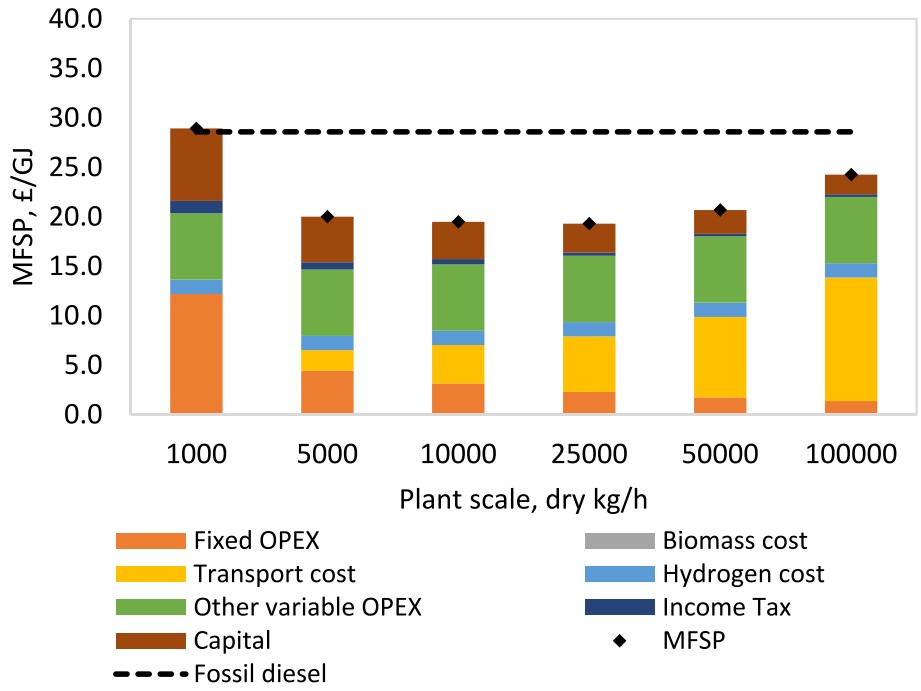


Fig. 4. Effects of plant scale with price breakdown for fuel production from food waste over England, based on Centralised, Grey H2 scenario and assuming the plant is located in Leicester, UK. The MFSPs are displayed in comparison with fossil diesel's price of £28.58 per GJ, based on 2021 wholesale prices of diesel published by RAC [76]. Prices in this study are driven by factors such as feedstock cost (which is zero or negative in some cases) and product yield. Royal Society [77] published biofuel prices from HTL of forest residues in the range of £20.2 – 29.1 per GJ.

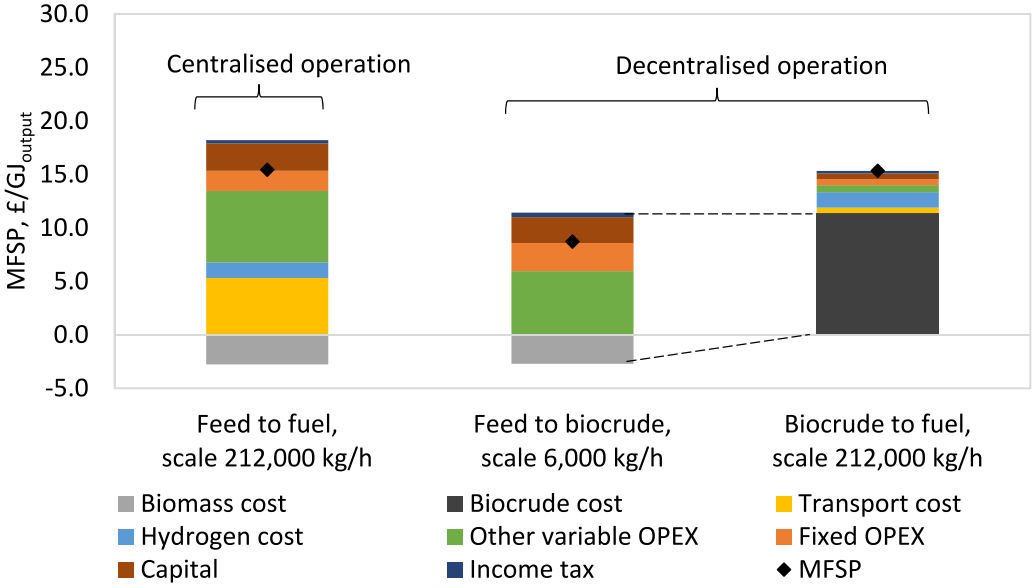


Fig. 5. Comparison between centralised and decentralised approaches for the co-processing of the feedstocks using grey hydrogen for upgrading. The graph shows the price from the conversion of biomass to fuel along various supply chains [units of MFSP in £/GJ_{fuel} for final fuel output and £/$GJ_{biocrude}$ for biocrude output].

biocrude production and upgrading and wastewater treatment can be found in SI [Section 1.2.4].

2.3. Material and energy balance

The material and energy balance of the fuel production processes were based on the biocrude yields shown in Table 3 and the process model by Snowden-Swan et al. [27]. HTL is an endothermic process which becomes slightly exothermic above certain temperatures (e.g., at 240 °C for cellulose, glucose, and wood HTL) [53,54]. As a result, the off-gases and char produced from the HTL of the feedstocks are used to provide the heating demand of the HTL. Additionally, natural gas is used to supply the remainder of the heating requirement of the process. Also, another place in which natural gas was consumed is in the thermal oxidation (THROX) unit for wastewater treatment. In the THROX unit, ammonia/air stream from the HTL aqueous stream is treated, as ammonia and organics are catalytically combusted to CO_2, nitrogen and water. No heating from natural gas is assumed to be used in the upgrading plant, as off-gases and heavy fuel oil from the upgrading unit are utilised, in line with the process model by Snowden-Swan et al. [27].

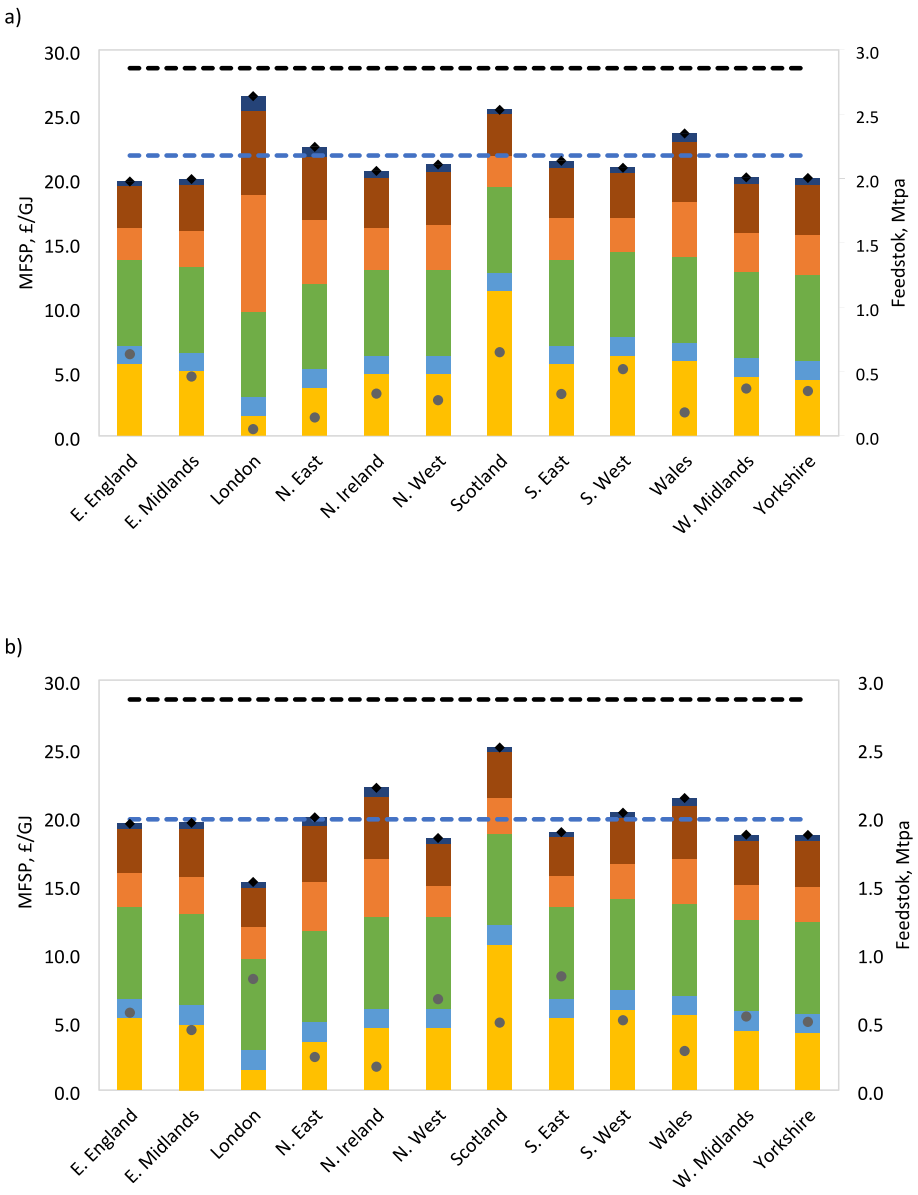


Fig. 6. UK regional distribution of MFSP for HTL processing of (a) digestates (b) food waste (c) BMW (d) SS and (e) co-processing the digestates, food waste, BMW and SS, based on the Centralised, Grey H2 scenario.

Fig. 3 shows the energy balance of food waste processing. More details of the mass and energy balance of the various feedstocks and processes including hydrogen and natural gas consumption are shown in SI [Section 1.2.4].

2.4. Feedstocks and current treatment

The feedstocks are assumed to be generated and collected in waste collection sites such as AD plants, councils' waste collection sites, and wastewater treatment facilities. Feedstocks which have high moisture contents, as shown in Table 3, are dewatered to 75 % moisture content at the waste collection sites, as this is the current practice with digestates and SS. They are then transported to the fuel production plant in the centralised approach or converted into biocrude at a local biocrude plant which is co-located with the waste generation or collection sites in the decentralised approach, see SI [Section 1] for details. Food waste and BMW do not need dewatering, due to their lower moisture content. However, it is assumed that BMW is diluted with water into 75 % moisture content at the biocrude production plant, to improve its pumpability prior to biocrude production due to pumping demands [27].

A key variable which has a strong impact on this economic analysis is the cost of the various waste biomass feedstocks, which varied from average values of -£25 to £0, based on data on feedstock cost/gate fees published in the literature [11,20,55–57]. Current feedstock cost/disposal gate fees are shown in Table 3, where a negative feedstock cost value indicates a payment would be received for accepting the feedstock. Because the prices of these feedstocks vary depending on factors such as season and location, there is a high level of uncertainty in the feedstock cost. For example, the price of food waste is reported to vary between -£15 and £15, based on the time of the year [57]. This variation leads to some uncertainty in the analysis. Also, it is not known what the

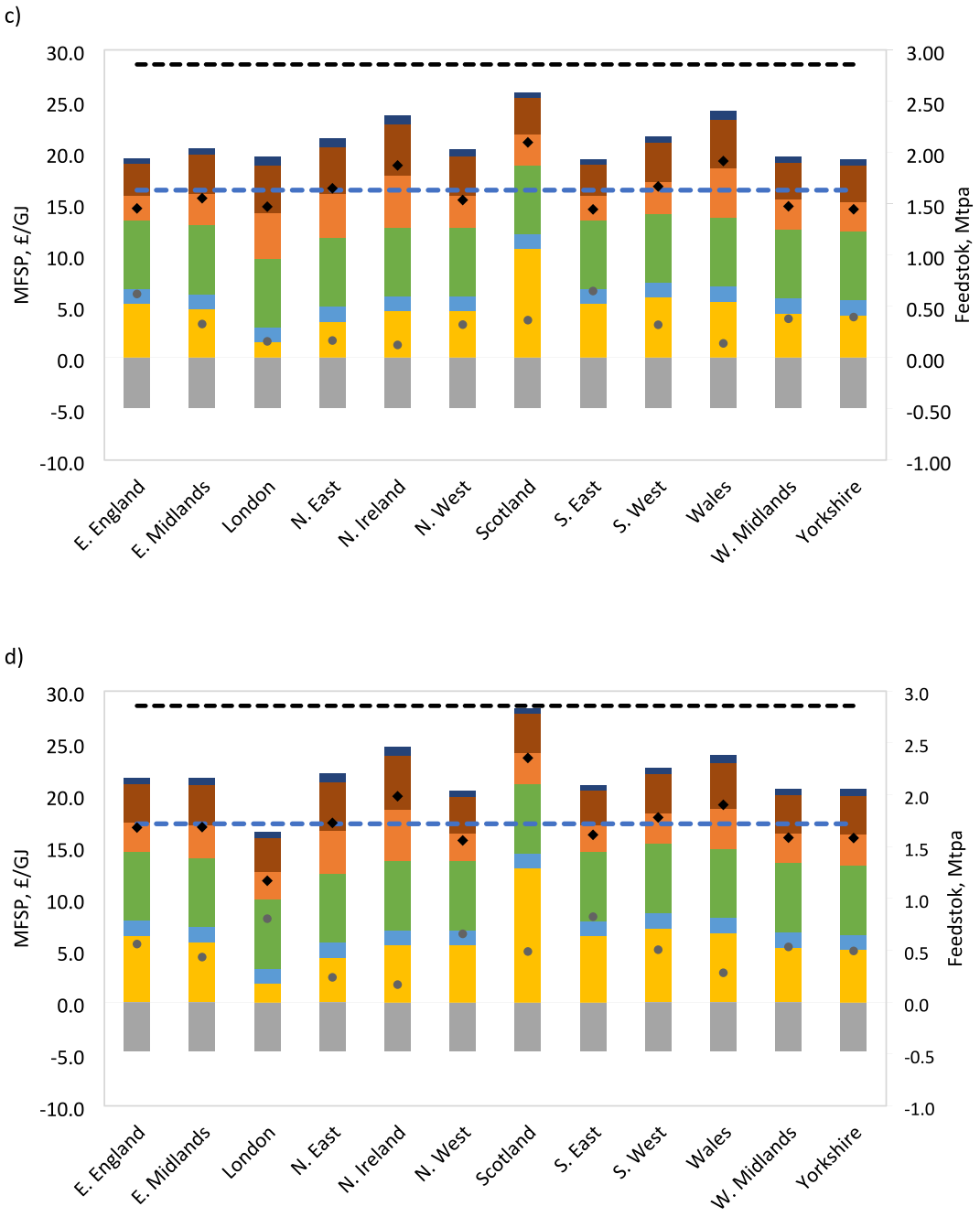


Fig. 6. (*continued*).

prices of these biomass feedstocks in the future will be, as other potential competing uses come into operation. Therefore, a sensitivity analysis based on the expected range of feedstock prices was done to determine the impact of changes in feedstock prices and presented in SI Section 4.4.

Current feedstock treatment methods are considered in the analysis of the GHG emissions, as utilisation of the wet feedstocks in fuel production can lead to direct and indirect impacts along the waste supply chain. Thus, several factors associated with using these feedstocks such as foregone electricity from current waste-to-energy technologies, foregone fertiliser credits from diverting wastes used as nutrients, and avoided treatment emissions from landfilled waste diversion were also considered, see SI [Section 3.1] for details. Hence, a consequential approach to the LCA is taken.

Because there is a trade-off between the economy of scale of facility size and feedstock transportation costs, it was assumed that the conversion of the waste feedstocks into fuel is done on a regional basis, with one central facility per region. The scale of the central facility in any region was based on the availability of the wet biomass feedstocks in the region. The trade-offs between facility capacity (economy of scale) and feedstock transportation cost were investigated to ensure this assumption is appropriate, see Section 3.1.1 for the impact of facility size and SI Section 4.4 for sensitivity analysis. It is important to note that this work does not propose sites where these facilities will be located nor consider the exact location where the waste sources are currently located. However, it attempts to estimate where these wastes will come from, based on the nature of the generation of these wastes and published national data.

In the centralised approach, the area of each region was used to determine the average transportation distance. Each region of the UK was assumed to be a circle, where the area-weighted average radius

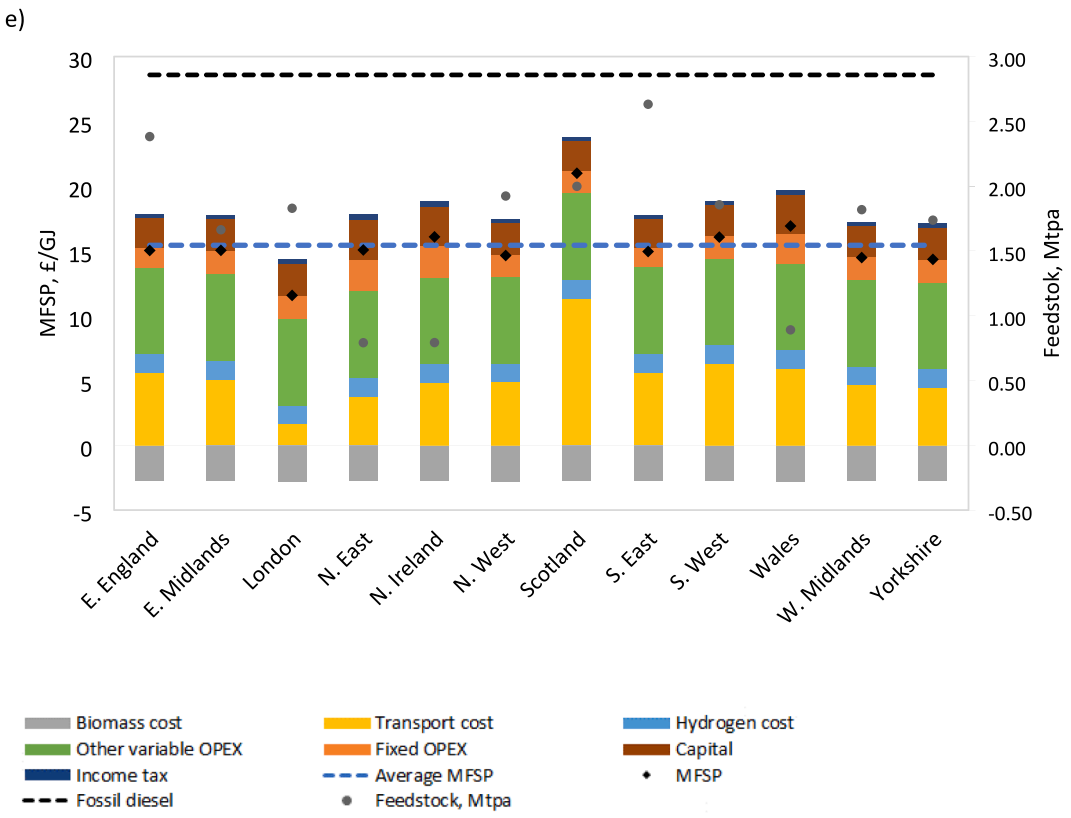


Fig. 6. (*continued*).

(two-thirds of the radius) of the circle is the average transport distance, see SI Section 1.2.2 for details. Since the various regions of the UK are not perfect circles, a sensitivity analysis is performed on the transportation distance to determine the impact of the uncertainty of the transportation distance on the MFSP, see SI Section 4.4 for details. Also, regional transportation cost is factored in the plant economics as this regional transportation of wet waste feedstocks may not be what is currently practised. The cost of transportation was estimated at £0.26 per km per ton of waste, based on reported data by Kocher [62].

In the decentralised approach, the transportation of biocrude produced from the feedstocks to a central drop-in fuel production plant is assumed to be part of the operating cost of the central plant and the distances involved are the same as in the central approach. However, in the decentralised processing of the feedstocks at local locations into biocrude, it was assumed that the local biocrude plants are co-located with the waste collection or treatment sites in local areas so that the transportation distance to the biocrude plant is negligible. Also, the assumption of a negligible impact of transportation of waste into biocrude in the local processing of wet feedstocks is supported by current applications, as currently waste gathering or collection is done via councils for food waste and the waste generator (including for digestates) pays for the transportation of the waste locally.

2.5. Hydrogen source

The hydrogen for hydroprocessing of biocrude can be obtained from a variety of sources such as natural gas and electricity. Grey hydrogen is the most widely available hydrogen currently, accounting for 95 – 99.5 % of the world's hydrogen supply [63,64]. The production of green and blue hydrogen is highly uncertain currently, as they make up only a negligible portion of world hydrogen production volumes, less than 1 %. However, scenarios considering the use of green and blue hydrogen are also analysed, assuming these will become available in the future, in line with current policies on hydrogen. The average of the cost values reported by IEA [65] and the emissions factors reported by BEIS [66], as shown in Table 4 were used in this study.

2.6. Economic analysis

The key approach adopted in the economic model for the estimation of the price of drop-in fuels is highlighted in this section. Data, such as equipment costs and costing methodology by authors such as Snowden-Swan et al. [27], Jones et al. [39] and Aierzhati et al. [37] were adopted for this analysis.

2.6.1. General assumptions and approach

The economic assessment was based on the nth plant costing analysis methodology, which represents a typical future costing, and this does not account for additional expenses such as equipment redundancies and longer start-up associated with designing and operating a first-of-a-kind plant [27,42], see Table 5 for details.

The cost analysis is performed based on the 2021 constant Pound Sterling (£) basis, therefore, equipment costs are updated to 2021, where necessary, using the chemical engineering plant cost indices. Conversions between £ and the US dollar ($) were made on the average 2021 exchange rate of £1 to $1.3496. The production costs determined are adjusted in line with inflation, and these are used to determine MFSP, based on a 25-year discounted cash flow rate of return, to assess discounted fuel selling cost and enable comparison with current fuel prices for potential financial viability.

2.6.2. Capital cost

Capital costs are usually based on estimates, as it is somewhat difficult and unrealistic to get the exact capital costs for a specific plant capacity, especially one which has not been commercially developed like HTL plants. In the estimation of the capital cost, original equipment costs are scaled to the current equipment/plant size, using a scaling factor (n) which is based on Equation (1), where n the scaling factor is

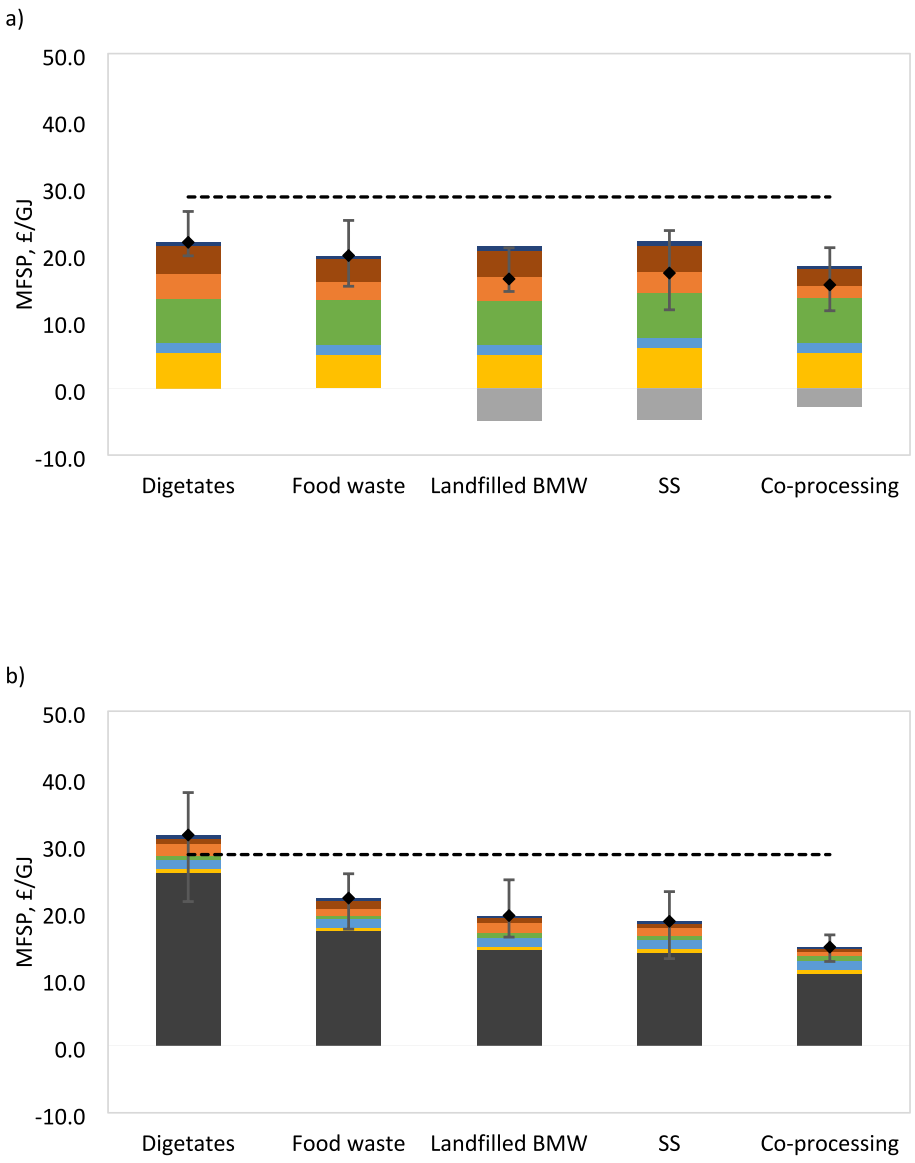


Fig. 7. Average MFSP distribution of various feedstocks using (a) Centralised approach based on grey hydrogen use (b) Decentralised approach based on grey hydrogen use (c) Centralised approach based on blue hydrogen use (d) Decentralised approach based on blue hydrogen use (e) Centralised approach based on green hydrogen use (f) Decentralised approach based on green hydrogen use. Error bars represent the variations in MFSPs across the various regions of the UK. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

typically between 0.6 and 0.7, based on reported values by Jones [39] and Snowden–Swan [27], see SI Section 2 for details. Adjustments were also made to account for the installation factors of various equipment.

$$\text{Scaled equipment cost} = \text{Cost at original scale} \times \left(\frac{\text{Scale up capacity}}{\text{Original capacity}}\right)^{n} \quad (1)$$

Furthermore, the capital costs of scaled equipment, which are typically in their respective cost years, are adjusted to the cost analysis base year of 2021 using the indices from the Chemical Engineering (CE) Index, by applying Equation (2)

$$\text{Cost in 2021 USD} = \text{Equipment cost in quote year} \times \frac{\text{2021 index}}{\text{Quote cost year index}} \quad (2)$$

The total installed cost (TIC) sums the various equipment cost, and this is used to calculate the total capital investment (TCI), which is the sum of the direct and indirect costs obtained using estimates based on the TIC. Table 6 shows the various cost factors used for direct and indirect cost analysis.

2.6.3. *Production costs*

The production cost also referred to as operating cost can be divided into fixed operating expenditure (fixed OPEX) and variable operating expenditure (variable OPEX) and is calculated on an annual basis from the cost of operating the plant. The fixed OPEX consists mainly of the labour cost, while the variable OPEX consist mainly of the feedstock and transportation costs, raw materials costs, and utilities. These costs were adjusted each year to account for inflation. An inflation rate of 2 % per year was used in this analysis.

The variable and the fixed OPEX basis of this analysis are shown in Table 7 and Table 8, respectively. The variable OPEX calculations were based on the literature data on the consumption of raw materials, chemicals, wastes, and utilities. The costs of the feedstocks used are based on Table 3.

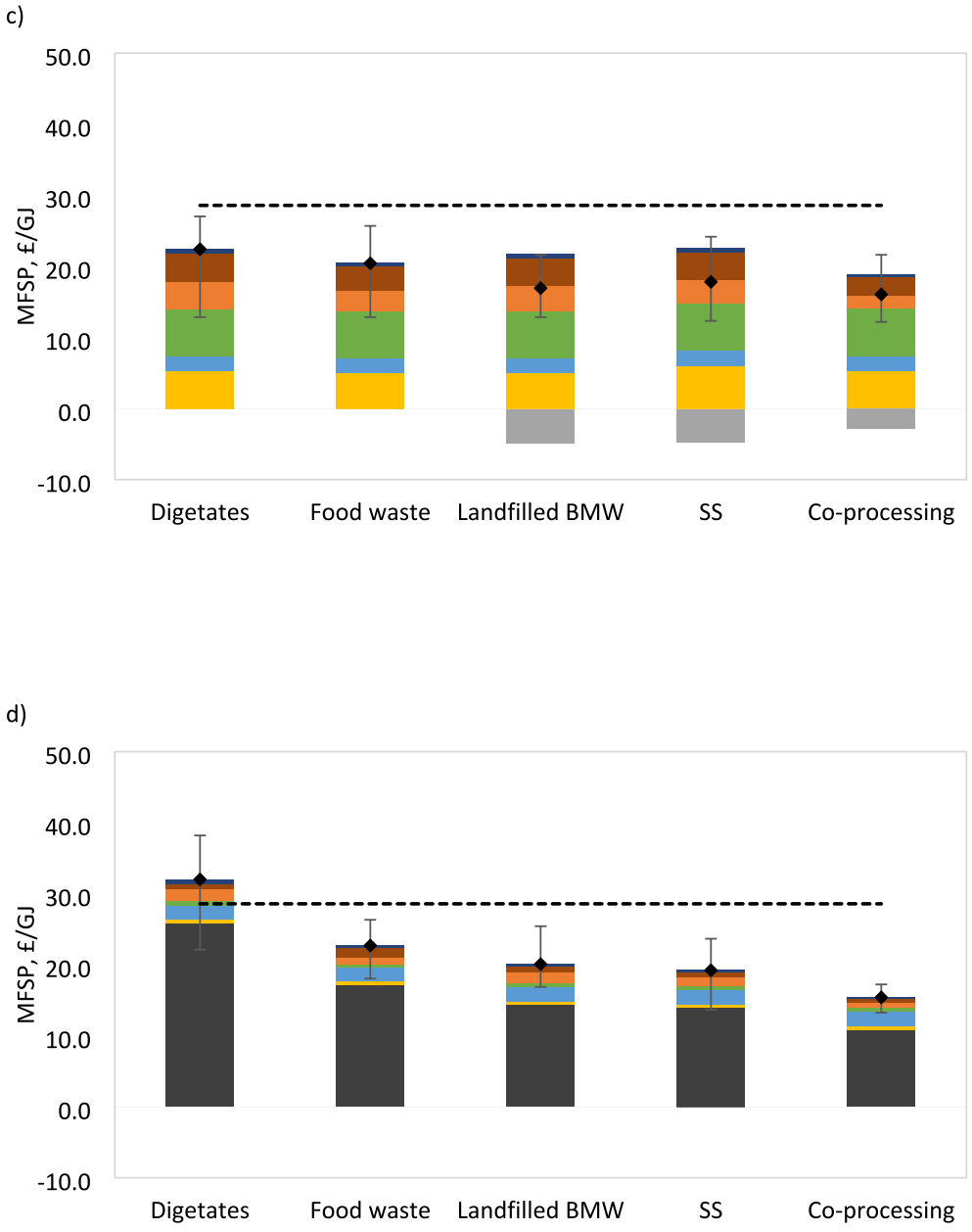


Fig. 7. (*continued*).

2.6.4. MFSP

A 25-year discounted cash flow rate of return, at a rate of 10 %, was used in the evaluation of the MFSP. The MFSP is the selling price of the fuel product at the factory gate that makes the net present value (NPV) of the project equal to zero, over the plant life. It was calculated based on Equation (3), where CF is the cash flow in any year (t) and r is the discount rate. In addition, economic cost factors that are found in Table 6 such as depreciation and tax were factored into the price analysis. The MFSP calculated is referenced to the factory gate as the sales point, hence, the MFSP here does not include other downstream costs factors such as the fuel distribution cost and retailer's margin.

$$NPV = \sum_{t=1}^{n} \frac{CF_t}{(1+r)^t} - CF_0 \quad (3)$$

2.7. LCA

The drop-in fuel life cycle, as shown in Fig. 1, consists of various stages such as the waste generation and the fuel production stages, and this defined the boundary conditions of the work. Various inventory data and emission factors from the literature were used to estimate the life cycle emissions involving the fuel production and utilisation processes, see SI Section 3 for details.

2.7.1. LCA goal and scope

This study aims to estimate the life cycle emissions of producing drop-in fuels using various UK wet feedstocks and fuel production scenarios. The analysis undertaken is similar to well-to-wheel LCA analysis where the emissions from the point the feedstocks become waste (raw materials) to the point the fuel is combusted are evaluated. Emissions

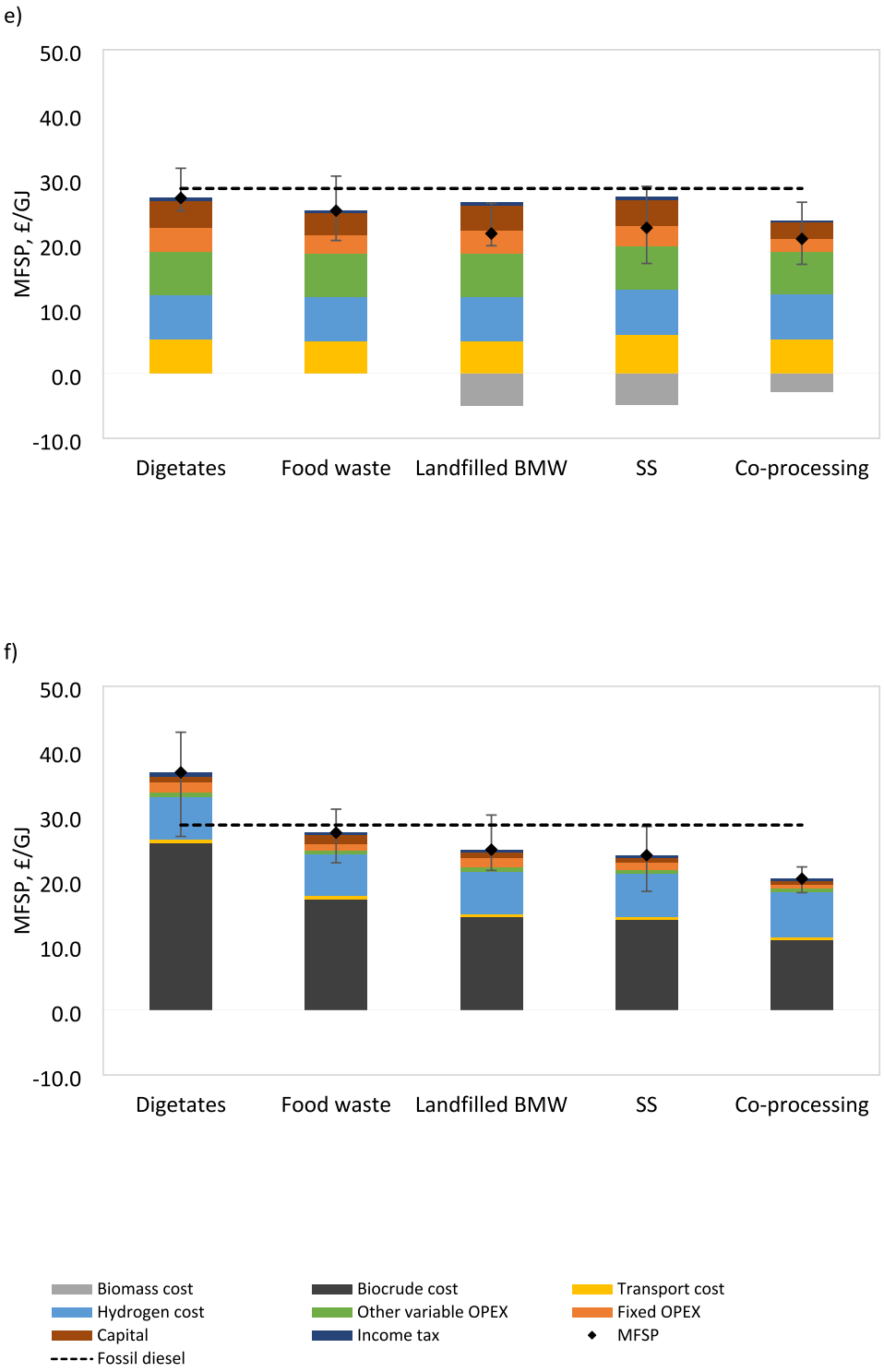


Fig. 7. (*continued*).

associated with building the infrastructures (process plant and vehicles) were not considered. Due to the nature of the various biomass feedstocks being waste materials, it is taken that the waste biomass materials carry a GHG emission rate of 0 g CO_2eq/kg at the point of collection. The functional unit of this study is 1 MJ of liquid (gasoline and diesel) fuel produced, while the GHG emissions are reported in kg CO_2eq per GJ fuel. The emissions in g CO_2eq per MJ of fuel can be converted to kg CO_2eq per GJ by using a factor of 1. The LCA approach is to determine both attributional and consequential GHG emissions of the drop-in fuels. Attributional LCA analyses the emissions impact directly associated with a process or product. While consequential LCA analyses the emissions impacts which may, directly and indirectly, arise from using a process or product. Generally, attributional LCA assigns an estimate of the share of global environmental burdens that belong to a process or product, while consequential LCA assigns an estimate of how a process or product affects the global environmental burdens [73]. In this study, emissions directly in the fuel production supply chain which were evaluated include emissions from feedstock transportation and fuel production, while emissions taken to come indirectly from the fuel including foregone electricity credits and foregone fertiliser credits were also

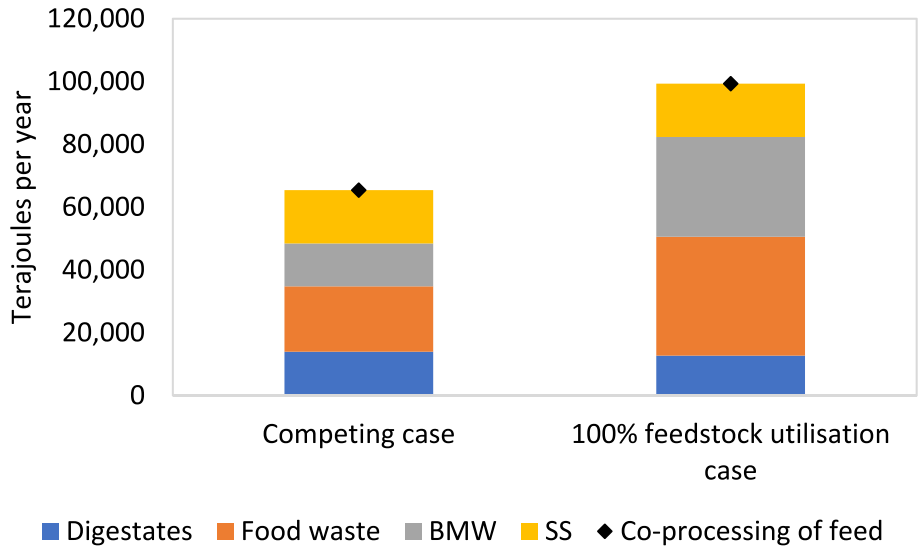


Fig. 8. The total drop-in fuel production volumes from the UK wet feedstock, based on the competing and 100% feedstock utilisation case.

evaluated. Other details on the assumptions about the LCA methodology can be found in the SI file [Section 3].

2.7.2. Avoided waste management

In the consequential LCA analysis, the indirect emissions associated with the diversion of the feedstocks from the existing waste management systems (shown in Table 1) were considered. The existing waste management systems' potential benefits and emissions that were analysed include electricity (for AD and incineration processes), soil benefits from fertiliser and carbon sequestration (for AD and composting processes), and avoided waste treatment emissions (for composting and landfilling processes). These benefits and emissions can be foregone when these feedstocks are used in fuel production. See Section 3.1 in the SI for more information on the indirect emissions factors of these processes.

2.7.3. Life cycle emissions outlook

Life cycle emissions outlook over the various fuel production approaches were analysed based on the BEIS [74] electricity emissions outlook for the UK. The BEIS outlook takes into account the energy policies in the UK in estimating future emissions. The electricity emission and heat emission factors, hydrogen emissions factors and sodium carbonate emissions factors were adjusted, based on BEIS publications [66,74], to develop the GHG emissions outlook in this study, with the year 2021 as the base year. Also, it was assumed that grid electricity instead of natural gas will be used to make up the heating demand of the fuel process from 2030, as heat generation shifts from natural gas to a lower carbon option. It is important to note that potential changes in competing uses in the future were not accounted for in the analysis.

2.7.4. Inventory data

The summary of the inventory data used in the LCA is outlined in SI Table 22. The data from the literature were collected on the various stages of fuel production ranging from feedstock collection and transportation to fuel transportation and distribution.

3. Results and discussions

3.1. Economic analysis

The results of the cost estimation for the various feedstocks, plant configurations and hydrogen sources are presented here. The impact of design and operating parameters such as plant scale and feed distribution are evaluated with respect to the MFSP. In addition, a sensitivity analysis of the key parameters impacting fuel production is also presented.

3.1.1. Plant scale

The effect of plant scale on the MFSP was evaluated for food waste processing as shown in Fig. 4. The MFSP decreases with an increase in plant scale as the economy of scale favours larger plant capacity until the transportation cost of the feedstocks becomes significantly dominant, then an increase in the MFSP is obtained with an increase in plant scale. At smaller production scales, the breakdown of the cost components of the MFSP, as shown in Fig. 4, is dominated by capital and fixed OPEX costs. However, as the production scale increases, the dominant cost components changed to transportation costs and other variable costs. As it is previously known, MFSP is highly dependent on the production scale, due to economy of scale, as reported by several authors such as Zhu et al. [42] and Snowden-Swan [75]. However, with wet biomass feedstocks being high in moisture content and consequently exhibiting very high transportation costs when long distances are involved, increasing the scale of the fuel production plant makes it less economical above certain plant capacity. Thus, a certain scale of operation is needed to reconcile the huge cost of transporting very high moisture content feedstocks. Fig. 4 suggests the optimum plant capacity for the centralised processing of the various wet biomass feedstocks is within 5,000 to 50,000 kg/h, as the MFSPs from these plant scales yield the best fuel prices. Furthermore, the scales of these drop-in fuel plants are expected to play a crucial role in the prices of fuel produced using either a centralised or decentralised production approach, as both approaches may vary with plant scale and subsequently in the MFSP. This can be seen in Fig. 5 when the plant scale for the decentralised conversion of the wet biomass to biocrude at localised locations is above a certain capacity, about 6000 kg/h. In this configuration, the decentralised case for the wet biomass feedstock becomes more economically favourable than the centralised approach. Thus, the benefit of using either a centralised or decentralised approach in wet biomass processing depends on the local availability of the feed and the distribution of the feedstock across locations.

3.1.2. Feedstocks

The MFSP of the drop-in fuels from any feedstock varied over different regions in the UK. As seen from Fig. 6a, for fuel production from food waste via Centralised, Grey H2, the MFSP varied from £15.23 per GJ in London to £25.07 per GJ in Scotland. The variation in the price of fuels over the various regions is highly driven by the

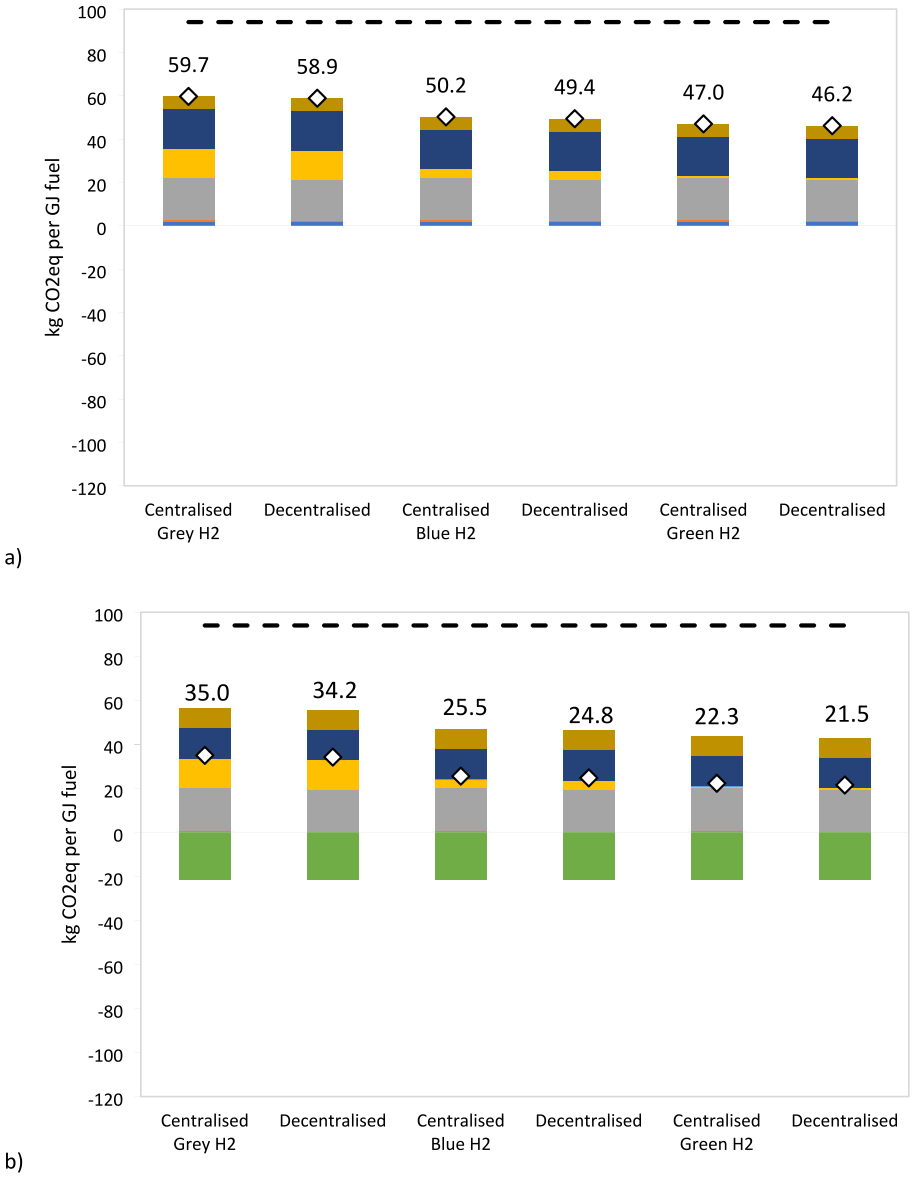


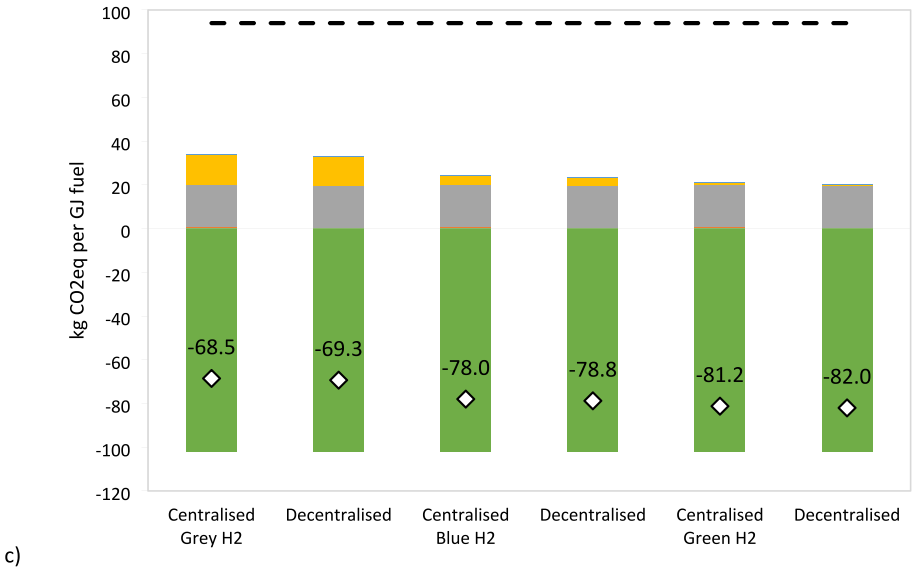
Fig. 9. Life cycle GHG emissions results of drop-in (gasoline and diesel) fuels from various production approaches for (a) Digestates (b) Food waste (c) BMW (d) SS and (e) co-processing of the feedstocks. The fossil diesel reference value by EU RED-II is 94 kg CO_2eq per GJ. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

availability and distribution of the feedstocks. London, which has the lowest MFSP for food waste processing, has one of the highest food waste availabilities. Also, the average transportation distance across London is significantly lower compared to the other regions. Conversely, Scotland which has a very high average transportation distance has the highest MFSP. Transportation distance constitutes a significant portion of the MFSP, up to 42 % of the MFSP for food waste processing, in the Centralised, Grey H2 scenario. Thus, the location of biofuel plants in any region can result in different MFSPs.

Also, the MFSP varied with the feedstock types, as seen in Fig. 6a–e, which showed the price distribution of fuel from the various feedstocks. The national average MFSP ranged from £14.76 to £36.71 per GJ (£0.47 – 1.17 per GLE) over different feedstocks and production approaches, see Fig. 7a–f and SI Section 4.3 for further details. All the feedstocks, except digestates in the decentralised cases, had prices which are competitive with 2021 wholesale fossil diesel's price of £28.58 per GJ. Therefore, excluding the decentralised scenarios for digestates, as digestates are very distributed, the average price is in the range of £14.76 to £27.11 per GJ (£0.47 – 0.86 per GLE). The significant variations in the MFSPs from the various feedstocks are due to factors such as feedstock cost/gate fees, product yield, feedstock availability and distribution over a location. The cost of feedstock/gate fee is expected to be different for the various feedstocks, as shown in Table 3. These feedstock costs are based on the current disposal methods, and there is no certainty about what the waste management market will look like in the future, considering the potential change that could come, such as in the use of new and emerging technologies. The uncertainty in the feedstock cost is further evaluated in the sensitivity analysis in SI Section 4.3.

3.1.3. *Centralised vs decentralised operation*

The distribution of the MFSP of fuel from the various feedstocks using centralised and decentralised approaches is shown in Fig. 7a–f. For the processing of the feedstocks, centralised production achieved the lower prices, while in the co-processing case, the decentralised approach achieved better prices. This is because the processing of digestates, food waste, landfilled BMW or SS into biocrude at localised areas prior to



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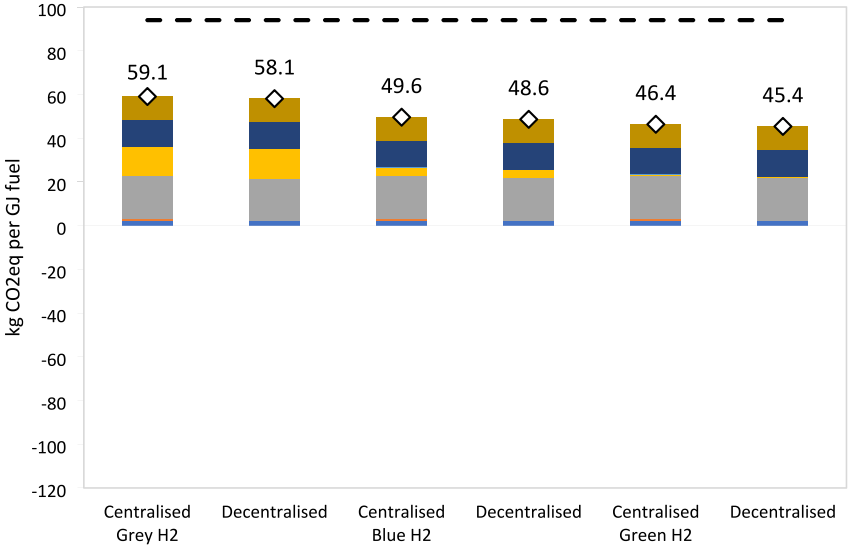


d)

Fig. 9. (*continued*).

conversion to fuel at a central site, requires many smaller scale HTL plants to be distributed over a much wider area, which is economically less favourable compared to the centralised approach. However, in the co-processing case, local conversion of the feedstocks is done at better plant scales since the decentralised case combines the various wet feedstocks (such as digestates, food waste and SS) that are available, thereby performing more optimally. As highlighted in Section 3.1.1, for localised processing of the feedstocks with volumes above 6000 kg/h, the decentralised approach performs better than a similar plant scale using the centralised approach. This shows how the economy of scale, distribution and transportation of feedstocks are key considerations when adopting production approaches in relation to wet biomass feedstocks. Where there is a low local availability of feedstocks, the centralised approach performs better but where there is ample local availability of feedstocks, the decentralised approach performs better. The average fuel price in the centralised approach for the grey hydrogen case is in the range of £15.44 – 21.79 per GJ compared to the decentralised approach which is in the range of £14.76 – 31.50 per GJ.

3.1.4. *Hydrogen sources*

The MFSP of drop-in fuels is highly dependent on the cost of hydrogen, with green hydrogen resulting in the highest fuel price, followed by blue hydrogen and grey hydrogen. As seen from Fig. 7a–f, the average prices of the fuel from the blue hydrogen scenarios for the various feedstocks are marginally higher (2 – 4 %) than those of grey hydrogen, while average prices of the fuel from the green hydrogen scenarios are significantly higher (17 – 38 %) than those of grey hydrogen. According to the IEA, the levelized cost of green hydrogen is about 3 – 5 times higher than the costs of blue and grey hydrogen, meanwhile, the incremental levelized cost of blue hydrogen is relatively smaller. While renewable hydrogen has a lower carbon intensity, it comes with a cost penalty. The price range of fuel from the grey hydrogen centralised scenarios of £14.76 – £31.5 per GJ (£0.47 – 1.00 per GLE) agrees with the prices of £15.39 – 29.1 per GJ (2021 prices) published by the Royal Society [77] and Jiang et al. [78], which used grey hydrogen for HTL of forest residues and SS. Also, the results of this study agree with Alamo et al. [79] drop-in fuel prices for SS HTL of

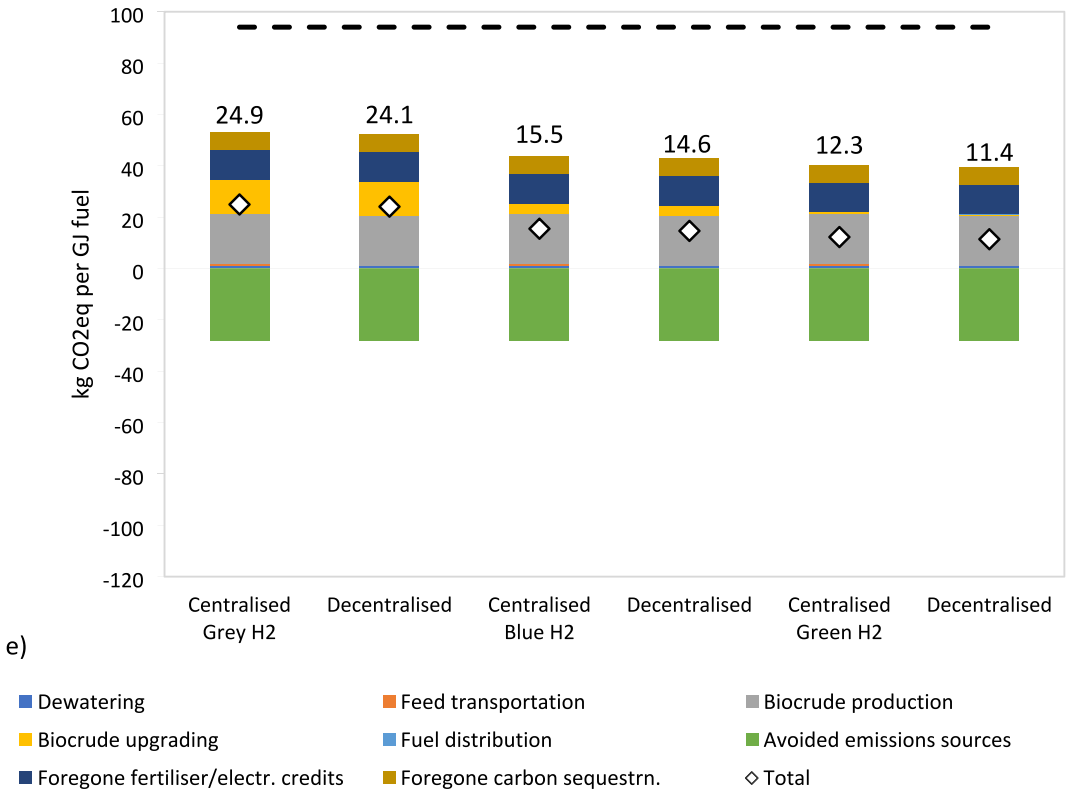


Fig. 9. (*continued*).

£18.48 – 30.10 per GJ over similar plant scales (100 – 400 tons/day). The prices of fuel from SS for this study using grey hydrogen centralised scenarios are in the range of £17.20 – 23.92 per GJ. Analyses by Jiang et al. [78] and Alamo et al. [79] also assumed negative feedstock prices for SS like the assumptions used here. However, these studies and many others in the literature do not consider the impact of using blue or green hydrogen in drop-in fuel production. Royal Society [77], Jiang et al. [78] and Alamo et al. [79] did not present a cost breakdown in their analysis but our study suggests that the fuel prices can increase by up to £5.40 per GJ when switching the hydrogen source from grey to green hydrogen. Additionally, the prices of drop-in fuel production via HTL are competitive with fossil diesel of £28.58 per GJ, based on 2021 wholesale prices of diesel published by RAC [76].

3.1.5. Total fuel quantities

Estimating the total volume of fuels that can be produced based on the UK wet feedstock is non-trivial, so here we assessed two bounding cases to serve as upper and lower limits. The competing case serves as the likely lower limit, reflecting the competitive use of biomass resources in line with current waste management techniques. Here, we assumed the use of 75 % of digestates (i.e., some digestates have low accessibility and poor quality), 46 % of food waste (i.e., some portion of the food waste is recycled or used in an AD), 30 % of landfilled BMW (i.e., due to food waste being landfilled and growth in competing uses), and 100 % of SS (i.e., new opportunity as current SS treatment is avoided due to high cost and safety concerns associated with sludge disposal). On the other hand, the upper limit assumed 100 % feedstock utilisation to reflect the theoretical maximum.

The volume of fuels which can be produced from the UK wet feedstocks is shown in Fig. 8. The competing case and 100 % feedstock utilization case resulted in a total potential volume of 1,865 ML/yr (65,395 TJ/yr) and 2,830 ML/yr (99,315 TJ/yr), respectively, at an MFSP of less than £20.80 per GJ (£0.66 per gasoline litre equivalent, see Fig. 7). This is approximately 4.5 % and 6.8 %, respectively, of the UK's total gasoline and diesel fuel consumption of 41,835 ML/yr in 2021 [80]. Importantly, these volumes are much lower than the 14 % target for biofuel consumption set by the EU RED-II [5,6] for 2030. While they can contribute to the current UK fuel mix, on top of the existing biofuel volumes of 5 % [6], this study highlights the need for complementary low-carbon fuel alternatives to close the supply gap in the mid and long-term. Here, the UK could consider low-carbon synthetic fuel often referred to as electro-fuel, produced from captured CO_2 and green hydrogen, as a complementary drop-in solution. However, the prices of electro-fuel of £72 – 95 per GJ estimated by the Royal Society [77] are significantly higher than those of drop-in biofuel from green hydrogen of £20.30 – 36.71 per GJ estimated in this study.

3.2. LCA

The life cycle GHG emissions of drop-in fuels from digestates, food waste, landfilled BMW and SS, based on the various scenarios analysed are represented in Fig. 9a–e. The impacts of plant configurations involving centralised and decentralised operations, and hydrogen sources were analysed, as shown in Fig. 9a–e. As seen from the figures, the GHG emissions were majorly driven by the biocrude production and upgrading stages, which require significant amounts of energy, chemicals, electricity and hydrogen. Also, depending on the waste types, other factors such as avoided emissions and foregone electricity credits, fertiliser credits and carbon sequestration significantly impact GHG emissions.

3.2.1. Feedstocks

All investigated fuels achieve lower emissions than conventional petroleum diesel, but the life cycle GHG emissions of the drop-in fuels are highly affected by the nature of the biomass feedstocks (Fig. 9). Diverting landfilled BMW to fuel production achieves significantly negative GHG emissions, due to avoided methane gas emissions associated with existing landfill management practices. Currently, about 17

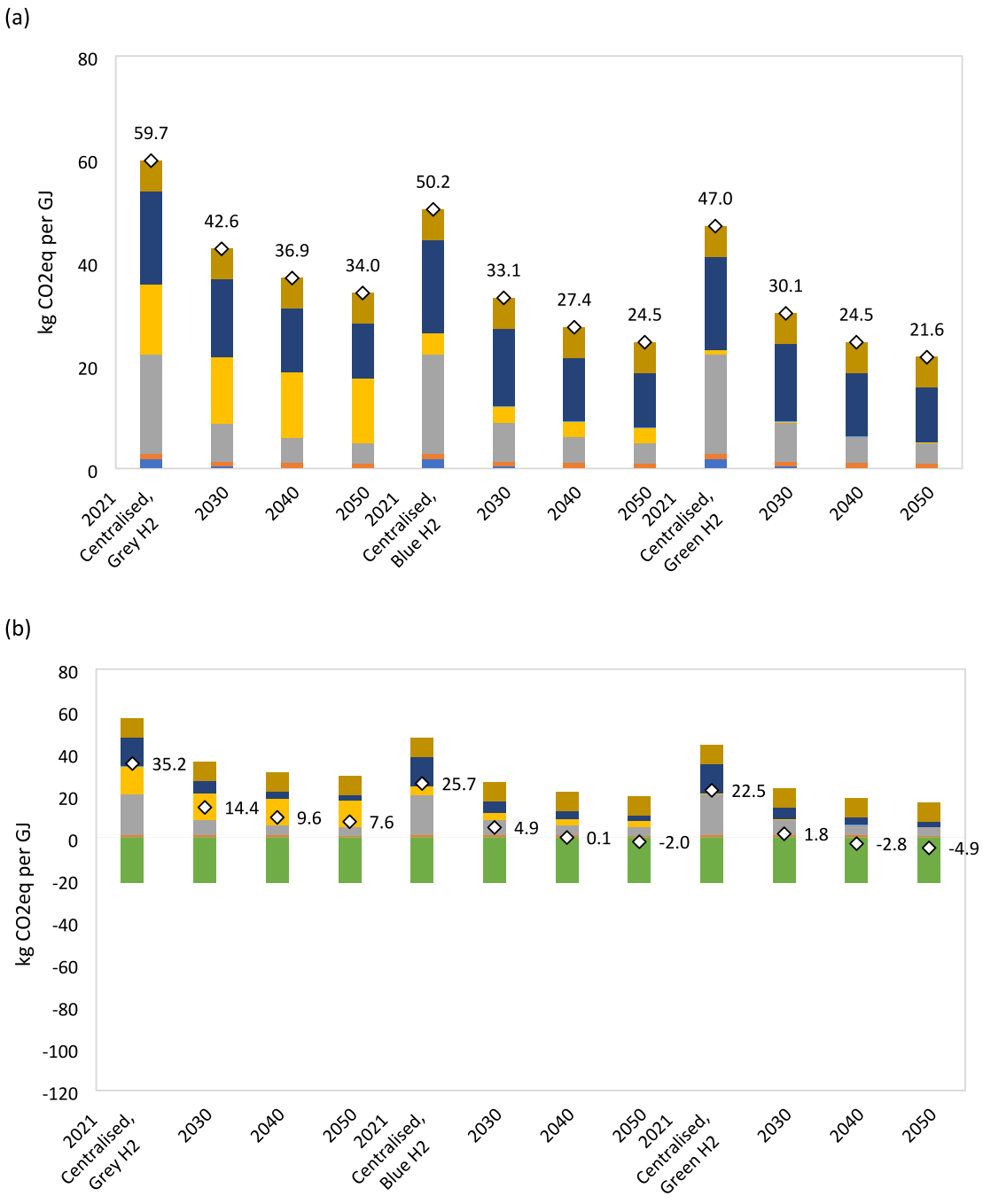


Fig. 10. Life cycle GHG emissions outlook scenarios for (a) digestates (b) food waste (c) Landfilled BMW (d) SS and (e) co-processing of the feedstocks, based on a consequential LCA approach.

% of landfilled MSW is food waste [9] and approximately 50 % of landfilled MSW is BMW [16]. A significant amount of methane is released from landfills despite some degree of methane recovery at these sites, and Nordahl et al. estimates about 400 g CO_2eq is released per tonne MSW [10]. Hence, −21.5 kg CO_2eq per GJ and −102.3 kg CO_2eq per GJ fuel contributes to the avoided emissions in the utilisation of landfilled food waste and BMW for fuel production, respectively. On the other hand, the much higher emissions for digestates and SS feedstocks are also driven by other consequential factors associated with the diversion from their existing uses as soil fertilizers to fuel use, foregoing fertilizer credit and carbon sequestration, and thus contributing about 11.1 – 17.9 kg CO_2eq per GJ fuel and 5.9 – 10.7 kg CO_2eq per GJ fuel, respectively. The total emissions from the digestates, food waste, landfilled BMW and SS feedstocks are 36 – 187 % lower than the 94 kg CO_2eq per GJ (94 g CO_2eq per MJ) fossil baseline under the EU RED-II [51]. This shows there is a strong benefit from diverting these waste materials into fuel.

However, it is important to note that the CO_2 accounting methodology under the EU RED-II is largely based on an attributional approach. Moreover, the RED-II requires that these advanced renewable fuels achieve at least 65 % (or 70 % if they are of non-biological origin) CO_2 reduction relative to conventional fuel for them to qualify under the regulation. Therefore, as part of the sensitivity analysis, we quantified the lifecycle emissions of these fuels by excluding the avoided emissions

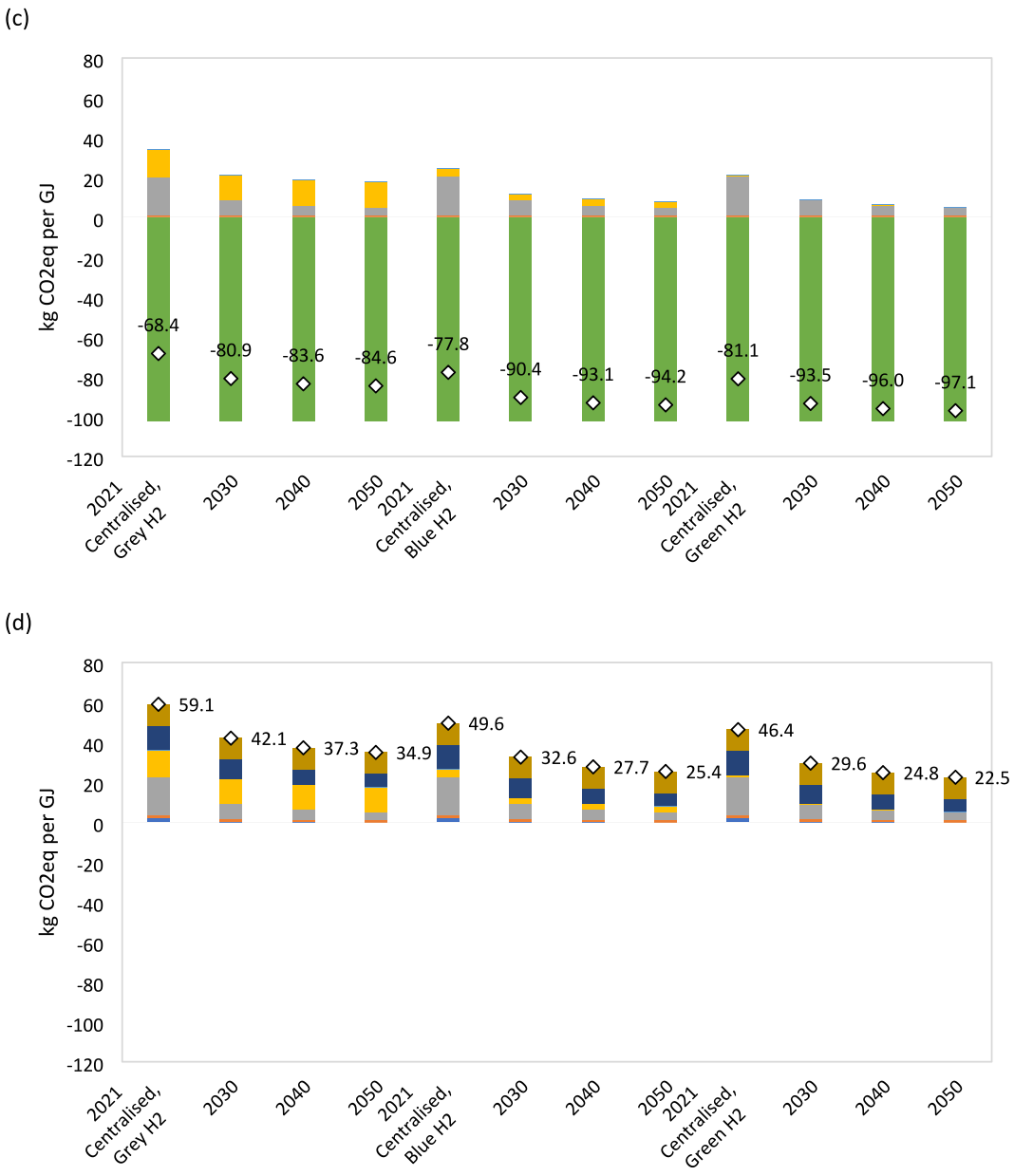


Fig. 10. (*continued*).

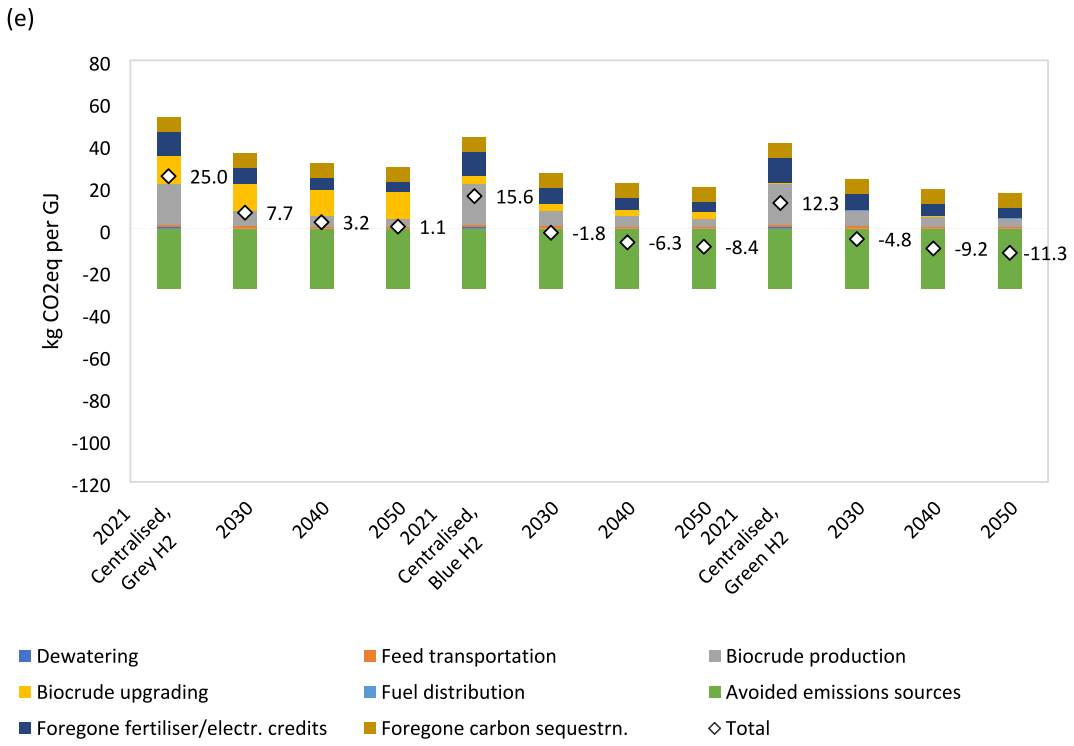
associated with current waste management practices. Without the consequential element of the analysis (i.e., the adoption of an attributional approach), the fuels' carbon intensities vary from a high range of 33.7 – 36.1 kg CO_2eq per GJ (for a centralised production with Grey H2) to a low range of 20.3 – 22.5 kg CO_2eq per GJ (for a decentralised production with Green H2). This translates to a CO_2 reduction potential of 62 – 78 % relative to conventional fuels (see SI Section 4.3 for detailed emissions for each route). Our overall lifecycle emissions are comparable to the literature values for similar HTL processes using woody and algae biomass as feedstocks that resulted in 27 kg CO_2eq per GJ and 35 kg CO_2eq per GJ, as reported by Fortier et al. [81] and Tews et al. [40], respectively.

3.2.2. Centralised and decentralised approaches

The use of a decentralised approach compared to a centralised approach is found to have only a marginal impact on the GHG emissions of the final fuel. As seen from Fig. 9a–e, the change in the mode of operation from centralised to decentralised resulted in about 1 kg CO_2eq per GJ difference, which is small compared to the overall life cycle GHG emissions of the fuel. The emissions associated with feedstock and fuel product transportation over distances are negligible compared to the overall fuel's life cycle emissions, hence, either a centralised or decentralised approach does not offer any strong advantage in GHG emission reduction. Moreover, in the future, the use of renewable fuel in feedstock and/or product transportation could lead to lower overall emissions.

3.2.3. Hydrogen source

Given that biocrude upgrading accounts for ca. 40 % of the total attributional lifecycle emissions, the use of a lower carbon intensity hydrogen in the hydroprocessing stage resulted in a lower overall lifecycle emission. As seen from Fig. 9a–e, the green hydrogen scenarios produced GHG emissions which are 18–37 % (12.7 kg CO_2eq per GJ) less than those produced using grey hydrogen, while the blue hydrogen scenarios produced 14–28 % (9.5 kg CO_2eq per GJ) less than those produced using grey hydrogen. As hydroprocessing requires a significant amount of hydrogen, about 4.4 kg hydrogen per 100 kg of biocrude, considerable emissions reductions can be achieved by switching to a less CO2-intensive hydrogen source during biocrude upgrading. However,



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this comes with high production price implications, as seen previously in Section 3.1.4, which demonstrated the impact of hydrogen sources on MFSP.

3.2.4. *Total emission quantities*

The use of these drop-in fuels has a significant potential to reduce emissions from the UK's road transport sector, which currently emits about 133.7 Mt CO_2eq [1]. Substituting conventional fuels with these drop-in alternatives could reduce emissions by about 4.5 – 5.4 Mt CO_2eq per annum and 8.4 – 9.8 Mt CO_2eq per annum, based on the competing and 100 % feedstock cases, respectively. This is a 3.4 – 7.3 % reduction in the UK's total road transport emission attributable to the displacement of 4.5 % (competing case) and 6.8 % (100 % feedstock case) of conventional fuels by these alternatives. A further reduction will require larger quantities of drop-in fuels, however, our initial estimate suggests that there are limited feedstocks available in the UK, and therefore the UK would benefit from other low-carbon synthetic fuels that can be scaled up to facilitate decarbonisation of the transport sector.

3.2.5. *Life cycle emissions outlook*

The lifecycle GHG emissions for the fuels are expected to reduce over time as manufacturing processes shift to lower carbon electricity and feedstocks (Fig. 10). Based on the competing case, the drop-in fuels could achieve as low as 1.1 kg CO_2eq per GJ, −8.4 kg CO_2eq per GJ and –11.3 kg CO_2eq per GJ of fuels from a centralised co-processing configuration in 2050 using grey, blue and green hydrogen, respectively. Because the consequential LCA approach is highly dependent on both the direct emissions from the drop-in fuel and indirect emissions associated with other processes and products related to drop-in fuel's production and use, there is a high degree of uncertainty in the future emissions estimated using the consequential approach. Furthermore, as the global economy decarbonises in the future, the consequential factors (such as foregone fertiliser and electricity generation) would likely have a lower impact on the total lifecycle GHG emissions. As part of the sensitivity analysis, we repeated the analyses and adopted the attributional LCA approach, which considers only the emissions from processes directly related to the fuel production and use (Fig. 11). The emissions from the centralised processing of the feedstocks based on an attributional approach in 2050 are in the range of 17.6 – 17.7 kg CO_2eq per GJ, 8.0 – 8.2 kg CO_2eq per GJ and 5.1 – 5.3 kg CO_2eq per GJ for grey, blue and green hydrogen use, respectively. Interestingly, by 2050, the lifecycle GHG emissions of these drop-in fuels can be lower than the limits for low carbon hydrogen in the UK of 20 kg CO_2eq per GJ (LHV), and potentially achieving an 81 – 95 % GHG reduction relative to the EU RED-II baseline.

4. Conclusion

This study demonstrates the potential for economically viable production of drop-in fuels from wet waste feedstocks, capable of achieving low – and even negative – life cycle GHG emissions. The HTL of digestates, food waste, BMW, and SS into drop-in fuels using various production approaches, such as plant configurations and hydrogen sources, were studied using TEA and LCA methodologies.

Our analysis estimated the MFSP of the fuel to be in the range of £14.76 to £27.11 per GJ (£0.47 – 0.86 per GLE), which is lower than the current fuel prices in the UK. However, the MFSP metric should be interpreted with caution. The main intention of the metric is to provide a simple "rule of thumb" method for comparing different types of fuel production technologies, which may not consider other relevant issues, including the revenue stream and margin for the producers. From a CO_2 perspective, the fuels are estimated to have a carbon intensity in the range of −82.0 to 59.7 kg CO_2eq per GJ, which translates to a benefit in the range of 36 – 187 % relative to a conventional fuel baseline of 94 kg CO_2eq per GJ. However, the LCA approach adopted here is based on the consequential method, which covers a broader, market-mediated effect beyond the typical fuel's production boundary. By adopting an attributional LCA approach, the CO_2 reduction potential of the fuels are in the range of 62 – 78 % relative to a similar conventional fuel baseline. Furthermore, the lifecycle GHG emissions for the fuels are expected to reduce over time as manufacturing processes shift to lower carbon electricity and feedstocks.

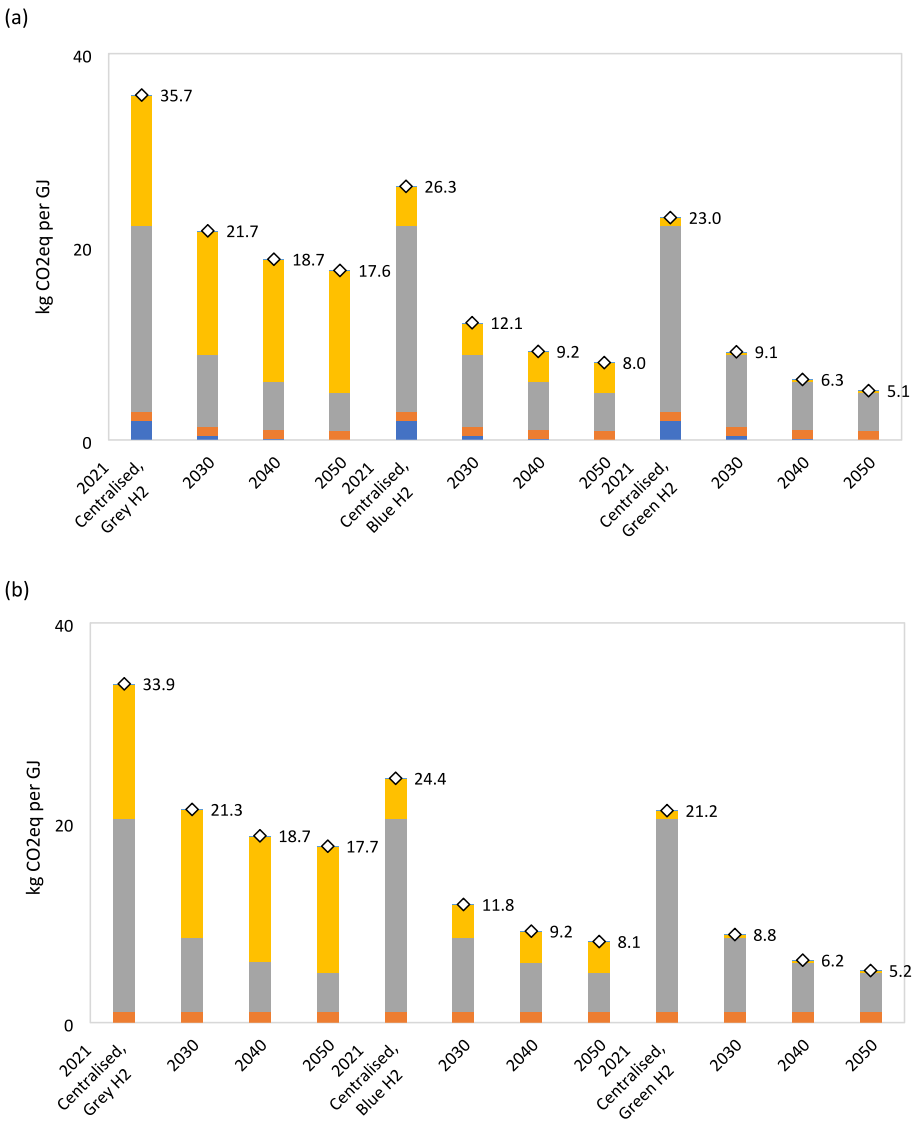
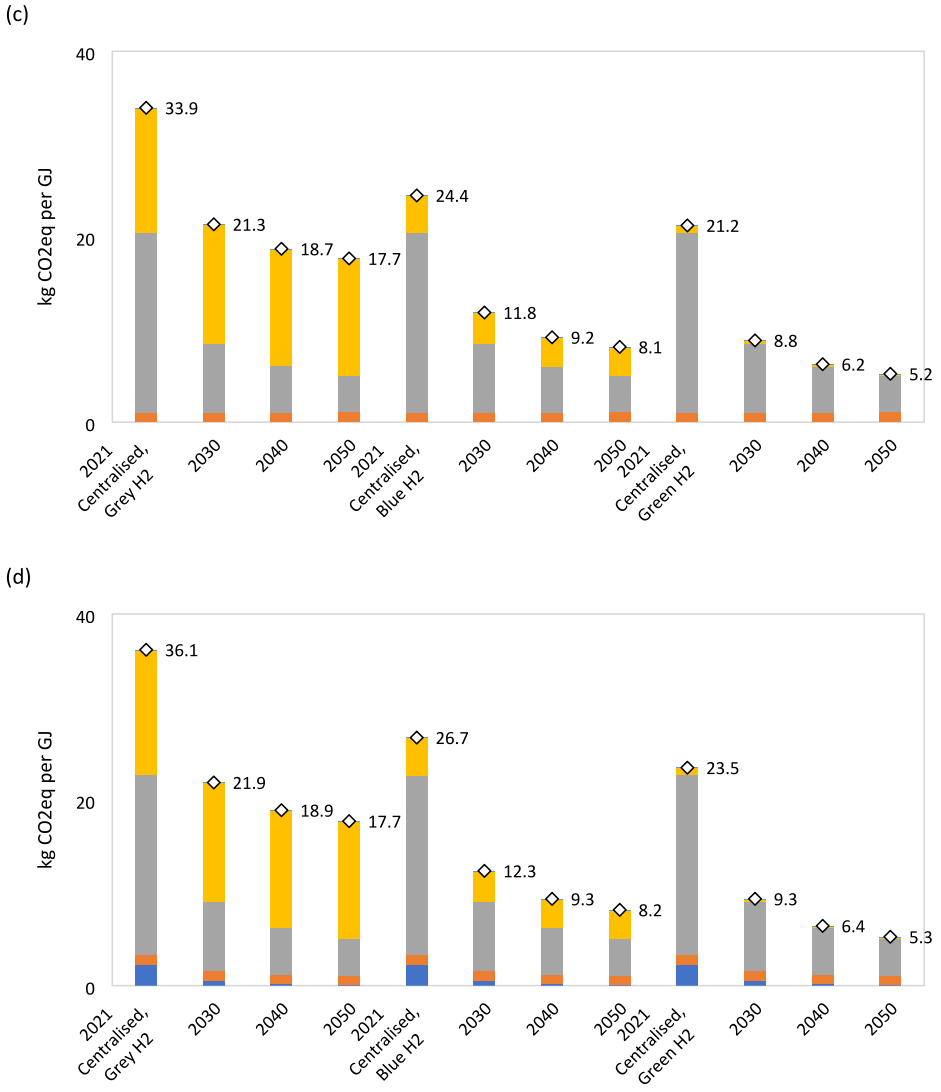


Fig. 11. Life cycle GHG emissions outlook for (a) digestates (b) food waste (c) Landfilled BMW (d) SS and (e) co-processing of the feedstocks, based on an attributional LCA approach.

Several key elements, such as plant configuration (e.g., centralised and decentralised operations) and feedstocks, as well as fuel production stages and supply chain factors, can have a significant influence on the MFSP and lifecycle GHG emissions of the fuels. The use of either a centralised or decentralised approach for the optimum processing of wet biomass is highly dependent on the availability, distribution and transportation of the wet biomass feedstocks, as both approaches can be beneficial. For the wet biomass feedstocks studied, when the local availability of feedstocks is less than 6000 kg/h of dry feed, the use of a centralised approach has significant cost advantages over the use of a decentralised approach. However, when the local availability of the feedstocks is above 6000 kg/h (dry), a decentralised approach provides better cost advantages over a centralised approach. The choice of centralised or decentralised configurations requires an optimal balancing between plant scaling and feed transportation distance, as both factors play important roles in the economics of the drop-in fuel production from wet biomass feedstocks in the UK. On the other hand, in terms of GHG emissions, the choice between a decentralised and a centralised approach has a marginal impact on the overall lifecycle emissions of the fuels. Similarly, the choice of hydrogen production methods can influence the cost and CO_2 impacts of the drop-in fuel, demonstrating the trade-off between the CO_2 benefit of utilizing a low-carbon hydrogen supply and its higher cost of production and supply. An additional production cost of up to £5.40 per GJ can be added due to the high costs of low-carbon hydrogen. However, a GHG emissions reduction of up to 40 % relative to the corresponding grey hydrogen scenarios can be achieved using low-carbon hydrogen.

There are significant opportunities for the production of drop-in fuels by diverting the UK's wet waste feedstocks from conventional waste treatments into transport fuels as a means to increase renewable energy penetration and mitigate transport emissions. However, our study estimated that the UK's wet biomass feedstocks could supply only about 4.5 – 6.8 % of the total gasoline and diesel consumption in 2021, potentially resulting in a 3.4 – 7.3 % reduction in the UK's total road transport emission. While they can contribute to the current UK fuel mix on top of the existing biofuel volumes of 5 %, this study also highlights



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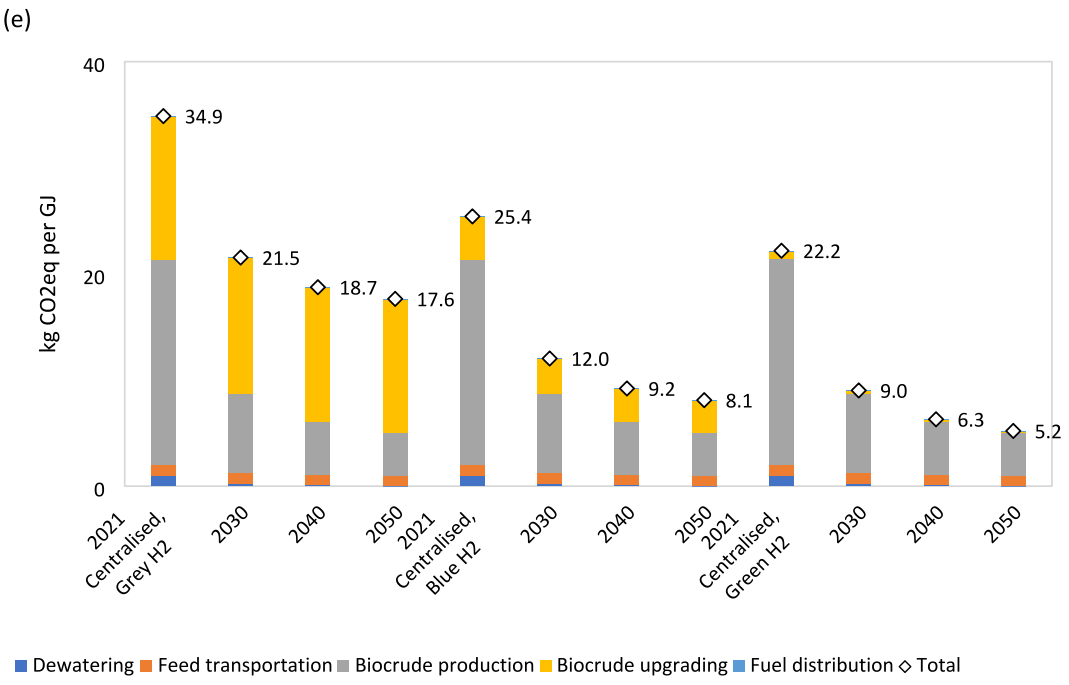

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the need for other complementary low-carbon fuel alternatives to close the supply gap in the mid and long-term towards achieving a net-zero future. As a complementary measure, the UK could consider other synthetic fuel pathways, for example, the production of drop-in fuel from green hydrogen and CO_2 captured from existing, CO_2-intensive industries in the UK. This is an emerging technology that could potentially be scaled up. Synthetic electro-fuel has gained regulatory attention in the EU, which has recently allowed combustion engine vehicles to be sold after the 2035 ban as long as the vehicles operate exclusively on low-carbon, synthetic electro-fuel. This is a technology area that is worth considering for the UK and will require further investigation.

CRediT authorship contribution statement

Sylvanus Lilonfe: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Project administration, Software, Visualization, Writing – original draft, Writing – review & editing. **Ioanna Dimitriou:** Conceptualization, Methodology, Supervision, Validation, Writing – review & editing. **Ben Davies:** Conceptualization, Supervision, Writing – review & editing. **Amir F.N. Abdul-Manan:** Conceptualization, Funding acquisition, Writing – review & editing. **Jon McKechnie:** Conceptualization, Funding acquisition, Resources, Methodology, Project administration, Resources, Supervision, Validation, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.cej.2023.147516.

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6 Techno-economic and life cycle assessments of direct air capture-related technologies

This chapter contributes to the overall thesis aim of assessing low-carbon fuel and chemical technologies by examining direct air capture technologies, including the technical, economic and life cycle assessments of solid sorbent manufacturing and CO_2 capture plants. Direct air capture CO_2 can form part of low-carbon fuel and chemical technologies for producing low-carbon fuels/chemicals by providing carbon-negative CO_2, enabling a circular economy, or can be an entirely standalone low-carbon technology for permanent CO_2 storage in geological reservoirs and as rocks (mineralisation).

The paper presents technical, economic, and life cycle assessments of solid sorbent manufacturing and CO_2 capture technologies from different technological, geographical, and temporal perspectives. It delivers important and original contributions by: 1) creating an innovative integrated manufacturing, techno-economic and life cycle assessment methodology; 2) directly linking the integrated methodology to the kinetics of adsorption and other key sorbent properties, providing new insights of how technical factors influence CO_2 cost and net removals; 3) charting development routes for sorbent technologies towards commercialisation; 4) evaluating a breadth of system options, including energy sources, sorbents, markets, system boundaries, and time to provide global relevant results. In summary, more than 150 key design and operational scenarios were analysed to understand the pathways that reduce the cost of direct air capture while maintaining its CO_2 removal benefits. The chapter reported that net capture costs within \$100/tCO_2 are achievable using certain approaches, including sorbent development and using a combination of US wind energy and grid electricity. This is consistent with claims by direct air capture startups, such as Climeworks, which reported capture costs of \$1,000 to \$2,000/tCO_2 for a 36,000 tCO_2/annum plant (vs \$600 to \$2,000/tCO_2 for a 36,000 tCO_2/annum plant in this work), as well as Carbon Engineering estimates of \$100 to \$250/tCO_2 using a 1 Mtpa capture plant (vs \$90 to \$170/tCO_2 using a 1 to 1.5 Mtpa CO_2 capture plant from the best technology pathways in this work). Additionally, unlike prior future-looking assessments, which mainly apply learning rates to project future costs, we provide, for the first time, clarity on how specific design and operational details must be leveraged to achieve the necessary cost reductions.

Furthermore, due to the scope of this work, some assumptions had to be made. The methodologies assumed that direct air capture could be achieved at a temperature of up to 75 °C at the end of adsorption, based on evidence from the literature, such as (i) Sinha et al. (2017), *Industrial & Engineering Chemistry Research*, which reported no changes in adsorption rates of mmen-Mg_2(dobpdc) adsorbent up to 75 °C, and (ii) Jamei et al. (2024), *Chemical Engineering Journal*, which reported marginal to significant changes (5% to 30%) in adsorption rates of polyethylenimine (PEI)-based adsorbents between 40 °C and 80 °C. The generic sorbent used in the commercial model in this work assumed that the best experimental breakthrough data from existing literature apply to the generic "commercial" sorbent. Future work could model how cases where adsorption rates vary significantly with temperature might affect the operations, costs, and emissions of direct air capture.

The work was published in the Carbon Capture Science & Technology journal in June 2025. The published work is titled "Technical, economic and lifecycle greenhouse gas emissions analyses of solid sorbent direct air capture technologies" and is presented as Chapter 5 in this work. The supplementary information for the work, published alongside the paper, is reprinted in Appendix A3.

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Full Length Article

Technical, economic and lifecycle greenhouse gas emissions analyses of solid sorbent direct air capture technologies

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ABSTRACT

Achieving net zero emissions by 2050 will require the development of cost-effective and CO_2-efficient direct air capture (DAC) technology to remove atmospheric CO_2. This study presents a comprehensive assessment of five solid sorbents under different technology scenarios to determine the design, operations, cost and greenhouse gas (GHG) emissions of DAC technologies. The cost and GHG emissions of the five solid sorbents ranged from $\$_{2024}$1,200–40,400/t sorbent and 3.1–12.3 tCO_2e/t sorbent in 2024, respectively, mainly driven by the raw materials used for sorbent manufacture. Cost estimates for the best capture technologies ranged from $\$_{2024}$97–168/gross tCO_2 captured [$\$_{2024}$126–170/net tCO_2 captured] in 2025 and can be further reduced to $\$_{2024}$87–140/gross tCO_2 captured [$\$_{2024}$93–142/net tCO_2 captured] in 2050. The costs of DAC are heavily influenced by: (i) economic factors (i.e. capital expenses and energy costs), (ii) design elements (i.e. plant scale) and (iii) technical parameters (i.e. sorbent's adsorption rate and time). Conversely, the GHG emissions of DAC are mostly determined by the source of energy. Price signals in existing carbon markets are inadequate to support a DAC project, but a forecasted carbon price increase to \$140–240/tCO_2 by 2030–2050 could make DAC commercially viable.

Abbreviations

CDR	Carbon dioxide removal
CEPCI	Chemical engineering plant cost indices
DAC	Direct air capture
DEA	Diethanolamine
ETS	Emissions Trading System
FCI	Fixed capital investment
FU	Functional unit
GHG	Greenhouse gas
GWP	Global warming potential
ISBL	Inside Battery Limit
LCA	Life cycle assessment
LCOC	Levelised cost of capture
MOF	Metal-organic framework
MSP	Minimum selling price
NG	Natural gas
NPV	Net present value
NZE	Net zero emissions
OSBL	Outside Battery Limit
PEI	Polyethyleneimine
Pz	Piperazine
TCI	Total capital investment
TVSA	Temperature vacuum swing adsorption
SI	Supplementary Information

1. Introduction

Achieving net zero emissions (NZE) and limiting global warming to 1.5 °C or even 2 °C above the pre-industrial level, requires gigaton-scale carbon dioxide removals (CDR) to drawdown atmospheric stock CO_2 (IPCC, 2014, 2023). Direct air capture (DAC) is an engineering-based CDR technology that directly extracts CO_2 from air using chemical or physical processes. Key advantages of DAC over other CDR methods include its ability to capture CO_2 at very high rates using significantly lower land area and process cycle time. A DAC plant that captures 1 $MtCO_2$ per year using a land area of 0.4–1.5 km^2 (99–371 acres) is equivalent to the CO_2 capture rates of roughly 46 million trees, requiring approximately 3098–4647 km^2 (765,494–1148,241 acres) of land (The Environmentor, no date; Fasihi et al., 2019). Additionally, the CO_2 captured by DAC can be utilised in low-carbon chemicals and fuels syntheses to meet society's growing demand for energy and materials in our existing carbon-based economy. Crucially, however, as many earlier

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studies have pointed out, the cost of DAC must be reduced significantly for it to play an important role in our net-zero strategy, whereby several sorbent-related parameters (e.g., cost, adsorption rate, cycle time) can be major contributing factors.

Amine liquid sorbent capture, the conventional CO_2 capture technology, has been used for CO_2 capture from flue gas since 1930 (Wang et al., 2022). Aqueous amines such as monoethanolamine and diethanolamine (DEA) have typically been used for CO_2 capture due to their suitable properties such as high adsorption rates, low regeneration temperatures, and relatively lower cost (Aghel et al., 2022; Wang et al., 2022). However, amine capture could be faced with problems such as corrosion due to the corrosive nature of liquid amines and evaporative (capacity) loss due to amines' high vapour pressure (Erans et al., 2022; Wang et al., 2022; Singh et al., 2024). Hence, solid sorbents have been developed to address some of the challenges associated with liquid amines and the high regeneration temperatures required for other liquid sorbents in DAC. These solid sorbents use physisorption, chemisorption, or a combination of both, and are made of various porous materials such as zeolites and metal-organic frameworks (MOFs). Physical adsorbents have also been combined with amines, resulting in amine-modified solid sorbents like amine-modified zeolites and amine-modified MOFs (Sinha et al., 2017; Erans et al., 2022; Wang et al., 2022; Zhang et al., 2023). Therefore, amine-modified adsorbents could combine the low regeneration temperature of solid sorbents and amines, the lower corrosion effect of amines in amine-modified adsorbents and the improved stability of amines in solid sorbents.

Despite the noteworthy prospect of zeolite sorbents, information in the literature related to their cost and greenhouse gas (GHG) emissions is uncertain. The costs of solid sorbents reported in the literature span orders of magnitude, from $200–80,000/t (Sinha et al., 2017; Azarabadi and Lackner, 2019; Valentine et al., 2022; Nagapurkar, Thirumaran and Kidder, 2024) while the GHG emissions of adsorbents were reported to be in the range of 1.2–50 tCO_2e/t sorbent (Deutz and Bardow, 2021; Leonzio et al., 2022). Generally, sorbent costs and GHG emissions are highly dependent on raw material costs and composition because sorbent manufacturing is a transforming process that modifies raw materials like zeolites and silica into high-quality adsorbents. Other factors that can significantly impact solid sorbent cost include plant capital cost and fixed operating cost (Nagapurkar, Thirumaran and Kidder, 2024). However, methodologies used in previous studies do not often reflect feasible industrial manufacturing processes e.g., not accounting for capital and investment factors (Sinha et al., 2017), no recovery and reuse of reagents which are used for conditioning the sorbent's raw materials but are not themselves consumed in the process (Sinha et al., 2017; Leonzio et al., 2022), limited sorbent types (silica, alumina, carbon and ionic resin sorbents) (Azarabadi and Lackner, 2019; Deutz and Bardow, 2021), and no details on the assumptions for cost estimate (Valentine et al., 2022). This study assessed the cost and associated life cycle GHG emissions of two new amine-modified zeolite sorbents and two amine-modified MOFs across different markets to understand DAC using amine-modified sorbents, see Table 1 for additional details. These sorbents developed by Lin et al. (2013), Sinha et al. (2017), Fashi, Ghaemi and Behroozi (2021), Bahmanzadegan, Pordsari and Ghaemi (2023) were selected in this study owing to their excellent adsorption rates and time.

Importantly, the deployment configuration of DAC facilities can substantially impact net CO_2 removals and levelised costs. However, despite indications that DAC costs can be significantly influenced by sorbent parameters such as adsorption rates and cycle time, there is a lack of comprehensive studies in the literature evaluating their impact. Solid sorbents such as zeolites and MOFs are modified physically and chemically to improve their adsorption rates, even if this modification has additional cost implications. Also, since CO_2 captured by sorbents is a kinetic process, it is important to understand the impact of the adsorption rates and times on CO_2 capture to reduce the cost of DAC. Generally, the energy emission factor (McQueen et al., 2020; Deutz and Bardow, 2021) is the most influential factor in DAC's GHG emissions, while the economics of DAC is highly sensitive to factors such as the energy demand of DAC (Fasihi, Efimova and Breyer, 2019), cost of energy (McQueen et al., 2020), plant capacity factor (Valentine et al., 2022), sorbent adsorption rates (Sinha et al., 2017) and cycle time. Prior work has estimated the life cycle GHG emissions of DAC to range from 0.01 tCO_2 emitted per tCO_2 captured when renewable electricity is used to 0.65 tCO_2 emitted per tCO_2 captured when grid electricity and natural gas (NG) heating are used (McQueen et al., 2020; Deutz and Bardow, 2021; Chauvy and Dubois, 2022; Hu et al., 2024). The cost of DAC, which is currently expensive, is estimated in the range of $\$_{2024}$145–400 per tCO_2 captured gross (cost adjusted to 2024 US dollars) (Keith et al., 2018; Fasihi, Efimova and Breyer, 2019; McQueen et al., 2020; Daniel et al., 2022). However, Fasihi et al. (Fasihi, Efimova and Breyer, 2019) estimate that the cost of DAC could decrease significantly to $\$_{2024}$20–130 per tonne of CO_2 captured by 2050. These estimates, based on learning-by-doing, highlight the importance of understanding design parameters and strategies that have the largest impact on DAC to enable targeted research and development to facilitate cost reduction and enable its wider deployment. Furthermore, because DAC processes generate their own GHG emissions, economic models that present DAC costs in terms of cost per mass of CO_2 captured (gross) are often misleading and underestimated. Therefore, in this study, DAC costs are presented in US dollars per net CO_2 captured, with life cycle GHG emissions fully integrated into the cost estimate.

This study designed and modelled the production of different solid sorbents and a DAC plant using Aspen HYSYS and Microsoft Excel in a manner not found in existing literature (see Table 1 for details). It assessed 1) the cost and GHG emissions impact of sorbent manufacture, 2) the impacts of sorbent properties/kinetics and 3) the cost and GHG emissions impacts of different DAC technologies used in CO_2 capture. A minimum selling price (MSP) and levelised cost of capture (LCOC) approaches were used to present the prices of sorbent and CO_2 captured, respectively.

2. Methods

The methodology developed in this work can be classified into process modelling, economic analysis, and life cycle GHG emissions analysis approaches. The process model developed in Aspen HYSYS was linked using MATLAB to the sorbent adsorption process, economic analysis and life cycle GHG emissions models developed in Microsoft Excel. These models were developed using data from several sources, including (Bahmanzadegan, Pordsari and Ghaemi, 2023) and (Seider et al., 2017). The study's boundaries start at energy generation and sorbent production and terminate at either CO_2 capture or storage (scenario depending), as shown in Fig. 1. In chemical production and CO_2 mineralisation, it was assumed that the chemical and CO_2 mineralisation plants would be co-located with the DAC plant, making the CO_2 transportation distance zero, based on these sources (Infinium, 2021; Concawe and Aramco, 2024; Wang, Ting and Zhao, 2024), while the average transport distance of CO_2 from the plant to the reservoir was assumed to be 400 km. This paper presents a cradle-to-grave cost and life cycle GHG assessment of solid sorbents and DAC, covering the UK and US markets.

The DAC scenarios analysed in this paper are summarised in Table 2. The experimental model, which may not be representative of operational plants, uses experimental data obtained from the literature. The commercial plant model, which represents the nth plant, uses a generic sorbent that is based on zeolite 4A-DEA experimental adsorption rate, an improved cycle time of 15 mins based on Sinha et al. (2017) experimental desorption time of 15–20 mins, and average of zeolites and MOFs sorbent heat capacities [Supplementary Information (SI) *Table S29*]. The Wind & Grid scenario was constrained to maximum GHG emissions of 0.1 tCO_2/tCO_2 captured to maintain the high CDR benefits of DAC since carbon credits are based on net CO_2 captured volumes.

Table 1
The scope and limitations of existing literature, with key literature referenced for presentation.

Reference	Sorbent type	Sorbent process modelling	Sorbent cost	Sorbent emissions	DAC process modelling	DAC cost	DAC emissions	Temporal	Geospatial	Additional comments
Leonzio et al. (2022)	Solid sorbents (MOFs and amine-modified silica and cellulose	Not assessed	Not assessed	Assessed	Not assessed	Not assessed	Assessed	Not assessed	Not assessed	No recovery and reuse of reagents which are used for conditioning the sorbent's raw materials but are not themselves
Deutz and Bardow (2021)	Solid sorbents (amine-modified silica, alumina and cellulose, carbonate-modified silica and carbon, and anionic resin)	Not assessed	Not assessed	Assessed	Not assessed	Not assessed	Assessed	Partly assessed	Partly assessed	General assessment of electricity emissions factors made for temporal and spatial. Changes in other input materials and energy emission factors not assessed
Nagapurkar, Thirumaran and Kidder (2024)	Solid sorbents (polymer)	Not assessed	Assessed	Assessed	Not assessed	Assessed	Not assessed	Not assessed	Not assessed	■ Only 2 polymer sorbents assessed ■ Only DAC capital estimated in the study
Sinha et al. (2017)	Solid sorbents (amine-modified MOFs)	Assessed	Assessed	Not assessed	Assessed	Assessed	Not assessed	Not assessed	Not assessed	Process modelling considered limit parameters, e.g., the impact of sorbent kinetic model not assessed) Sorbent costing has no account for capital and investment factors, e.g., fixed operating cost and discount rates
An, Farooqui and McCoy (2022)	Liquid sorbent (potassium hydroxide)	Not assessed	Not assessed	Not assessed	Assessed	Assessed	Assessed	Not assessed	Not assessed	Limited scenarios considered in this work, e.g., limited range of energy sources, sorbents, location and temporal factors
Fasihi, Efimova and Breyer (2019)	Solid and liquid sorbents (generic)	Not assessed	Not assessed	Not assessed	Not assessed	Assessed	Not assessed	Assessed	Not assessed	■ No process modelling and future cost estimations strictly based on learning rates alone. ■ No extensive evaluation of the technical parameters and strategies (e.g., sorbent properties) required to achieve future cost estimates
Sievert, Schmidt and Steffen (2024)	Solid and liquid sorbents (generic)	Not assessed	Not assessed	Not assessed	Not assessed	Assessed	Not assessed	Assessed	Not assessed	■ No process modelling and future cost estimations strictly based on learning rates alone. ■ No extensive evaluation of the technical parameters and strategies (e.g., sorbent properties) required to achieve future cost estimates
McQueen et al. (2020)	Solid sorbent (generic)	Not assessed	Not assessed	Not assessed	Assessed	Assessed	Assessed	Not assessed	Assessed	■ Limited process modelling parameters assessed: No modelling of the impacts of sorbent properties, which are key in DAC costing. ■ No sorbent costing. Assumed sorbent cost has no assessment of capital and investment factors ■ Geospatial location is limited to the US only
This work	Solid sorbents (amine-modified zeolites and MOFs)	Assessed	Assessed	Assessed	Assessed	Assessed	Assessed	Assessed	Assessed	■ Assessed comprehensively process operations and designs of sorbent manufacture and DAC plants, including the impact of sorbent kinetics and plant scale on DAC cost and GHG emissions ■ Developed robust methodology for assessing the cost and GHG emissions of sorbent manufacture and DAC plants, including methods for experimental and commercial plant assessments ■ New type of sorbent was assessed: Amine-modified zeolites. Existing amine-modified MOFs were also assessed ■ Extensively assessed the technical parameters and strategies (e.g., sorbent properties) required to achieve future cost estimates beyond just learning rates assumptions.

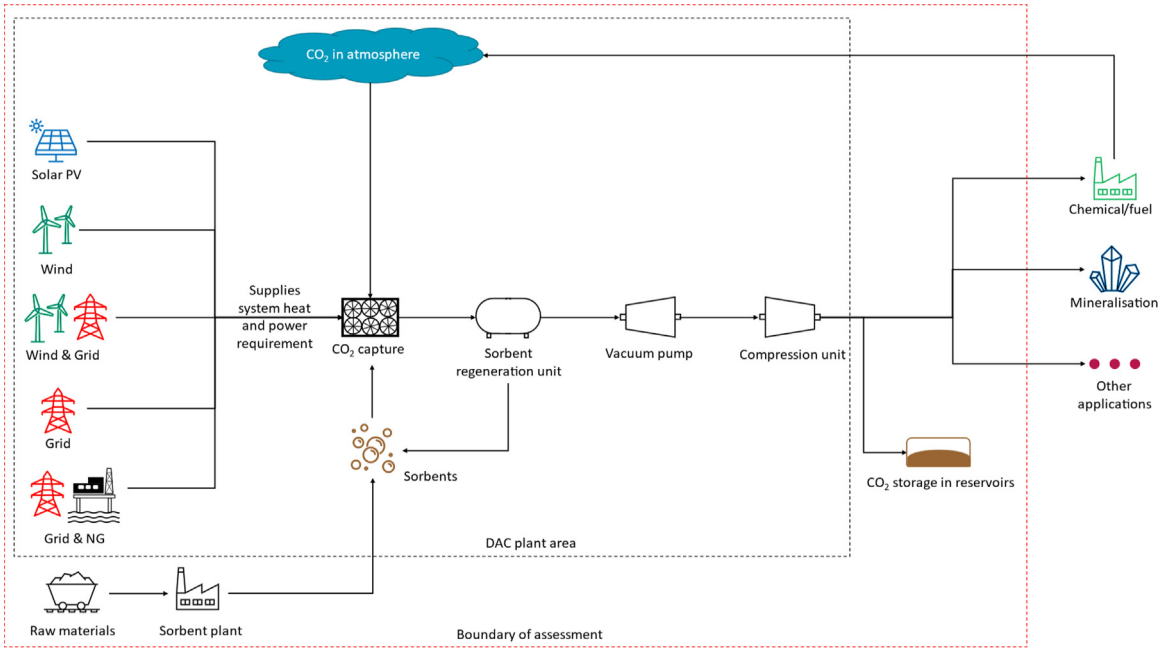

Fig. 1. The simplified flow diagram of DAC showing the scope of the study.

Table 2
Summary of the DAC scenarios considered.

Year	Country	Energy source	Boundary	Sorbent	Adsorption time model
2025	UK	Wind	DAC plant gate	Zeolite 4A-DEA	Experimental plant model
2030	US	Solar	CO_2 reservoir	Zeolite 13X-piperazine (Pz)	Commercial plant model
2040		Wind & Grid		MIL-101(Cr)-polyethyleneimine (PEI)	
2050		Grid		Mmen-Mg_2(dobpdc)	
		Grid & NG		Generic sorbent	

2.1. Process modelling

The process modelling of the solid sorbent DAC system included the air contactor, sorbent adsorption and regeneration unit, vacuum pump, heat exchangers and compressors (Fig. 1). The air contacting unit (sorbent, monolith and fans) and sorbent adsorption and regeneration unit were modelled in Microsoft Excel using data found in Table 3, SI *Table S5* and equations S1–S9. The other sections of the plant, including the vacuum pump and compression unit (compressors and heat exchangers), were modelled in the commercial process simulator Aspen HYSYS. The Microsoft Excel and Aspen HYSYS models were integrated using MATLAB code to automate data transfer, reducing the need for manual input and ensuring synchronisation between Aspen HYSYS and Excel, as shown in Fig. 2. The design parameters of the sorbent and other plant sections modelled are discussed further in Table 4 and SI. In the operation of the DAC plant, air from the atmosphere is captured in the air contacting unit as the fans pump air into the monolith which contains the sorbent. The sorbent captures the CO_2 while the CO_2-depleted air is released back into the atmosphere. The sorbent is regenerated based on temperature vacuum swing adsorption (TVSA) through the five-step TVSA cycle described by Sinha et al. (2017). Steam is passed through the monolith channels during the TVSA cycle to release the CO_2 in the sorbent. The oxidation of the amine sorbents at high temperatures is managed by limiting the temperature and oxygen concentration in the monolith channels using methods described by Sinha et al. (2017). Using the integrated HYSYS/Excel process model, the effects of sorbent properties, such as the adsorption rate and time of the five selected sorbents, on the volume and cost of CO_2 captured were evaluated. This assessment was based on adsorption kinetics data published by Lin et al. (2013), Sinha et al. (2017), Bahmanzadegan, Pordsari and Ghaemi (2023) and Fashi, Ghaemi and Behroozi (2021), as shown in SI *Table S1* to *Table S4*. The base case for the annual capacity of the plant modelled is 1 $MtCO_2$ captured per annum.

Table 3
Process modelling parameter based on Sinha et al. (2017), McQueen et al. (2020).

Parameter	Value	Unit
Adsorbent channel inner radius, d_1	0.000525	[m]
Adsorbent channel outer radius, d_2	0.000585	[m]
Channel diameter, d_3	0.00127	[m]
Contactor width side 1, w_1	1.1	[m]
Contactor width side 2, w_2	1.1	[m]
Channel Length (m), l	0.3	[m]
Desorption swing capacity, θ	0.8	[mol/mol]
Air velocity, v	3	[m/s]
Air viscosity, μ	1.84E-05	[kg/m.s]
Air density	1.29	[kg/m^3]
Adsorbent density	See Table S14	[kg/m^3]
Wall density	2050	[kg/m^3]
CO_2 desorption	55	[KJ/mol]
H_2O:CO_2 uptake	2.2	[mol/mol]
Temperature at end of adsorption	348	[K]
Temperature for desorption	373	[K]
Channels per contactor	400	[cpsi]
Monolith heat capacity	840	[J/kg.K]
CO_2vol in air	0.04 %	
CO_2 capture efficiency	75 %	
CO_2 final outlet pressure	70	bar

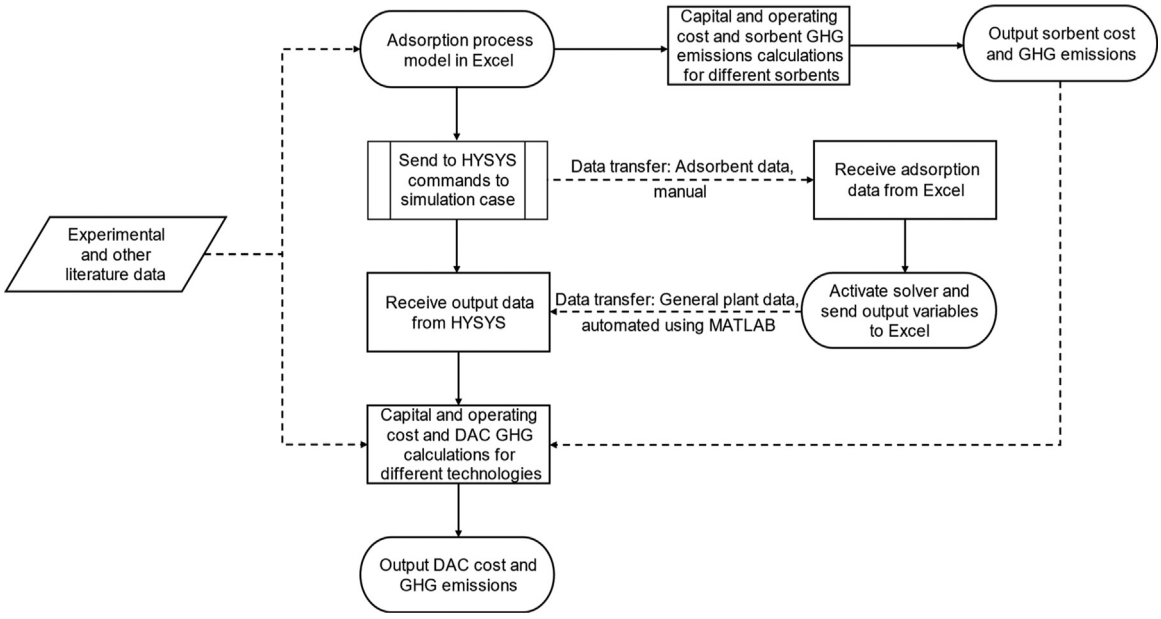

Fig. 2. Schematic of the integrated techno-economic and life cycle assessment methodology adopted in the study.

Table 4
Design and economic parameters for the economic assessment (Seider et al., 2017; Towler and Sinnott, 2021; Maxwell, 2024).

Economic parameters	Reference values
Sorbent/DAC plant capacity	0.012 Mtpa (sorbent), 1 Mtpa (DAC)
CEPCI, 3-year average of 2021 to 2023	774.2
Free onboard equipment purchase cost	See SI Table S7, S8 and S25
Installed capital cost	Hand method
Capital spending	Sorbent $\frac{1}{2}$ in 2 years, DAC ⅓ for 3 years
Sorbent/DAC plant construction period	2 (sorbent) years, 3 years (DAC)
Plant commissioning year	2024/2025, 2030, 2040 and 2050
Plant operating hours	8400 h
Plant life	30 years
Depreciation	10-year linear
Plant salvage value	Zero
Installed cost – Inside Battery Limit (ISBL) Factor	See SI Table S7, S8, S9 and S25
Outside Battery Limit (OSBL)	25 % of ISBL
Commissioning cost	5 % of ISBL
Fixed capital investment (FCI)	ISBL + OSBL + Commissioning
Working capital	10 % of ISBL + OSBL
Total capital investment (TCI)	FCI + Working Capital
Discount rate	10 %
Inflation rate	2 %
Corporate tax rate [Sorbent plant only]	25 %
Exchange rate	£1 to $1.2438

2.2. Economic assessment

Capital costs were estimated using the Hand factor method (Towler and Sinnott, 2021) with the equipment cost equations provided by Seider et al. (2017). Table 4 summarises the general assumptions used for the economic assessment. The sorbents and CO_2 capture costs were estimated using mass and energy data along with cost and emission factors from the process modelling and literature. It was assumed that reagents not consumed in the main process are reused in the sorbent manufacture, in line with existing industrial manufacturing approaches. A make-up amount of fresh reagents was also assumed to be added over the functional unit (FU) to replenish any depletion, see *Table S10* to *Table S13* for details. The details on the mass and energy balance for the sorbent can be found in the SI. The sorbent plant capacity selected was 0.012 Mtpa, which is 5 to 106 times the annual sorbent demand for a 1 Mtpa DAC plant. Sensitivity analysis of the sorbent plant showed little change in the sorbent prices with plant capacity up to 0.5 Mtpa. Using the estimated sorbent cost, other cost factors, and the DAC process plant model, the cost of DAC was estimated for each technology scenario, as shown in Fig. 2 for the methodologies. The cost analysis is performed based on the 2024 United States dollar ($\$_{2024}$), therefore, equipment cost estimations were adjusted using a 3-year average of 2021 to 2023 chemical engineering plant cost indices (CEPCI).

The fixed operating cost estimates were based on the costing methodologies by Rodgers et al. (2022) and Sinnott and Towler (2009) and are shown in Table 5. The labour costs for US and UK operators in 2024 were obtained from SalaryExpert (SalaryExpert, 2024).

The estimations of variable operating costs were based on material and energy balances derived from the DAC process model, as shown in SI *Table S5* to *Table S27*. Wind and solar electricity costs were obtained from DESNZ (DESNZ, 2023a) and NREL (NREL, no date) publications for offshore wind (UK), onshore wind (US) and utility PV. The costs of grid electricity and NG used were the average during the plant operation years up to 2050 electricity cost estimates, based on the electricity

Table 5
Economic factors for fixed operating cost estimation.

Economic parameters	Sorbent plant	DAC plant
Operating Labour	3 shift teams 3 operators per shift $44,321 (UK), $62,127 (US)	4.8 shift teams 3 operators per shift
Supervisory Labour	25 % of Operating labour	
Direct Salary Overhead	50 % of Operating + Supervisory	
Maintenance	3 % of ISBL	
Property taxes & insurance	1 % of ISBL	
Rent of land/buildings	1 % of FCI	
General plant overhead	65 % of total labour + maintenance	
Allocated environmental charges	1 % of FCI	

and NG forecast by DESNZ (DESNZ, 2023b) and EIA (EIA, 2023). Due to the sorbent plant's small electricity demand, only grid electricity was assumed to be used in sorbent production. For DAC, more energy scenarios were considered, including wind, solar, and grid electricity with NG heating, to evaluate and compare the CO_2 capture cost from these technologies, as shown in Fig. 1.

For the scenario involving the injection of CO_2 into geological reservoirs, the cost of a CO_2 transport pipeline of $62,352/km/($MtCO_2$/yr) and compression energy for injection of 11.82 kWh/tCO_2 were incorporated into the cost model, based on the data published by DNV (DNV, 2020) when adjusted for inflation using CEPCI. An injection pressure of near critical point of 70 bar and a mean transport distance of 400 km were used in the analysis.

2.3. Sorbent minimum selling price and DAC levelised cost of capture

An MSP approach was adopted for the sorbent cost analysis according to the convention generally used for chemical products. The MSP is the selling price of the sorbent at the plant gate that makes the project's net present value (NPV) equal to zero over the plant life [Eq. (1)]. In contrast, according to the convention generally used for DAC, an LCOC was used for CO_2 capture cost analysis. The LCOC is the discounted lifetime cost of constructing and operating the DAC plant [Eqs. (2) and (3)]. The sorbent MSP and DAC LCOC were expressed in $/t sorbent and $/t$CO_2$ captured, respectively. The sorbent MSP and DAC LCOC were determined using Eqs. (1)-(3), where CF is the total cash flow in any year (t), M is the mass of CO_2 captured in any year (t), and r is the discount rate.

$$\textbf{Selling price subject to NPV} = \sum_{t=0}^{n} \frac{CF_t}{(1+r)^t} = 0 \tag{1}$$

$$LCOC_{gross}\ [\$/tCO_2 captured] = \frac{\sum_{t=0}^{n} \frac{CF_t}{(1+r)^t}}{\sum_{t=0}^{n} \frac{M}{(1+r)^t}} \tag{2}$$

The $LCOC_{gross}$ calculated using Eq. (2) presents the gross cost of capture of CO_2, as CO_2 is the DAC product and the GHG emissions indicator. This creates ambiguity in the cost numbers since the GHG emissions from the plant represent a form of loss, thereby, making the cost from different technologies incomparable due to their different GHG emissions. Hence, the net cost of CO_2 capture was determined using Eq. (3), where EF is the GHG emissions associated with the CO_2 captured.

$$LCOC_{net}\ [\$/tCO_2 captured] = \left(\frac{\sum_{t=0}^{n} \frac{CF_t}{(1+r)^t}}{\sum_{t=0}^{n} \frac{M}{(1+r)^t}} \right) \frac{}{1-EF} = \frac{LCOC_{gross}\ [\$/tCO_2 captured]}{1-EF} \tag{3}$$

2.4. Life cycle assessment

A life cycle assessment (LCA) was performed to determine the life cycle GHG emissions of the sorbents. The mass and energy data and emission factors for the sorbent manufacture were derived from the literature, including (Bahmanzadegan, Pordsari and Ghaemi, 2023) and Ecoinvent. Additionally, the life cycle GHG emissions of CO_2 captured by DAC were assessed based on process modelling and literature data. Cradle-to-grave LCA models were developed based on the ISO Standards 14040 and 14044, which include goal and scope definition, inventory analysis and impact assessment (ISO, 2006b, 2006a; Matthews, Hendrickson and Matthews, 2014). The goal and scope of the study for the sorbent and DAC plants are shown in Fig. 1. The global warming potentials (GWPs) were based on 100-year GWP factors. The FUs used in the assessment for the sorbents and CO_2 captured were 1 kg of sorbent and 1 tonne of CO_2 captured, respectively. The GHG emissions are reported in units of tCO_2e emitted/t sorbent and tCO_2e emitted/tCO_2 captured for the sorbents and captured CO_2, respectively. In estimating emissions factors in the future, a hybrid of prospective-LCA and conventional-LCA approaches was taken, with the impact of changes in emissions factors from energy and materials accounted as practical as possible. Due to the scope of the work and data availability, as the authors estimated the emission factors of several sub-components of the sorbents, some of the emissions factors of the materials were based on the conventional-LCA approach. The data in the literature justify the methodology adopted since the GHG emissions of DAC are mostly determined by the energy source (McQueen et al., 2020; Deutz and Bardow, 2021). The mass and energy balance and inventory data used in the LCA analysis can be found in SI *Table S10* to *Table S28*.

2.5. Future estimates

The commercial plant model scenario for the best sorbent was used to develop future DAC scenarios. The future cost estimates were derived using the methodology proposed by Fasihi, Efimova and Breyer (2019), which adopts the standard learning curve approach outlined in Eq. (4). Fasihi, Efimova and Breyer (2019) assumed learning rates of 15 % for DAC based on the learning rates of sulphur removal systems of large-scale centralised coal-fired power plants (10 %) and modular technologies such as water electrolysers (18 %) and seawater reverse osmosis desalination (15 %). However, this very high learning rate may not reflect the nature of DAC technology because the components of DAC plants are mature except for the sorbent and monolith. For example, the energy plant is matured, and learning rates of 5 % have been applied in 2030 and 2050 estimations of onshore wind power (Concawe and Aramco, 2024). Additionally, other key equipment, such as fans and compressors, are mature technologies. The Carbon Engineering liquid sorbent DAC analysis by Keith et al. (2018) shows that fans are the costliest equipment in a DAC plant, making up 25–30 % of the equipment cost even in the nth plant model. This is because pumping any volume of CO_2 in the air, say 1 Mtpa of CO_2, will have the same fan design and cost parameters regardless of any improvement in the adsorption process (monolith and sorbents for solid sorbent DAC). Likewise, advancements in the adsorption process do not impact the equipment downstream, as these improvements primarily reduce the cost of monolith equipment rather than affecting the plant's downstream CO_2 handling capacity. The monolith is a key DAC plant equipment that learning by doing can notably impact. The sorbent adsorption rate and cycle time can significantly influence the cost of the monolith. However, since the monolith is assumed to be replaced every 10 years, it was treated as a variable cost in the economic analysis. Hence, a 2 % learning rate was assumed for the whole DAC equipment (including monolith) in this analysis, consistent with the learning rates of mature technologies previously suggested (McDonald and Schrattenholzer, 2001; Jamasb, 2007; Rubin et al., 2015). The capacities of DAC in 2030, 2040 and 2050 deployed, as shown in Table 6, were based on the DAC capacity estimates

Table 6
The total capacities of DAC deployment from 2025 to 2050.

Year	Total capacity, $MtCO_2/a$	Comment
2025	3	IEA (IEA, 2022a)
2030	85	IEA NZE Scenario DAC capacity (IEA, 2021, 2022b)
2040	383	Interpolation of IEA NZE Scenario
2050	980	IEA NZE Scenario minimum DAC capacity (IEA, 2021, 2022b)

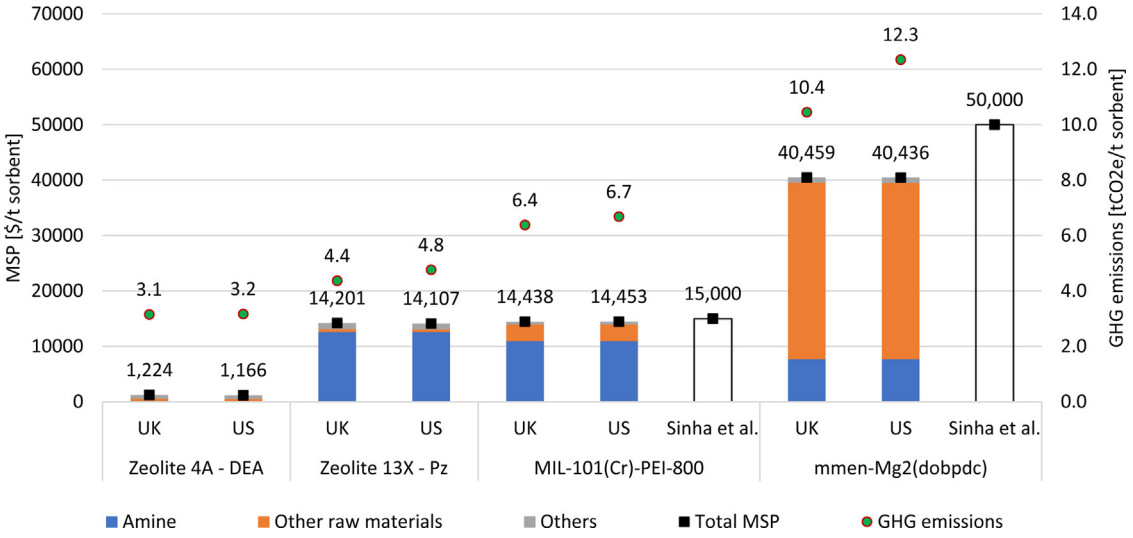

Fig. 3. The cost and GHG emissions of the DAC sorbents evaluated across different locations (UK and US).

by IEA (IEA, 2021, 2022b, 2022a).

$$(\boldsymbol{Capital\ cost})_{year\ n} = (\boldsymbol{Capital\ cost})_{initial} \cdot \left(\frac{\boldsymbol{Production}_{year\ n}}{\boldsymbol{Production}_{initial}}\right)^{\frac{\log(1-LR)}{\log 2}} \quad (4)$$

The energy design, cost and emissions data between 2030 and 2050 were based on estimates by DESNZ (2023a, 2023b), EIA (2023), IEA, and NREL (2021), no date, as shown in SI *Table S20* and *Table S21*. Grid electricity emissions factors were based on a weighted average of the IEA Stated Policies and Sustainable Development scenarios. The average emission factor of 2030 consisted of 70 % Stated Policies and 30 % Sustainable Development numbers, those in 2040 assumed 50 % Stated Policies and 50 % Sustainable Development numbers and those in 2050 assumed 30 % Stated Policies and 70 % Sustainable Development numbers (see *Table S20*). This is to account for the increased likelihood of meeting sustainable development goals, in line with IEA estimates and government commitments to achieving net-zero emissions by 2050.

3. Results

3.1. Sorbent costs and greenhouse gas emissions

Fig. 3 shows the costs of the considered sorbents are estimated to be in the range of $\$_{2024}$1,200–40,400/t sorbent in 2024, varying significantly based on the raw materials composition and sorbent type, with MOFs sorbents showing higher cost than zeolite sorbents. Raw materials make up a significant portion of the sorbent cost, ranging from 45 % in zeolite 4A-DEA to 98 % in mmen-Mg2(dobpdc). Therefore, optimising the performance of amines (e.g., adsorption rate) when used to modify solid sorbents is crucial for maximising their benefits. Furthermore, there is negligible variation between the sorbent cost in the UK and the US, as shown in Fig. 3. This is due to the balancing effects of location-specific factors, such as cheaper electricity and raw material costs in the US compared to cheaper labour costs in the UK. GHG emissions from sorbent manufacturing, estimated to range from 3.1 to 12.3 tCO_2e/t sorbent in 2024, vary significantly depending on the composition of raw materials and emission factors.

Sorbent manufacturing that utilises materials with lower GHG emission factors and requires fewer raw materials and reagents demonstrates better performance in terms of emissions. Emissions from amines account for 10–77 % of the total life cycle GHG emissions of the sorbents. Furthermore, GHG emissions from the UK are lower than those from the corresponding US scenarios due to the higher emission factors associated with energy and materials in the US.

The estimated costs and GHG emissions fall within the ranges previously reported in the literature, $200–80,000/t (Sinha et al., 2017; Azarabadi and Lackner, 2019; Valentine et al., 2022; Nagapurkar, Thirumaran and Kidder, 2024) and 1.0–50 tCO_2e/t sorbent (Deutz and Bardow, 2021; Leonzio et al., 2022). The costs estimated in this analysis of MIL-101(Cr)-PEI and mmen-Mg2(dobpdc) were lower than the average cost reported by Sinha et al. (2017) by 4 % and 19 %, respectively. This difference can be attributed to the present analysis methodologies, such as the reuse of reagents in sorbent manufacturing, investment factors in cost analysis and the variation in raw material costs over time.

3.2. Cost and greenhouse gas impacts of sorbent properties

The kinetics of adsorption has a considerable impact on the performance of DAC. As shown in Fig. 4, *SI Figures S1 and S2*, the cost and GHG emissions of DAC initially decrease with increasing adsorption rate and time, reaching a minimum point. Beyond this point, further increases in adsorption rates and time lead to a rise in costs and GHG emissions. This is because longer times are required to capture CO_2 at near-equilibrium adsorption rates. Despite the high near-equilibrium adsorption rates, the longer time it takes to reach these rates significantly affects the cycle time (adsorption and desorption time) and, consequently, the monolith design capacity and cost and DAC GHG emissions. The cost of the monolith, which can contribute 4–28 % of the total capture cost in the best experimental cases, is highly sensitive to the adsorption rate and cycle

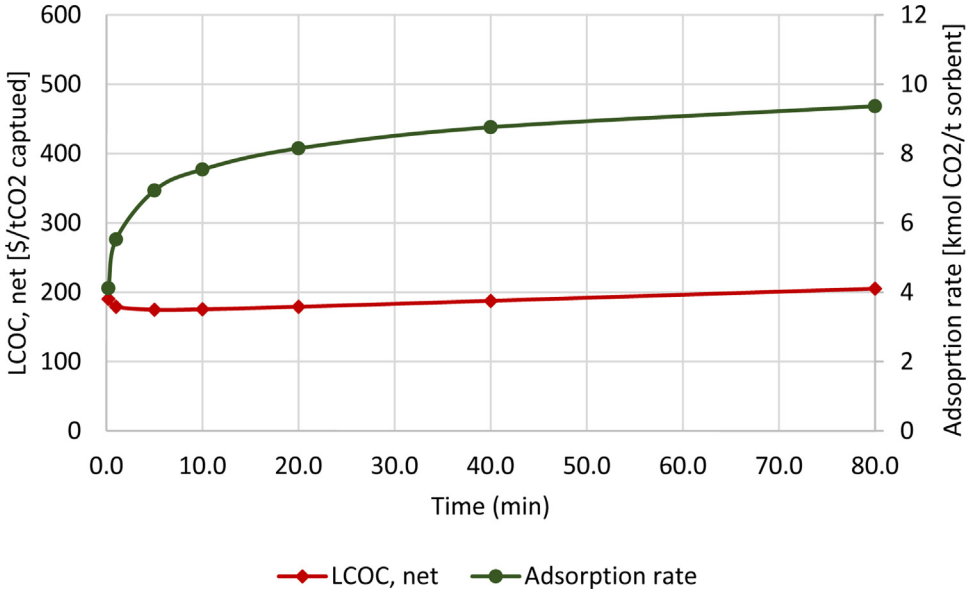

Fig. 4. Variation in DAC cost and GHG emissions with adsorption rate and time, based on the 2025 commissioning year using UK Wind for Zeolite 4A-DEA with kinetic data from Bahmanzadegan, Pordsari and Ghaemi (2023). Additional details on the other sorbents can be found in SI Figures S1 and S2.

time. Hence, developing sorbents with high adsorption and short cycle time is critical to DAC cost minimisation. As shown in Fig. 4 and SI *Figure S1*, the best operating point of the sorbents differs, with zeolite 4A-DEA performing the best at an adsorption rate of 6.9 mol/kg and an adsorption time of 5 mins. Consequently, a generic sorbent generated for the commercial plant model was based on zeolite 4A-DEA adsorption rate, zeolite 4A-DEA cycle time and zeolite 4A-DEA and MOFs sorbent heat capacities [SI *Table S29*].

3.3. Present day cost and greenhouse gas impact of commercial dac

Fig. 5 shows that the cost of DAC is heavily influenced by economic parameters such as capital (15–50 %), fixed operating (10–35 %), electricity (5–50 %), heat (5–40 %), and monolith (2–6 %) costs in the 2025 commercial plant model. Additionally, design factors such as energy source, plant boundary, and market location have significant impacts on the cost of DAC. The LCOC for injection to the reservoir is higher than the corresponding cost at the plant gate by 2–10 % due to the additional capital and operating cost required to compress CO_2 into reservoirs [SI *Table S30*]. The $LCOC_{gross}$ of DAC in 2025 ranged from $\$_{2024}106–597/tCO_2$ captured [$LCOC_{net}$ of $\$_{2024}148–623/tCO_2$ captured], with the best cost estimates obtained from US Grid & NG and UK Wind. Unlike sorbent cost in the UK and US, which balances out with location factors, the broader range of location-specific parameters in DAC (such as energy cost and location and technology-specific capacity factors) significantly influence the cost of DAC across the two regions. The DAC $LCOC_{gross}$ of $\$_{2024}106–597/tCO_2$ captured as estimated in this study is in-line

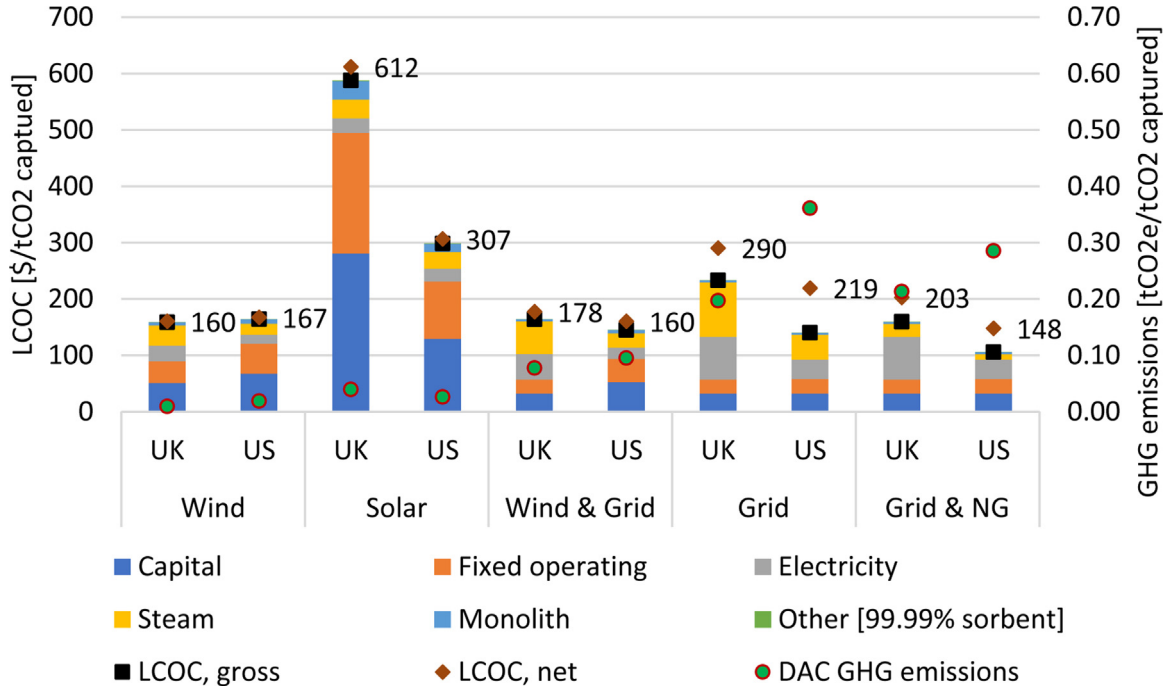

Fig. 5. DAC cost at plant gate in 2025 based on the commercial model. The Wind & Grid scenario was constrained to a maximum GHG emissions of 0.1 tCO_2/tCO_2 captured. In practice, most of the Wind & Grid scenarios are limited by the plant operational hours of 8400 h rather than GHG emissions limits.

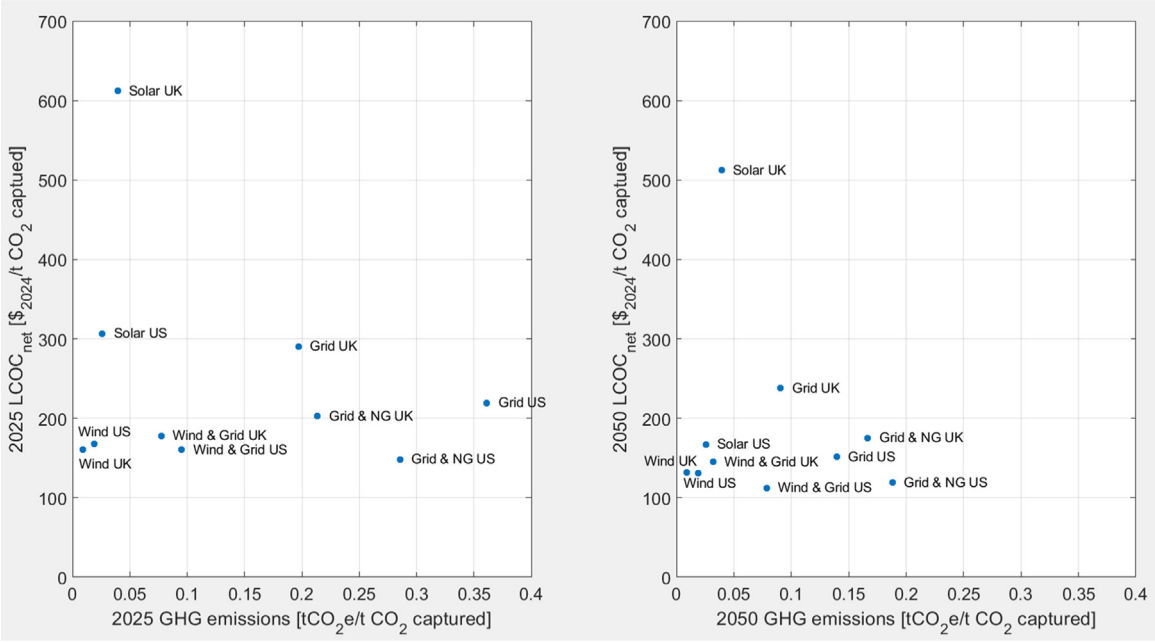

Fig. 6. The cost of DAC in 2025 and 2050 based on the commercial 1 Mtpa plant model. The Wind & Grid scenario was constrained to a maximum GHG emissions of 0.1 tCO_2/tCO_2 captured. In practice, most of the Wind & Grid scenarios are limited by the plant operational hours of 8400 h rather than GHG emissions limits.

with previous $LCOC_{gross}$ estimates of $\$_{2024}$145–400 per tCO_2 captured (adjusted to 2024 US dollars) (Keith et al., 2018; Fasihi, Efimova and Breyer, 2019; McQueen et al., 2020). However, some of the cost estimates in this analysis are significantly lower, owing to the methodologies used in this study, including novel sorbents as well as the design and operational strategies discussed in the Introduction and Methodology sections.

3.4. Cost and greenhouse gas impact of plant commissioning year and scale

There is a significant variation in the cost of DAC due to energy source, plant commissioning year and plant scale, as shown in Fig. 6. The LCOC vary considerably by energy source and plant commissioning year, with the best cost estimates for 2025 obtained from US Grid & NG and UK Wind and the best estimates for 2050 obtained from US Wind & Grid and UK Wind. The LCOC varies by energy source and plant commissioning year due to the changes in plant load factors, the cost and emissions associated with energy sources, and capital infrastructure cost over time. Also, the cost can vary by plant size, making it possible to capture CO_2 at $LCOC_{gross}$ as low as $\$_{2024}87/tCO_2$ captured [$LCOC_{net}$ of $\$_{2024}93/tCO_2$ captured] for a 1.5 Mtpa plant in 2050 using US Wind & Grid electricity (see Fig. 8). This is because economies of scale provide substantial cost-saving benefits. Based on this forecast, it would be highly unlikely for future DAC costs to be lower than $\$50/tCO_2$ captured in 2050 as forecasted by some studies (Fasihi, Efimova and Breyer, 2019) due to the significant contribution of key cost components, such as the cost of capital infrastructures (gross $\$_{2024}$25–37/$tCO_2$), fixed operating cost (gross $\$_{2024}$19–29/$tCO_2$) and energy cost (gross $\$_{2024}$39–60/$tCO_2$), which account for approximately 95 % of the total DAC cost for 1–1.5 Mtpa plant scales. These cost components are mature and have inherent minimum practical requirements. For example, substantial reductions in the capital infrastructure of DAC are highly unlikely due to the maturity of most DAC plant equipment, such as fans and compressors. The only area where substantial cost reductions are possible is the adsorption unit (monolith and sorbent), which remains a novel component in DAC technology. It is important to note that in this analysis, most of the Wind & Grid scenarios are constrained by the practical plant operational hours rather than by the condition imposed on Wind & Grid GHG emissions of not exceeding 0.1 tCO_2 per tCO_2.

Similarly, there is a significant variation in the GHG emissions of DAC mainly due to energy sources, including the emission factor of grid electricity, which changes significantly with the plant commissioning and operational years. The key contributing parameters to DAC GHG emissions are energy (49–99 %), capital infrastructure (1–45 %), and type of sorbent (0–10 %). The best GHG emissions benefits of lower than or equal to 0.01 tCO_2/tCO_2 captured are realised from renewable wind, while high emissions are obtained from the Grid scenarios with emissions up to 0.37 tCO_2/tCO_2 captured in 2025 and 0.19 tCO_2/tCO_2 captured in 2050, based on the commercial plant model. This study's commercial plant GHG emissions calculations of 0.01–0.37 tCO_2 emitted per tCO_2, agreed with previously published estimates of 0.01–0.65 tCO_2 emitted per tCO_2 for Wind, Grid, Grid & NG (McQueen et al., 2020; Deutz and Bardow, 2021; Chauvy and Dubois, 2022; Hu et al., 2024). However, the life cycle GHG emission estimates in this study are slightly more favourable due to improved sorbent performance (including higher adsorption rates and optimised cycle times), emissions factors for 2025 compared with previous studies, and the specific methodology employed (i.e., yearly averaged grid electricity emissions factor over the plant's lifetime).

3.5. DAC and carbon pricing

The carbon markets today, whether voluntary or compliance, are rather fragmented, where the price signals do not reflect the durability, reliability, and verifiability of the different carbon removal schemes. Nature-based removal projects in the voluntary markets typically range below $\$20/tCO_2$ removed. The carbon allowance price under a compliance market can be quite volatile, with the EU's Emissions Trading System (ETS) currently trading at about $\$70/tCO_2$ and only briefly exceeding the $\$100/tCO_2$ threshold in 2023 (Trading Economics, no date). Presently, this is £65/tCO_2 ($81/$tCO_2$) in the UK while ranging about $42–46/$tCO_2$ in California, US (Bloomberg NEF, 2024; DESNZ, 2024). Comparing the UK and US carbon pricing with the 2025 estimates of $LCOC_{net}$ of $\$_{2024}$116–139/$tCO_2$ captured (Fig. 5 and Fig. 8), DAC plants may struggle to operate economically between 2025 and 2030, even

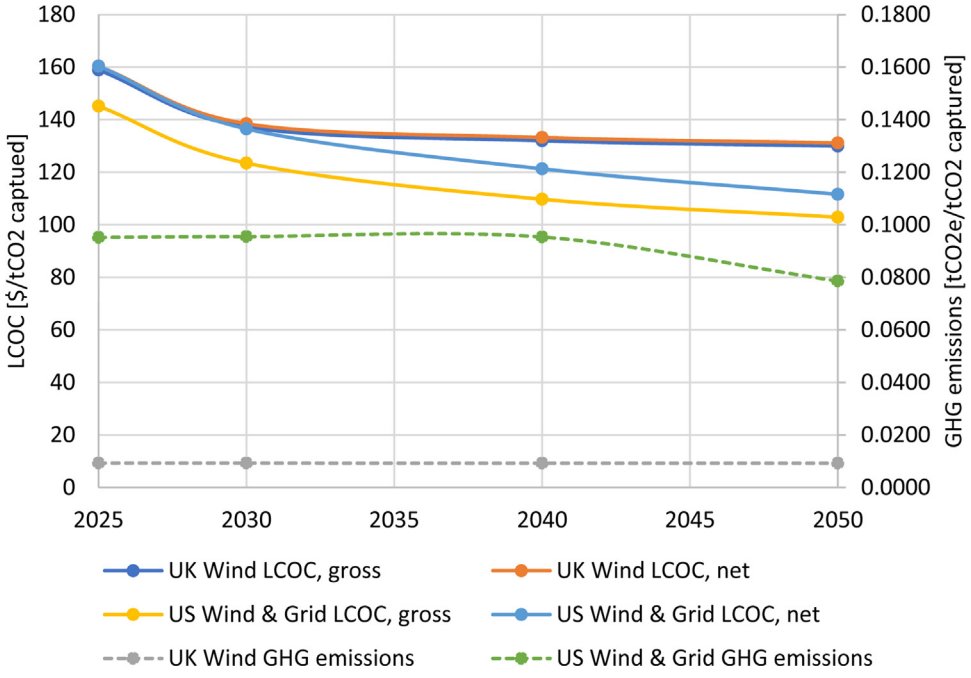

Fig. 7. The cost of DAC for 1 Mtpa plant across different plant commissioning years using the best-performing energy sources in the respective countries. The Wind & Grid scenario was constrained to a maximum GHG emissions of 0.1 tCO_2/tCO_2 captured. In practice, most of the Wind & Grid scenarios are limited by the plant operational hours of 8400 h rather than GHG emissions limits.

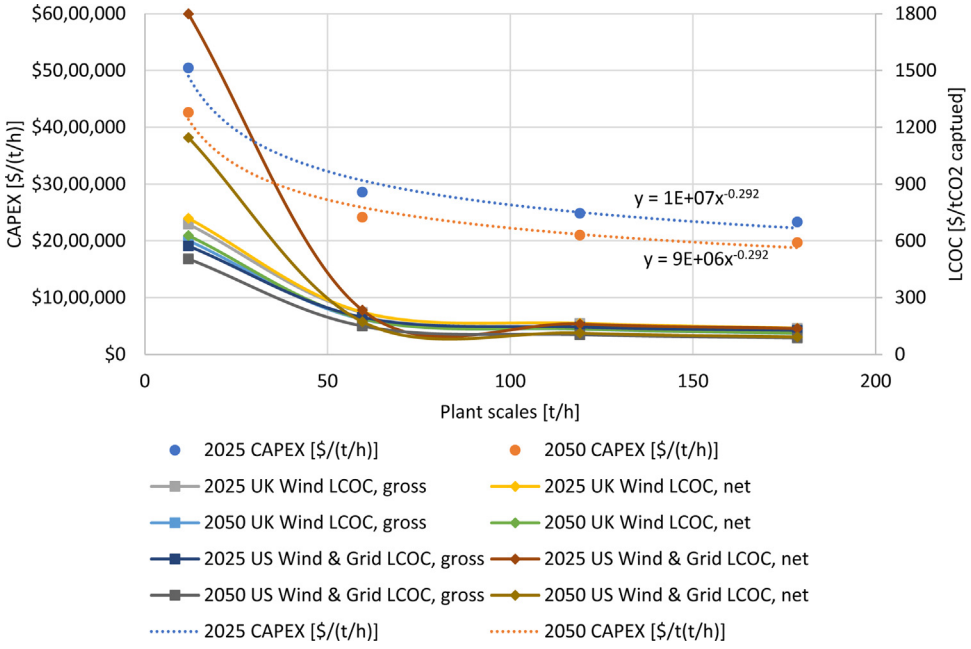

Fig. 8. The variation of DAC capital cost and LCOC with plant capacity and commissioning year for a commercial plant model. The Wind & Grid scenario was constrained to a maximum GHG emissions of 0.1 tCO_2/tCO_2 captured. In practice, most of the Wind & Grid scenarios are limited by the plant operational hours of 8400 h rather than GHG emissions limits.

with a 1.5 Mtpa scale plant. However, today, there are already over 2 $MtCO_2$ of DAC-based CDR credits sold, reflecting the growing desire for high-quality CDR credits (CDR.fyi, no date). Google (Google, 2024), for instance, recently announced a $10 million DAC-based CO_2 credit offtake agreement for delivery by 2030, equivalent to 100 kt CO_2 removed at a record-low price of $\$100/tCO_2$, which benefits from the US' 45Q subsidy support. Nevertheless, as the projected carbon price exceeds $\$140/tCO_2$ from 2030 (Bloomberg NEF, 2024), DAC could be commercially viable given the 2030–2050 LCOC estimate for DAC would reduce to $LCOC_{net}$ of $\$_{2024}93–139/tCO_2$ captured (Fig. 7 and Fig. 8).

3.6. Targets for sorbent innovation to drive down future capture costs

A sensitivity analysis of key sorbent parameters was performed to determine the required sorbent properties to achieve an $LCOC_{gross}$ within $\$_{2024}100$ per tCO_2 captured ($LCOC_{net}$ within $\$_{2024}110$ per tCO_2 captured) in 2050. Since the study evaluated the impacts of several sorbent and DAC parameters, including concurrent variations of multiple parameters, only a limited sensitivity scenarios are presented in Table 7. To achieve LCOC targets in 2050 using a 1 Mtpa plant, a sorbent cost of $\$_{2024}1–25/t$ sorbent and a minimum adsorption rate of 12.0 mol CO_2/kg sorbent (2.4 mol CO_2/kg sorbent/min) is required. Increasing adsorption rates beyond 12.0 mol CO_2/kg sorbent provides only a small benefit compared to those of 9–10 mol CO_2/kg sorbent (Fig. 5). Consequently, it may likely be easier to obtain an $LCOC_{net}$ of less than $\$_{2024}100$ per tCO_2 captured in 2050 by scaling the DAC plant to 1.5 Mtpa than by improving adsorption rates beyond 12.0 mol CO_2/kg sorbent because of the greater impact of economy of scale on capital and operating cost on the overall capture cost. Another design and operational approach, using US NG with carbon capture and storage (including capturing of the

Table 7
Results from the parametric sensitivity analysis of key sorbent factors for 1 Mtpa plant using US Wind & Grid in 2050.

Parameter	Value
Adsorption rate [mol/kg]	12–18
Sorbent cost [$/kg]	1–25
Sorbent lifetime [y]	0.5–3
Sorbent density [kg/m^3]	500
Sorbent heat capacity [J/kg.K]	892.5
Cycle time [min]	10–15
Sorbent demand [kg sorbent/tCO_2]	0.0417–0.0626
LCOC, gross [$/t$CO_2$]	97–102
LCOC, net [$/t$CO_2$]	105–110
DAC GHG emissions [tCO_2/tCO_2 captured]	0.074–0.077

flue gas CO_2 from NG combustion), which is low-carbon for a scenario involving complete CO_2 storage in reservoirs, can also drive down DAC $LCOC_{gross}$ to $\$_{2024}94$ per tCO_2 captured ($LCOC_{net}$ $\$_{2024}97$ per tCO_2 captured) in 2050. However, this design would require roughly 0.25 Mtpa flue gas CO_2 captured for every 1 Mtpa air CO_2 captured.

4. Discussion/Conclusion

This study provides a comprehensive evaluation of the cost and GHG implications of a solid sorbent DAC system with emphases on the technical, geographical, temporal and operational aspects of an engineered CDR. Our assessment incorporated the effects of different solid sorbent chemistries, their adsorption kinetics, types of energy used, location-specific parameters including capacity factors across two countries, the end-use fate of captured CO_2, and their evolution over time.

The cost and GHG emissions of sorbents ranged from $\$_{2024}1{,}200$–40,400/t sorbent and 3.1–12.3 tCO_2e/t sorbent in 2024, respectively, which are mainly driven by raw materials used in their manufacturing. However, they contribute ca. 0.2 % and 0–10 % to the overall cost and GHG emissions of DAC given that sorbent consumption in DAC is relatively small compared to other parameters, including the cost and emissions associated with energy uses. However, depending on the design and operating parameters, such as the system boundary, energy source, location, commissioning year and plant size, the cost and CO_2 emissions can vary substantially.

From an LCA perspective, the GHG emissions could vary from 0.01 to 0.37 tCO_2e/tCO_2 captured, with wind energy resulting in the lowest emissions while the 2025 US grid electricity producing the highest carbon intensity. Consistent with earlier studies, the source of energy used is a key determining factor in the total lifecycle GHG emissions, accounting for about 49–99 % of the overall emissions. On the other hand, key factors influencing the cost of DAC include capital expenses, fixed operating costs, energy costs, monoliths costs, and sorbents costs. Consequently, DAC $LCOC_{net}$ ranged from $\$_{2024}148$–$623/tCO_2 captured in 2025, which can be reduced to $\$_{2024}112$–$523/tCO_2 captured in 2050, in which the best-performing DAC scenarios by country in 2050 being US Wind & Grid and UK Wind. Over time, technological improvements are expected to further reduce the cost of DAC, while increasing plant capacity could benefit from economy of scale, with the $LCOC_{net}$ as low as $\$_{2024}93/tCO_2 captured possible in 2050 using a 1.5 Mtpa plant. Importantly, though, our analyses also highlight the importance of chemical kinetics, specifically the adsorption rate and time, on the costs and CO_2 emissions of DAC. We demonstrated the opportunity to identify and develop an optimal adsorption rate and time to minimise the cost of DAC.

The cost of DAC from the best technological approaches assessed here are still generally above $LCOC_{net}$ of $\$_{2024}100/tCO_2 captured. Our cost estimates far exceed current CO_2 prices in the market, both, voluntary and compliance. Therefore, DAC is unlikely to be fully financed by the carbon market in their current forms and, in the short-term, will necessitate fiscal incentives to achieve gigaton-scale CDR buildouts. The US Inflation Reduction Act, for example, enhances the 45Q tax credit for DAC by increasing the incentives from $50/t$CO_2$ to $180/t$CO_2$ for geological sequestration of CO_2. While an engineered CDR like DAC is generally considered costly, it is important to situate this in the context of the social cost of carbon. The current US EPA's official cost of carbon is $51/t$CO_2$, however there is a growing recognition that this is a significant underestimate. Therefore, the latest EPA proposal is to increase it to $190/t$CO_2$, based on a more recent scientific estimate (Rennert et al., 2022). With this higher social cost of carbon, the high cost of DAC becomes even more justifiable. Furthermore, with carbon prices projected to increase from $40–100/t$CO_2$ in 2023 to $140–240/t$CO_2$ in 2030–2050, DAC could be a commercially profitable CDR option. Hence, well-designed policies encouraging investments in DAC are crucial for achieving gigaton-scale DAC buildouts.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Sylvanus Lilonfe reports financial support was provided by Engineering and Physical Sciences Research Council (EPSRC). Sylvanus Lilonfe reports financial support was provided by Saudi Aramco Technologies Company. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Sylvanus Lilonfe: Writing – original draft, Visualization, Validation, Software, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Sarah Rodgers:** Writing – review & editing, Validation, Software, Methodology, Data curation, Conceptualization. **Amir F.N. Abdul-Manan:** Writing – review & editing, Supervision, Funding acquisition. **Ioanna Dimitriou:** Writing – review & editing, Validation, Supervision, Conceptualization. **Jon McKechnie:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Funding acquisition, Conceptualization.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.ccst.2025.100380.

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7 Life cycle assessments of gaseous low-carbon fuels technologies

This chapter contributes to the overall thesis aim of assessing low-carbon fuel and chemical technologies by examining the life cycle environmental impacts of gaseous low-carbon fuels and chemicals supply chains – H_2 and synthetic natural gas supply chains – from different design, operational, geographical and temporal perspectives. The paper is the most comprehensive study to date on the life cycle greenhouse gas emissions impacts of H_2-related supply chains.

The paper summarises key insights drawn from over 10,000 cases, analysing the supply of H_2 from six renewables-rich regions and transporting it via different modes to two European markets, using six different chemical forms, including compressed-H_2, liquefied-H_2, synthetic natural gas, methylcyclohexane, ammonia, and methanol. It delivers important and original contributions in many ways, including 1) creating innovative and integrated methodologies for H_2 production, transportation, storage and life cycle assessment; 2) assessing the use of key centralised and decentralised approaches for low-carbon gaseous fuels life cycle energy demand and greenhouse gas emissions minimisation 3) analysing a set of H_2-related supply chain options over different continents to determine the impacts of international trade on the life cycle environmental impacts of low-carbon gaseous fuels. It incorporates the impact of location factors to offer specific insights, especially for renewable energy sources; and 4) assessing the dynamic impacts of low-carbon gaseous fuel emissions over 3-time horizons [2025, 2030, and 2050]. As a result, insights were drawn from over 10,000 cases as the manuscript reports that the lifecycle greenhouse emissions of H_2 and SNG supply chains typically range from 5–86 gCO_2e/MJ in 2025, and this could reduce to 2–40 gCO_2e/MJ in 2050.

The work was published in Energy Conversion and Management in June 2025. The published work is titled “Life cycle greenhouse gas implications of low-carbon gaseous fuel supply chains from technological, geospatial, and temporal perspectives” and is presented here as Chapter 7. The main supplementary information for the work, SI 1, published alongside the paper, is reprinted in Appendix A4. Other supplementary information, which provides specific details on the various scenarios assessed, SI 2 and 3, totalling approximately 380 pages, is provided in the online version of the published work and https://ars.els-cdn.com/content/image/1-s2.0-S0196890425003267-mmc2.xlsx.

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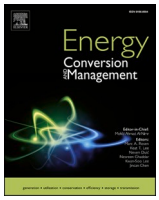

Research Paper



Life cycle greenhouse gas implications of low-carbon gaseous fuel supply chains from technological, geospatial, and temporal perspectives

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ABSTRACT

There is consensus that achieving net-zero emissions will require the use of low-carbon hydrogen (H_2) and its derivatives, particularly in the hard-to-abate sectors. This necessitates the development of a global H_2 supply chain, which can be complex given that there are limited experiences worldwide. While H_2 production emissions at the plant gate might be low, the emissions throughout their supply chains are not yet well understood. Here, we summarise key insights drawn from over 10,000 cases, analysing the supply of H_2 from six renewables-rich regions and transporting it via different modes to two European markets, using six different chemical forms, including compressed-H_2 (CH2), liquefied-H_2 (LH2), synthetic natural gas (SNG), methylcyclohexane (MCH), ammonia (NH_3), and methanol (MeOH). We discussed the implications on the overall energy efficiency, product losses throughout the supply chains, and life cycle greenhouse gas (GHG) emissions from temporal, geospatial, and technological perspectives. The total loss and energy efficiencies of H_2 and SNG throughout the supply chains were estimated to range from 0.8–11.0 %/kg and 1.8–3.6 MJ/MJ of gaseous fuel delivered, respectively. The lifecycle GHG emissions (without embodied emissions) ranged from 5–86 gCO_2e/MJ in 2025, and this could reduce to 2–40 gCO_2e/MJ in 2050, due to changes in technological, design and operational factors. Minimising the impact of fuel/carrier production, H_2/CH_4 losses, fuel and electricity emissions factors by combining centralised and decentralised supply chain approaches could result in a lower GHG estimate. The use of chemical carriers could increase GHG emissions due to the H_2 liberation step at the destination. Even when starting with a low carbon intensity H_2 at the plant gate, the emissions associated with the supply chain can drive the emissions above the EU and UK regulatory limits. This paper further adds to the body of evidence pointing to the need for life cycle assessment-based certification that is asset-specific and supply chain-specific for demonstrating compliance against regulatory limits or H_2 standards globally.

1. Introduction

The hard-to-abate sectors, like heavy-duty trucking, marine and aviation, as well as heavy industries involved in the manufacturing of iron, steel, and petrochemicals, account for over 7 $GtCO_2$ emissions worldwide in 2022 [1]. The consensus is that low-carbon hydrogen (H_2), and its derivatives, are promising abatement options that could play a pivotal complementary role to meet the high energy and chemical feedstock demands from these sectors while contributing towards the global net-zero ambition [2–4]. Currently, many government policies, including the European Union (EU) [4–6], the United Kingdom (UK) [7] and Germany [8], support the use of H_2, and its derivatives, for

Abbreviations: AL, Algeria; AU, Australia; BAT, Best available technology; CCS, Carbon capture and storage; CH2, Compressed H_2; CL, Chile; DAC, Direct air capture; E-fuel, Electro-fuels; EU, European Union; FU, Functional unit; GHG, Greenhouse gas; GWP, Global warming potential; LCA, Life cycle assessment; LCF, Low-carbon fuel; LH_2, Liquefied H_2; LOHC, Liquid organic H_2 carrier; MCH, Methylcyclohexane; MeOH, Methanol; MR, Morocco; NG, Nigeria/natural gas (depending on context); NL, Netherlands; NH_3, Ammonia; NOx, Nitrous oxides; RED, Renewable Energy Directive; RCF, Recycled carbon fuel; RFID, Radio frequency identification; RFNBO, Renewable fuels from non-biological origin; RTFO, Renewable Transport Fuel Obligation; SA, Saudi Arabia; SI, Supplementary information; SMR, Steam methane reforming; SNG, Synthetic natural gas; UK, United Kingdom.

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transport, as well as domestic and industrial applications. In the transport sector, low-carbon fuels (LCFs) derived from H_2, like renewable fuels of non-biological origins (RFNBOs) and recycled carbon fuels (RCFs), are gaining considerable interest, particularly for aviation and marine where direct electrification is less likely and considering the limited potentials of other alternatives [9–11]. Furthermore, the EU's H_2 and gas decarbonisation package aims to accelerate the uptake of low-carbon H_2 within the EU, consistent with the goals of REPowerEU [6,12]. Crucially, the EU Hydrogen Strategy [4,6,13] recognises the high likelihood that low-carbon H_2 will need to be imported from outside the EU, particularly from regions that could have cost-competitive advantages, to supplement domestic productions in meeting growing EU demands.

However, there are limited experiences of international H_2 trade globally. Although today H_2 demand globally exceeds 95 Mt, most of it is produced and consumed within the same location without the need for complex distribution infrastructures [14]. The emerging international H_2 trades can be complex as they require transboundary supply chains, certainly involving multimodal transportations, with current considerations including a range of different H_2 carriers that may necessitate conversion/re-conversion steps. Therefore, it is considered timely to assess the efficiency and greenhouse gas (GHG) emission implications of producing and transporting low-carbon H_2 across several geographical locations, using different carriers and the associated technologies for conversion/reconversion, and their future potentials over time. Importantly, this has to be performed within the context of meeting regulatory thresholds for low-carbon H_2.

The GHG emissions associated with the production of low-carbon H_2 such as e-H_2 and blue H_2 can be low, which according to the UK BEIS [15], Almena et al. [16], and IEA [17], should be within the range of −175 gCO_2e/MJ with renewables and carbon capture & storage (CCS) to 25 gCO_2e/MJ with steam methane reforming (SMR) and CCS. These emissions are within regulatory standards for H_2 production, such as the UK Low Carbon Hydrogen Standard [18] of 20 gCO_2e/MJ and the EU standard [17] of 28.2 gCO_2e/MJ. However, the emissions related to activities downstream of H_2 production, i.e., transformation, storage, and transportation of H_2-based fuels, can significantly increase the overall emissions, resulting in well-to-user emissions of 2–50 gCO_2e/MJ [15]. The regulatory limits (legal obligation) for well-to-user or lifecycle emissions of 32.9 gCO_2e/MJ by the UK Renewable Transport Fuel Obligation (RTFO) [7] and 28.2 gCO_2e/MJ by the EU [17] could be exceeded under some supply options. Additionally, many regulatory standards, such as the UK Low Carbon Hydrogen Standard [18] and EU Renewable Energy Directive (RED) II [5], do not account for embodied emissions from infrastructure, including production equipment and transport vehicles. As a result, even H_2 supply chains that comply with the regulatory limits may still incur significant emissions related to infrastructure, leading to higher overall GHG emissions. Generally, H_2 supply chains differ by design and operations, namely: H_2 production method; transformations for transport and storage; transportation modes and distances; and the form of fuel and dispensing method at the point of delivery to the user. These factors influence both the efficiency of the supply chain (H_2 losses) and energy use, where associated GHG emissions are further influenced by sources of energy inputs that may differ significantly by location (e.g., electricity grid mix). Hence, it is important to understand the impacts of these factors on the H_2 fuel supply chain using a comprehensive life cycle GHG emissions assessment approach. Prior studies of H_2 supply chains are typically limited to national perspectives [15,19–21], for instance, the production and use within the UK market, which requires a short transport distance [15]. Studies that consider long-distance international supply chains delivering H_2 and H_2 carriers such as ammonia (NH_3), often adopt generic assumptions for H_2 production, transformation and transport that do not necessarily account for location-specific factors such as renewable resource intensity, actual transportation distance, and energy source types (e.g., [22,23]). Others have considered very limited scenarios of H_2 states and carriers [21,24,25].

The transformation of H_2 into a higher-density form, either via liquefaction or chemical reaction to produce a carrier, allows for a safer and less costly transportation means [22,23,26], though these will likely have to be reconverted into H_2 further downstream in the end-use market. Due to the various physical states and chemical carriers that can be used in the H_2 supply chain, it remains unclear which conversion/reconversion approach is the most optimal from a GHG emissions perspective. Furthermore, a traditional fuel production approach, including H_2 production, has generally relied on a centralised production scheme. However, H_2 reconversion can occur at the import terminals or distribution centres in a centralised location or decentralised at fuel dispensing stations. The energy consumption of some reconversion technologies at distinct locations – import terminals, distribution centres or fuel dispensing stations – may vary significantly depending on the point of reconversion due to technological and operational factors (e.g., process integration). Different production approaches, such as centralised and decentralised production, have been reported by Lilonfe et al. [11,27] to significantly impact the economics of drop-in biofuels produced from wet biomass feedstocks, primarily due to the effects of economies of scale and transportation costs. Although the differences in the impacts of centralised and decentralised production approaches on GHG emissions of drop-in biofuels were shown to be negligible, this may not be the case with an international H_2 supply chain given that it could involve longer distances and conversion between liquids and gasses. Hence, it is important to understand the implications of adopting different downstream reconversion processes and approaches on the overall life cycle GHG emissions of the delivered H_2.

Critically, understanding the fugitive losses along various supply chains, from fuel production to consumption, would also be key to realising their GHG emissions benefits. Fugitive H_2 and CH_4 losses, including from synthetic natural gas (SNG) supply chains, can occur due to factors such as leakage along pipe casing, purging during plant startup and shutdown, and boil-off from a liquefied state. Importantly, H_2 and SNG (i.e., CH_4) are indirect and direct GHGs, with corresponding global warming potentials (GWPs) much higher than CO_2, roughly 11 and 28 times that of CO_2 over a 100-year period [28,29], respectively.

Here, we address the gaps in the literature by assessing the lifecycle GHG emissions of entire H_2 supply chains with and without infrastructure-embodied emissions, by adopting market-specific factors, and using a variety of H_2 carriers and physical states including compressed H_2 (CH2), liquefied H_2 (LH2), SNG, methylcyclohexane (MCH), NH_3, and methanol (MeOH). We consider the production of H_2 from key renewables-rich regions [Saudi Arabia (SA), Nigeria (NG), Chile (CL), Morocco (MR), Algeria (AL), and Australia (AU)] and transporting H_2 via various modes to European markets by ship and, from locations in Middle East and North Africa, by *trans*-continental pipelines. We could consider other countries, however, the intention here is not to evaluate all possible options but to focus on key representative supply chains. Nonetheless, the approach and models developed here could readily be applied to other production and consumption markets. Furthermore, we assess the GHG emission impacts of key H_2 downstream processes, novel H_2-delivery approaches, and the effects of dispensing H_2 as CH2 and LH2 in high-pressure cylinders. We develop a Microsoft Excel-based tool to model the H_2 and SNG losses along various supply chains, including those emitted during H_2 production, transmission, and distribution, which we then use to estimate mitigation benefits associated with strategies for managing H_2 and SNG losses. The analyses are performed for the years 2025, 2030, and 2050, whereby we present here summary findings and insights from 17 key scenarios drawn from over 10,000 scenarios and sensitivity cases.

2. Methodology

The methodologies used in the life cycle assessment (LCA) were based on the standards given by ISO 14 040 and 14 044, which include

goal and scope definition, inventory analysis, impact assessment and interpretation [30–32]. This study aims to evaluate key H_2-based fuel supply chains and estimate the life cycle GHG emissions associated with their production, delivery, and use. The flow diagram of the H_2-based supply chains assessed in the study is shown in Fig. 1 where the final fuel delivered is either H_2 (i.e., CH2 or LH2) or SNG. The boundary of the study starts at the electricity generation plant/natural gas (NG) extraction plant and terminates at the end-use stage in a vehicle/gas boiler where the fuel is oxidised. A Microsoft Excel-based tool was developed for this analysis, which was used to evaluate thousands of H_2 and SNG supply chains, as summarised in Fig. 1. The LCA performed considers the temporal, geospatial, and technological parameters, as it incorporates location-specific and technology-specific factors, and their changes over three time-horizons (2025, 2030, 2050). Also, the GHG emissions were estimated with and without accounting for embodied emissions from infrastructures to determine the impacts of new infrastructures. The GHG emissions factors used were 100-year GWPs obtained from the existing literature, including Ecoinvent (version 3.7.1) and DESNZ [33]. Where a considerable variation in data exists for a parameter in the literature, any or both of these approaches were adopted: a) Prioritisation of data from commercial applications over demonstration plants and experimental data and b) Use of averages of the most represented range in the literature. The study's functional unit (FU) is 1 kg of fuel at the fuel dispensing station/gas boiler while GHG emissions estimates were reported in gCO_2e per MJ of fuel.

In total, this study presents 17 key pathways for H_2-based fuel supply chains, summarising tens of thousands of scenarios and sensitivity cases that were evaluated; see Table 1 for details. Fig. 1 presents a graphic summary of the approaches used in the analysis, considering numerous scenarios to assess the impacts of:

(1) Technological factors and process improvements over time – 2025, 2030, and 2050. Key technological factors were assessed, including the use of fossil-fuelled vehicles in 2025, dual fuel engines and boil-off gas recovery systems from 2030 – 2050, improvement in electrolyser efficiency in 2050, and switching from NG heating to grid electricity, e-H_2 or SNG in 2050;
(2) Geographical-specific factors, like solar and wind resources for renewable fuel production and local electricity grid mix. This scenario considered the production and transportation of H_2 and SNG into Europe (UK and NL [Netherlands]) from various markets, namely: SA, NG, CL, MR, AL, and AU;
(3) H_2 sources including green, blue and grey H_2. The electrolysis of H_2 using alkaline electrolysers at efficiencies of 65.4 % in 2025 and 2030 and 75 % in 2050 were evaluated to account for improvements in efficiency over time;
(4) Two final delivered fuel products: H_2 and SNG;
(5) Physical states and chemical carriers for H_2 transportation, including CH2, LH2, MCH, NH_3 and MeOH (see Section 2.2 for details);
(6) Different transport modes, including ships, pipelines, rails and trucks and their return journey (see Section 2.3 for details);
(7) Boil-off and boil-off gas reduction approaches such as using H_2 reliquefaction and dual fuel in transport vehicles (see Section 2.3 and 2.5 for details);
(8) Reconversion approaches, including reconversion at import terminals, distribution centres or fuel dispensing stations;
(9) Downstream energy supply emission factors such as grid electricity and gaseous synthetic fuel in dehydrogenation energy demand;
(10) Various fuel application technologies: Transport vehicles and gas boilers, including CH2 and LH2 dispensing stations that can dispense H_2 as compressed or liquefied using compressors or pumps (see Section 2.5).

2.1. Fuel

The paper evaluates H_2 and SNG, which are produced using electrolysis and methanation, respectively. The electrolysis technology evaluated is the alkaline electrolyser with an efficiency of 65.4 % in 2025 and 2030 and 75 % in 2050 [34]. The reaction stoichiometries of electrolytic H_2 production and grey and blue H_2 production via SMR are shown in Eqs. (1) and (2) [34,35]. The energy technologies for green H_2 production analysed were solar and wind electricity. The embodied emissions factors for renewables and electrolysers were calculated as described in Section 2.4. Catalysts used in methanation and conversion of H_2 to carriers are estimated to be less than 0.2 gCO_2e/MJ fuel [27], and are considered small and therefore excluded from the analysis, consistent with the UK Low Carbon Hydrogen Standard materiality threshold of 0.2 gCO_2e/MJ H_2 [18]. Also, the volume of H_2 loss in the production stage due to activities, such as start-up, plant shutdown and H_2 crossover to the anode in electrolysers, was accounted for. The reaction stoichiometry of SNG production via methanation is shown in

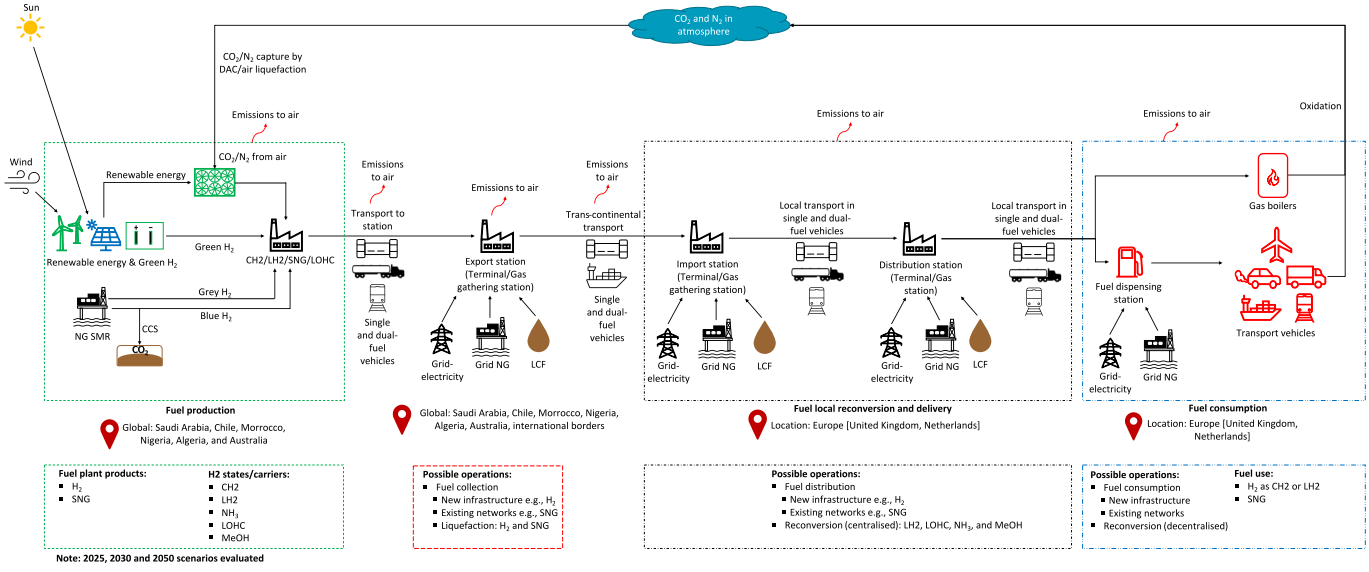

Fig. 1. Summary of key gaseous synthetic fuels' supply chain analysed.

Table 1
The summary of key scenarios of the gaseous synthetic fuel supply chains assessed in this work.

Scenario	Title	Fuel production approach	Transmission mode	Distribution mode	Reconversion	Final fuel consumed
1	Centr. LH2, Centr. H_2 (T2)	Centr. LH2	Ship	Rail/trucks	Centr. import terminal (T2)	H_2
2	Centr. LH2, Centr. H_2 (D)	Centr. LH2	Ship	Rail/trucks	Centr. distribution terminal (D)	H_2
3	Centr. LH2, Decentr. H_2 (V)	Centr. LH2	Ship	Rail/trucks	Decentr. vehicle (V)	H_2
4	Centr. LH2, Decentr. H_2 (S)	Centr. LH2	Ship	Rail/trucks	Decentr. fuel station (S)	H_2
5	Centr. LH2, Ship & Gas Line	Centr. LH2	Ship	Grid pipeline	Centralised	H_2
6	Centr. CH2, Gas Line	Centr. CH2	Pipeline	Grid pipeline		H_2
7	Centr. MCH, Centr. H_2 (T2)	Centr. MCH	Ship	Rail/trucks/ pipeline	Centr. import terminal (T2)	H_2
8	Centr. MCH, Centr. H_2 (D)	Centr. MCH	Ship	Rail/trucks/ pipeline	Centr. distribution terminal (D)	H_2
9	Centr. MCH, Decentr. H_2 (S)	Centr. MCH	Ship	Rail/trucks/ pipeline	Decentr. fuel station (S)	H_2
10	Centr. NH_3, Centr. H_2 (T2)	Centr. NH_3	Ship	Rail/trucks/ pipeline	Centr. import terminal (T2)	H_2
11	Centr. NH_3, Centr. H_2 (D)	Centr. NH_3	Ship	Rail/trucks/ pipeline	Centr. distribution terminal (D)	H_2
12	Centr. NH_3, Decentr. H_2 (S)	Centr. NH_3	Ship	Rail/trucks/ pipeline	Decentr. fuel station (S)	H_2
13	Centr. MeOH, Centr. H_2 (T2)	Centr. MeOH	Ship	Rail/trucks/ pipeline	Centr. import terminal (T2)	H_2
14	Centr. MeOH, Centr. H_2 (D)	Centr. MeOH	Ship	Rail/trucks/ pipeline	Centr. distribution terminal (D)	H_2
15	Centr. MeOH, Decentr. H_2 (S)	Centr. MeOH	Ship	Rail/trucks/ pipeline	Decentr. fuel station (S)	H_2
16	Centr. SNG, Ship & Gas Line	Centr. SNG	Ship	Grid pipeline	Centralised	SNG
17	Centr. SNG, Gas Line	Centr. SNG	Pipeline	Grid pipeline		SNG

Note: Scenarios 5, 6, 16 and 17 are compatible with domestic/industrial heating. Centr. stands for centralised and decentr. for decentralised.

Equation (2) [34,35]. The CO_2 scenarios assessed included CO_2 capture via DAC using renewable energy [34,36]. The embodied emissions factors for DAC and SNG production were based on NETL [37], Terlouw et al. [38] and Ecoinvent. Table 2 shows the process, material, energy, and emission factor data used in the analysis, including those for blue and grey H_2. The process yields and other key process data are shown in the supplementary information (SI) 1 Table S2 and Table S3. Fig. 1 presents the supply chain scenarios of H_2 and SNG evaluated.

$$2\,H_2O \rightarrow 2\,H_2 + O_2 \qquad \Delta H = +286\,kJ/mol \tag{1}$$

$$CH_4 + 2H_2O \leftrightarrow 4H_2 + CO_2 \qquad \Delta H = +165kJ/mol \tag{2}$$

2.2. Hydrogen carriers

Due to the low mass density of H_2, various models for H_2 carriers, such as NH_3 and liquid organic H_2 carriers (LOHCs), have been developed to minimise the transportation cost of delivering H_2. The cost of storing and transporting H_2 using NH_3 and LOHCs over moderate to large distances and capacities is reported to be lower than those using CH2 and LH2 [22,23,26]. LOHCs often analysed in the literature include MCH and MeOH. However, while NH_3 and MeOH can provide low GHG emissions when produced using low-carbon H_2, the GHG emissions of MCH and dibenzyltoluene carriers reported in the literature are often high, with emissions in the range of 20–50 $gCO_2e/MJ\ H_2$ [19,20,22], due to the non-renewable manufacturing processes of these LOHCs. In this work, the carriers analysed were MCH, NH_3 and MeOH. The productions of MCH, NH_3 and MeOH were based on toluene hydrogenation, nitrogen hydrogenation (Haber-Bosch process), and CO_2 hydrogenation to MeOH, respectively. The reaction equations for MCH, NH_3 and MeOH are shown in Equations (3)–(5) [34,45,47,58]. Table 2 provides the material, energy, and emissions data used in the analyses of H_2 carriers.

$$C_7H_8 + 3H_2 \leftrightarrow C_7H_{14} \qquad \Delta H = -205kJ/mol \tag{3}$$

$$CO_2 + 3\,H_2 \leftrightarrow CH_3OH + H_2O \qquad \Delta H = -49.4\,kJ/mol \tag{4}$$

$$N_2 + 3\,H_2 \leftrightarrow 2\,NH_3 \qquad \Delta H = -92\,kJ/mol \tag{5}$$

2.3. Transportation

The transportation of H_2 and SNG fuels using various modes of transportation, such as trucks, rails, pipelines, and ships, was assessed. Pipelines and ships were used in long-distance intercontinental transportation, while trucks, rails, and pipelines were used in local and regional fuel transportation. Intercontinental shipping distances were obtained from Port.com, while the pipeline distances were obtained from Haumann et al. [59], Google Maps, and Fluentcargo.com. The various modes of transporting the fuels considered included fossil (single) fuel vehicles in the 2025 scenarios and dual fuel (fossil fuel and H_2/SNG fuels) vehicles in the 2030–2050 scenarios. In the assessment of dual fuel engines, the base case assumed that LCF is the primary fuel used under standard operating conditions, allowing the engine to operate exclusively on synthetic fuel during normal operations and to utilize fossil fuel only when there is a shortfall in synthetic fuel supply. Additionally, boil-offs and vented gases in transport supply chain applications were considered. Boil-offs and venting of H_2 and SNG for safety reasons can form sources of losses for H_2 and SNG supply chains. Hence, we developed strategies to mitigate the impacts of boil-off and venting of H_2 and SNG by using gas recompression, re-liquefaction technologies and dual fuel engines, based on existing and anticipated technological developments [60–62]. The MCH transport scenarios included the return of toluene back to the fuel production plant for another process cycle. Furthermore, the fuel transportation by pipelines using pumps and compressors was assessed over different electricity sources such as renewables, grid mix and in-situ electricity generation. In-situ electricity from LCF was assumed to be the default mode in the case of remote *trans*-continental locations. The transport parameters used in the analysis are given in Table 3 and SI 1 Table S4 to Table S8. The embodied emissions for delivery vehicles and pipelines used in fuel transportation were based on data obtained from Ecoinvent and other literature for trailers, trains, liquefied NG tankers and NG pipelines (Table 3, Table S4 to Table S8). Fig. 1 shows the summary of the transport scenarios analysed.

Table 2
Material, energy, and embodied emission factor data for H_2 production, carrier production and reconversion.

Technology	Process conditions	Casing leaks/direct losses[a] [per kg H_2/ CH_4]	Electricity demand[a] [kWh/kg H_2 or kWh/kg SNG]	Fuel/Heat demand[a] [MJ per kg H_2 or MJ/kg SNG]	Embodied emissions[a] [kgCO_2e/kg H_2 or kgCO_2e/kg SNG]	Reference
H_2 and SNG production and regasification technologies						
Electrolysis 65.4 % (green)	T: 50–80 °C, P: Up to 30 bar	0.52 %	50.95	–	0.7167	[17,34,39]
Electrolysis 75 % (green)	T: 50–80 °C, P: Up to 30 bar	0.52 %	44.43	–	0.6249	[17,34,39]
SMR (grey)	T: 200–550 °C, P: 1– 100 bar	1.70 %	–	160.20	0.2999	[17,39,40]
SMR + CCS (blue)	T: 200–550 °C, P: 1– 100 bar	1.70 %	0.80	176.40	0.2999	[17,39,40]
Methanation: SNG	T: Up to 400 °C, P: 30 bar	0.40 %	0.32	–	Based on MeOH plant data on Ecoinvent	[34,39]
LH2 regasification	P: 1 bar	0.02 %		0.12	0.0000	[41,42]
Liquefied SNG regasification	P: 1 bar	0.04 %		2.5	0.0000	[43,44]
H_2 carrier production and reconversion technologies						
Toluene hydrogenation to MCH	T: 250–350 °C, P: 1–20 bar	0.20 %	0.20		Based on MeOH plant data on Ecoinvent	[45–47]
MCH dehydrogenation	T: 150–200 °C, P: 1–20 bar	0.20 %	1.50[b]/ 1.5[c]	37.96[b]/40.20[c]	Based on MeOH plant data on Ecoinvent	[45,48,49]
Haber-Bosch process (traditional): NH_3	T: 400–500 °C, P: 150– 250 bar	0.50 %	2.62		Based on MeOH plant data on Ecoinvent	[34,39]
Haber-Bosch process (electrochemical): NH_3	T: 25–250 °C, P: 1–10 bar	0.50 %	1.47		Based on MeOH plant data on Ecoinvent	[39,50,51]
NH_3 cracking with pressure swing adsorption	T: 400–900 °C, P: 1–10 bar	0.20 %	0.50[b]/0.50[c]	32.40[b]/36.00[c]	Based on MeOH plant data on Ecoinvent	[48,52,53]
NH_3 cracking with membrane separation	T: 400–900 °C, P: 1–10 bar	0.20 %	3.0[b]/5.0[c]		Based on MeOH plant data on Ecoinvent	[54,55,56]
NH_3 cracking with cryogenic separation	T: 400–900 °C, P: 1–10 bar	0.20 %	1.26[b]/9.06[c]	2.03[b]	Based on MeOH plant data on Ecoinvent	[54,55,56]
CO_2 hydrogenation: MeOH	T: 200–300 °C, P: 10– 100 bar	0.80 %	1.43	–	Based on MeOH plant data on Ecoinvent	[34,39,46]
MeOH reforming by steam cracking	T: 240–350 °C, P: 1– 10 bar	0.25 %	0.50[b]/0.50[c]	14.60[b]/18.25[c]	Based on MeOH plant data on Ecoinvent	[24,46,48,57]

Key: T- temperature, P- pressure
Note: The energy demands for the Haber-Bosch process and CO_2 hydrogenation to MeOH presented in this table are the energy demands for the process (excluding other processes such as H_2 production, nitrogen liquefaction and CO_2 capture via DAC). For details on other processes such as H_2 production, nitrogen liquefaction and CO_2 capture via DAC, see H_2 production in Table 2 and CO_2 and nitrogen capture in SI Table S3.
[a] Units of numbers are on a kg H_2 basis at the process gate except in SNG methanation, where the unit is on a kg SNG basis. See SI 1 Table S2 and Table S14 for additional details such as overall system losses that include by-product formation and blue H_2 emission factors at the plant.
[b] Centralised application
[c] Decentralised application

Table 3
Truck/trailer transportation parameters.

Trucks	Units	CH2	LH2	as MCH	as MeOH	as NH_3	Data based on ref.
Capacity	t (cargo)	1.1	4	34	36	32	[34,63,64]
Truck life	years	15	15	15	15	15	
Product stored pressure	bar	500	<5	1	1	1	[60,63]
Boil-off	Per h for CH2 and per kg H_2 for LH2	0.0075 %	0.43 %	N/A	N/A	N/A	[39,60]
Speed (loaded)	km/h	60	60	60	60	60	[46,65]
Speed (unloaded)	km/h	70	70	70	70	70	
Delivery distance	km	400	400	400	400	400	
Travel time (loaded)	h	6.67	6.67	6.67	6.67	6.67	
Travel time (unloaded)	h	5.71	5.71	5.71	5.71	5.71	
Loading/unloading time	h	1.75	3	3.5	1.75	1.75	[46,56,66]
Total time	h	8.42	9.67	10.17	8.42	8.42	
Total time with empty return	h	14.13	15.38	15.88	14.13	14.13	
Total time with toluene return	h	15.88	18.38	19.38	15.88	15.88	
Energy consumption	MJ/kg fuel product/km	0.00707	0.00200	0.01345	0.00433	0.01729	[34]
Energy consumption with empty return	MJ/kg fuel product/km	0.01406	0.00393		0.00544	0.02123	
Energy consumption with toluene return	MJ/kg fuel product/km	0.01096	0.00589	0.02690			
Embodied emissions (single trip basis)	kgCO_2e/kg fuel product	0.00363	0.00115	0.00218	0.00058	0.00204	Trailer, Ecoinvent

2.4. Electricity

In normal operations, both renewable and grid electricity were assumed to be used based on location, the type of process and point of use. Processes occurring at the fuel production plant location used renewable electricity (except in the case of blue or grey H_2), while downstream processes used grid electricity (except for remote pipeline applications), as detailed in SI 1 Table S15. The emissions factors for renewable electricity without embodied emissions were taken as zero, in line with the UK Low Carbon Hydrogen Standard [18]. However,

embodied emissions factors included emissions from infrastructures and were calculated using data from Ecoinvent, NREL [67], NASA wind and solar data [68]. The wind turbine and solar PV were designed using the methodologies detailed by Ligęza et al. [69], EPA [70] and Nizami et al. [71], as summarised in Eqs. *(6) and (7)*. Grid electricity emissions factors in 2025 were based on the Stated Policies scenarios by the IEA whereas future grid scenarios for 2030 and 2050 were based on IEA's Sustainable Development and Stated Policies scenarios. The grid electricity emissions factors of countries not found in the IEA report were calculated based on the assumptions or estimates found in the IEA's report for the region where the countries belong; see SI 1 Table S11 for details. Electricity emissions factors from using in-situ LCFs were calculated using the emission factor of that fuel and turbine efficiencies, such as H_2 gas turbine efficiency. SI 1 Table S9 to Table S14 summarised the electricity emission factors used in the study.

$$P_T = 0.5 \bullet \rho \bullet A_T \bullet C_P \bullet v^3 \quad (6)$$

where, P_T is the power generated by the turbine in MW, ρ is the air density at the hub height, A_T is the rotor swept area in m^2, C_P is the overall efficiency coefficient (power coefficient) that changes with both wind speed and turbine rotational speed, and v is the wind speed. The design parameters of the turbine are shown in Table 4.

$$E_{PV} = A_{PV} \bullet E_{sun} \bullet \eta_{PV} \bullet PR \quad (7)$$

where, E_{PV} is the energy produced by the solar PV in kWh, A_{PV} is the area of the solar PV in m^2, E_{sun} is the Global Horizontal Irradiation (GHI) in kWh/m^2, η_{PV} is the solar PV efficiency, and PR = (1 −system loss) is the performance ratio, coefficient for losses. The design parameters of the solar PV are shown in Table 5.

2.5. Refuelling stations

The different types of gaseous fuels refuelling stations analysed included: H_2 refuelling stations with CH2 storage and dispensing CH2 at high pressures using compressors; H_2 refuelling stations with LH2 storage and dispensing CH2 at high pressures using compressors; H_2 refuelling stations with LH2 storage and dispensing LH2 at low or high pressures using pumps; H_2 refuelling stations with NH_3 storage; and SNG refuelling stations with grid SNG/NG uptake. Additionally, H_2 refuelling stations were assessed for scenarios which use gas re-liquefication systems to mitigate boil-off and venting. The mass, energy and emissions data of refuelling stations, including embodied emissions, are shown in SI 1 Table S16.

2.6. Fuel use

The analysis of the fuel use stage assumed that the oxidation of 1 kg of fuel in any burner, fuel cell or engine type produces the same oxidation products (emissions) whether the engine is stationary or mobile. For SNG, the emissions factor for the combustion of SNG was obtained from DESNZ and BEIS [75], which assumes negligible variation in emissions by engine type. This approach further assumes fuel combustion returns the CO_2 initially captured at the initial fuel production stage and only accounts for other emissions, such as CH_4 and N_2O emissions, from the combustion of these fuels. The oxidation of H_2 is taken to emit zero GHG by emitting 100 % H_2O. This may be true for a fuel cell type of powertrain, however, in practice, according to Douglas et al. [76] and DESNZ and BEIS [75], 0.0017 $kgCO_2e/kg\ H_2$ (0.01391 gCO_2e/MJ) is emitted from nitrous oxides (NOx) during H_2 combustion, which is negligible. Furthermore, H_2 combustion engines can be equipped with selective catalytic reduction units to reduce NOx. In GHG emissions estimation with embodied emissions, the emissions for constructing vehicles and gas boilers were accounted for based on the data obtained from Ecoinvent (SI 1 Table S18). The vehicle models used for road, rail, water, and air transport fuel oxidations were truck, train, ship and aircraft, respectively. The model for a gas boiler is the 10-kW rated boiler for the European market. SI 1 Table S16 and Table S18 show the fuel oxidation, vehicle and gas boiler emissions factors used in the analysis.

Table 4
Key technical specifications of the IEA wind 15-MW turbine.

Parameter	Value	Units	Ref.
Rated power	15	MW	[72]
Cut-in wind speed	3	m/s	
Cut-out wind speed	25	m/s	
Rotor diameter	240	m	
Rotor swept area,A_T	45,239	m^2	
Aerodynamic brake	3	blades full feathering	
Frequency	50/60	Hz	
Hub height	150	m	
Air density,ρ	1.225	kg/m^3	
Power coefficient,C_P	35 %		[69]

Table 5
Key technical specifications of utility-grade solar PV.

Parameter	Value	Units	Ref.
Rated power	670	W	[73]
Maximum efficiency,η_{PV}	21.60 %		[73,74]
Dimensions	2384 × 1303	mm	[73]
Area,A_{PV}	3.106352	m^2	
Operational hours	8760	hours	
Performance ratio,PR	85.9 %		[70]

3. Results and discussions

3.1. Hydrogen and methane leakage

Generally, H_2 is a very small molecule with low viscosity, which makes its applications prone to leakage. The total supply chain leakage rate of gaseous fuel is generally in the range of 0.8–11.0 % per kg of gaseous fuel delivered at the station, with the AU to NL route having the highest loss rates due to the long transport distance involved, as shown in SI 1 Figs. S1–S14. The highest gaseous fuel leakage is obtained in H_2 systems using LH2 due to the boil-off of H_2 during storage and transportation. The boil-off of LH2 in transportation ships that are not equipped with boil-off recovery systems is responsible for the highest leakage in supply chains (SI 1 Figs. S1–S7). H_2 and CH_4 leakages due to boil-off during their delivery to the market have the potential to be reduced significantly by using re-liquefaction technologies and dual fuel delivery vehicles that can utilise H_2 for fuel (SI 1 Figs. S8–S14). Hence, the base case scenarios for product delivery in this analysis for 2030–2050 assumed H_2 supply chains equipped with H_2 re-liquefaction technologies and dual fuel delivery vehicles. Other scenarios with high H_2 and CH_4 losses are pipeline scenarios due to casing leaks, which could lead to losses that may be more difficult to manage. The lowest gaseous fuel leakage is obtained in H_2 systems using H_2 carriers since their major source of leakage is the H_2 production stage (70–85 %). In contrast, when H_2 is delivered as LH2 or CH2, the production (5–10 %), storage (0–50 %), and transportation (40–90 %) stages are the major sources of H_2 leakages.

3.2. Energy consumption

The total supply chain energy consumption varied from 1.8–3.6 MJ per MJ fuel product, as shown in SI 1 Figs. S15–S20. Supply chains delivering H_2 in its chemical form have the lowest energy consumption, while those using carriers, generally recorded the highest energy usage due to the inefficiency involved in the conversion/reconversion steps. In particular, MeOH and SNG have the highest energy intensity because up

to 50 wt% water per kg H_2 is produced as a by-product during MeOH and SNG production [see Eq. (4) and Eq. (2) for additional details].

3.3. Present day greenhouse gas emissions

The life cycle GHG emissions for all the key scenarios assessed in this study are presented in SI 2 & 3. Here, we present the results for the scenario where green H_2 and SNG are produced in SA and exported to the UK in 2025. The emission estimates for all the other scenarios are in SI 2 & 3 and the general insights drawn here are applicable for other scenarios too.

Fig. 2*a–b* shows that the GHG emissions of H_2 supply chains are heavily influenced by technology parameters, design and operational factors [such as production, compression, storage, transportation, reconversion (for carriers), and dispensing stations], and LCA methodology. In 2025, when excluding embodied emissions, the design and operational factors that majorly impact the overall emissions of green H_2 and SNG are fuel/carrier production (0.5–8.7 gCO_2e/MJ), compression (0–9.3 gCO_2e/MJ), storage (0–6.2 gCO_2e/MJ), transportation (2.5–37.6 gCO_2e/MJ), re-conversion (0–21.8 gCO_2e/MJ) and dispensing station (0.9–8.0 gCO_2e/MJ). These emission categories are driven primarily by fuel/carrier production methods, H_2/CH_4 losses, and fuel and electricity emissions factors. The energy consumption of H_2 compression in the distribution stage is typically related to the energy consumption of the

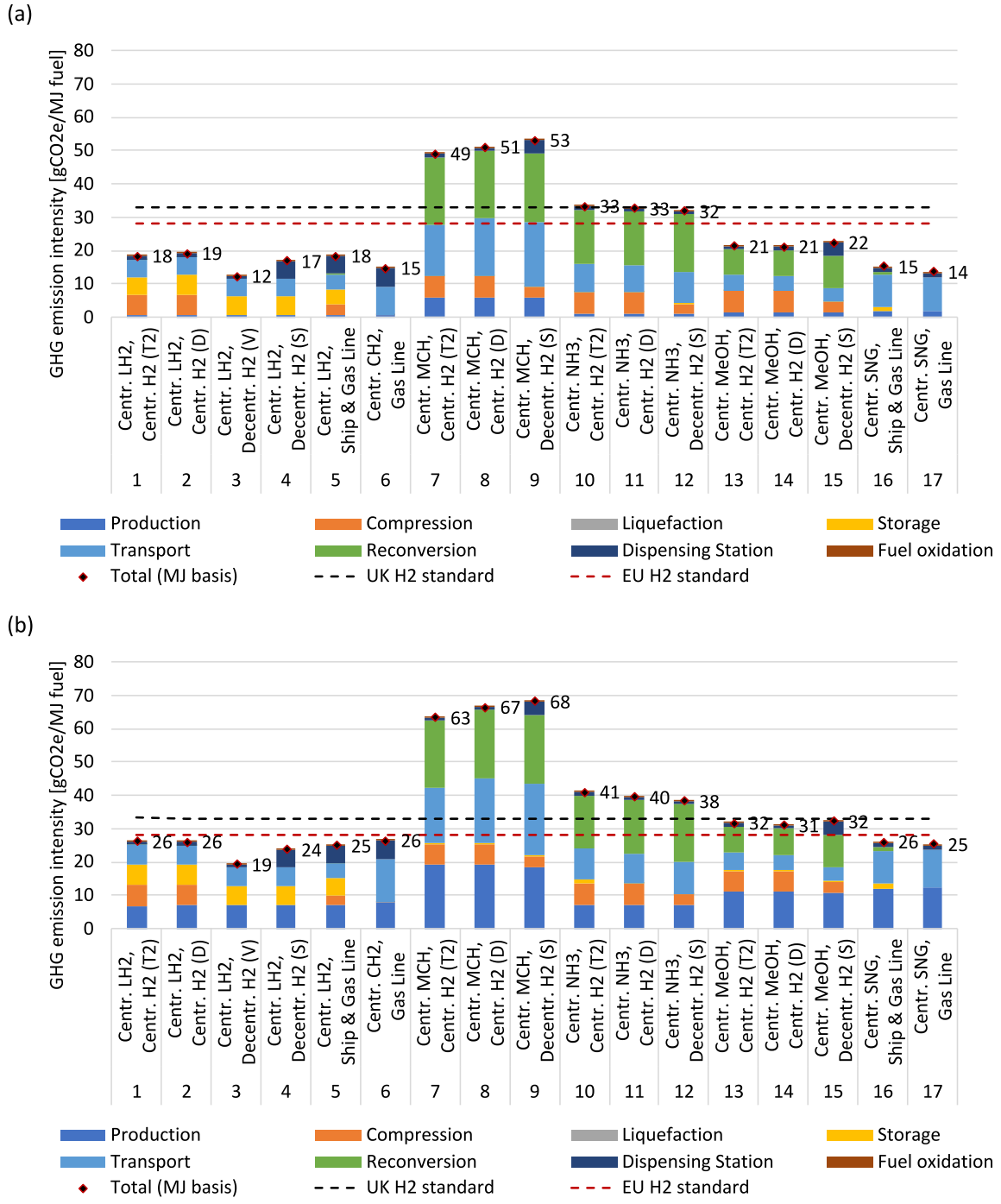

Fig. 2. GHG emissions of green H_2 supply chains for the SA to UK in 2025 (a) Excluding infrastructure embodied emissions and (b) Including infrastructure embodied emissions. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

transportation and dispensing stations because the latter were assumed to have no depressurisation in storage vessels (to maintain the volume factor of compressed H_2) during transportation and storage. Furthermore, there is no significant variation in GHG emissions from the end-use oxidation of H_2 and SNG fuel on road, rail, water, air transport or homes using combustion engines or fuel cell vehicles. This is because the differences in the oxidation products from these sources per MJ of fuel are negligible, as seen from the emission factors in SI 1 Table S18. The overall emissions with embodied emissions are higher than those without embodied emissions. It is worth noting that the embodied emissions from pipeline routes can significantly be reduced should *trans*-continental pipelines function like a grid where different production facilities utilise it for product transportation. Consequently, the GHG emissions of green H_2 and SNG supply chains in 2025 are estimated to range from 5–66 gCO_2e/MJ and 18–84 gCO_2e/MJ without and with embodied emissions, respectively. Other studies reported GHG emissions of green H_2 supply chains ranging from 0.1–85 gCO_2e/MJ [15,19,21,22] (embodied emissions not included), which aligns well with the estimates reported herein. However, the findings from this study may not be directly comparable with the literature values due to the approaches taken in this study differ from those in the literature, which assumed production and use within the national market, thus requiring a short transport distance [15,19,20,21]. The analysis by UK BEIS [15] for delivering renewable electro-CH2 over 150 km distance yielded life cycle emissions of 9, 5 and 3 gCO_2e/MJ for 2020, 2030 and 2050, respectively. These emissions are slightly lower than the renewable electro-CH2 estimates in this analysis of 10–18, 7–11 and 4–7 gCO_2e/MJ in 2025, 2030 and 2050, respectively, which considered *trans*-continental distances. Also, many literature [19–21,25], including those that analysed generic long-distance, used unclear or mixed LCA analysis approaches by accounting for embodied emissions of H_2 production while excluding those of downstream processes. This methodology is inconsistent and not in line with existing regulations [5,18], making direct comparisons challenging.

Generally, from all the scenarios for transport applications, Scenario 3 [Centr. LH2, Decentr. H_2 (V)] has the best range of GHG emissions, with emissions for green H_2 scenarios ranging from 10–18 gCO_2e/MJ without embodied emissions and from 19–31 gCO_2e/MJ with embodied emissions. The combination of centralised and decentralised approaches here provides an optimal solution for several reasons. First, H_2 liquefaction is done in the plant using renewable energy with very low emissions factors compared to grid electricity or any energy used downstream to reconvert the carriers. Although H_2 liquefaction may consume higher energy compared with H_2 carriers, the downstream re-gasification step consumes significantly less energy (0.1 kWh/kg H_2 [41]) than the liberation of H_2 from its carriers (4–13 kWh/kg H_2 [54–56]). Second, the transporting and dispensing of H_2 as LH2 provides the highest energy efficiency [SI 2], with minimal energy losses involved relative to other scenarios that require H_2 carrier production and reconversion and H_2/SNG pipeline. And third, during the dispensing of H_2, Scenario 3 [Centr. LH2, Decentr. H_2 (V)] utilised pumps instead of compressors to dispense LH2 at low pressures into LH2-tanked vehicles or at high pressures into CH2-tanked vehicles, thereby enabling significant energy savings from avoiding H_2 compression even when compared with other LH2 scenarios. The LH2 in the low- or high-pressure tanks can be vapourised to a gaseous state onboard a vehicle before its oxidation. Generally, gas compression to higher pressures consumes significantly more energy than pumping liquids to higher pressures. Consequently, technologies used at the dispensing stations can significantly impact the GHG emissions of H_2 and SNG supply chains based on their operational approach – compressing or pumping H_2. Dispensing stations alone produce emissions ranging from 0.8–8.0 gCO_2e/MJ in 2025. Hence, Scenario 3 [Centr. LH2, Decentr. H_2 (V)] leads to a considerably lower range of GHG emissions than the other scenarios assessed, even in the future. Furthermore, from all the key scenarios for heating applications (Scenarios 5, 6, 16 and 17) as presented in SI 3, Scenario 6 for H_2 pipeline transportation produced the lowest range of GHG emissions, with emissions for green H_2 scenarios of 5–20 gCO_2e/MJ without embodied emissions and 18–41 gCO_2e/MJ with embodied emissions in 2025. This is majorly due to in-situ H_2 use and the lower GWP of H_2 compared with SNG in the event of casing leaks. The future heating scenarios will see Scenario 5 produce the lowest GHG emissions as grid electricity emission factors reduce with time. This indicates the greater influence of electricity emission factors over energy demand in overall GHG emission estimates.

On the other hand, the scenarios using carriers had the highest GHG emissions due to the use of grid electricity to power the reconversion (or H_2 liberation) step and the energy requirements arising from the reconversion. Amongst the H_2 carriers considered, MCH Scenario 9 [Centr. MCH, Decentr. H_2 (S)] has the highest GHG emissions for two main reasons: First, the toluene carrier is derived from fossil feedstock, hence resulting in higher production emissions. Second, the toluene has to be transported back to the production plant to be reused as a carrier, which increases the total transport emissions. Other authors [46] have proposed using in-situ H_2 produced during reconversion to power the conversion process. However, this may not be economically feasible, especially from an H_2 volume and cost perspective. Using in-situ H_2 to power the reconversion process can lead to considerable reductions in the overall emissions of green H_2 scenarios from 20–39 gCO_2e/MJ to 12–33 gCO_2e/MJ without embodied emissions in 2025 [SI 2], excluding the MCH scenarios. However, this comes with a significant penalty in H_2 consumption of 15–70 % per kg of H_2 produced at the reconversion stage. Using in-situ H_2 in the MCH scenarios may not yield any emission reductions in some instances (32–66 gCO_2e/MJ vs 24–65 gCO_2e/MJ), as the benefits of using in-situ H_2 may be offset by the need to produce and return more toluene per kg H_2 delivered. Hence, we assumed that the base case energy for H_2 reconversion would be the cheaper grid electricity, whose emission factor is projected to improve with time. It is important to note that in the MCH scenarios, there is uncertainty regarding the future production of toluene, a byproduct derived from the production of gasoline from crude oil and of coke from coal, particularly given the rise of alternative feedstocks.

Currently, there are no emission limits for H_2 or SNG use in domestic or industrial applications, but there are several policies on their application in the transport sector. Without embodied emissions, which is the methodology currently adopted by EU and UK RTFO regulations in transport applications, the green H_2 and SNG fuel supply chains could meet the H_2 GHG emissions threshold in the EU and UK in 2025, except for some supply chain cases involving MCH and NH_3. This is due to the high emission factor of MCH (toluene carrier), the return of toluene to the fuel production plant to restart the supply chain cycle, and grid electricity used to meet carriers' high reconversion energy. The option for not returning toluene in MCH scenarios is impractical in terms of emissions, as the overall emissions are extremely high, generally above 200 gCO_2e/MJ, due to the low H_2 carrier rate of MCH (roughly 15 kg MCH per kg H_2) and its fossil nature. Generally, pipeline cases above 18,400 km transmission distance for e-SNG in 2025 will exceed the EU regulatory emission limit, while under the UK RTFO, they will meet the UK emission limit even above 18,400 km. Although this is an improbable scenario, theoretically, e-H_2 pipelines do not have practical distance limits to which their emissions will exceed the regulations considering the earth's antipodal distance of 20,000 km [SI 1 Table S21]. The scenarios for MCH (scenarios 7–9) and some NH_3 scenarios do not meet the EU and UK emission limits for H_2 [17] in 2025, but they could meet the regulations in 2050 (Fig. 3 and SI 2). This highlights the opportunities for process improvements and systems optimisation towards enabling a lower carbon H_2 supply option in the future. In the context of the regulatory limits, Fig. 2*b* also highlights the effects of embodied emissions in H_2 production, which can have a significant influence on the overall GHG emission of the delivered H_2. In fact, the total life cycle emissions, when accounting for embodied emissions, are 1.1–3.1 times higher than those of corresponding

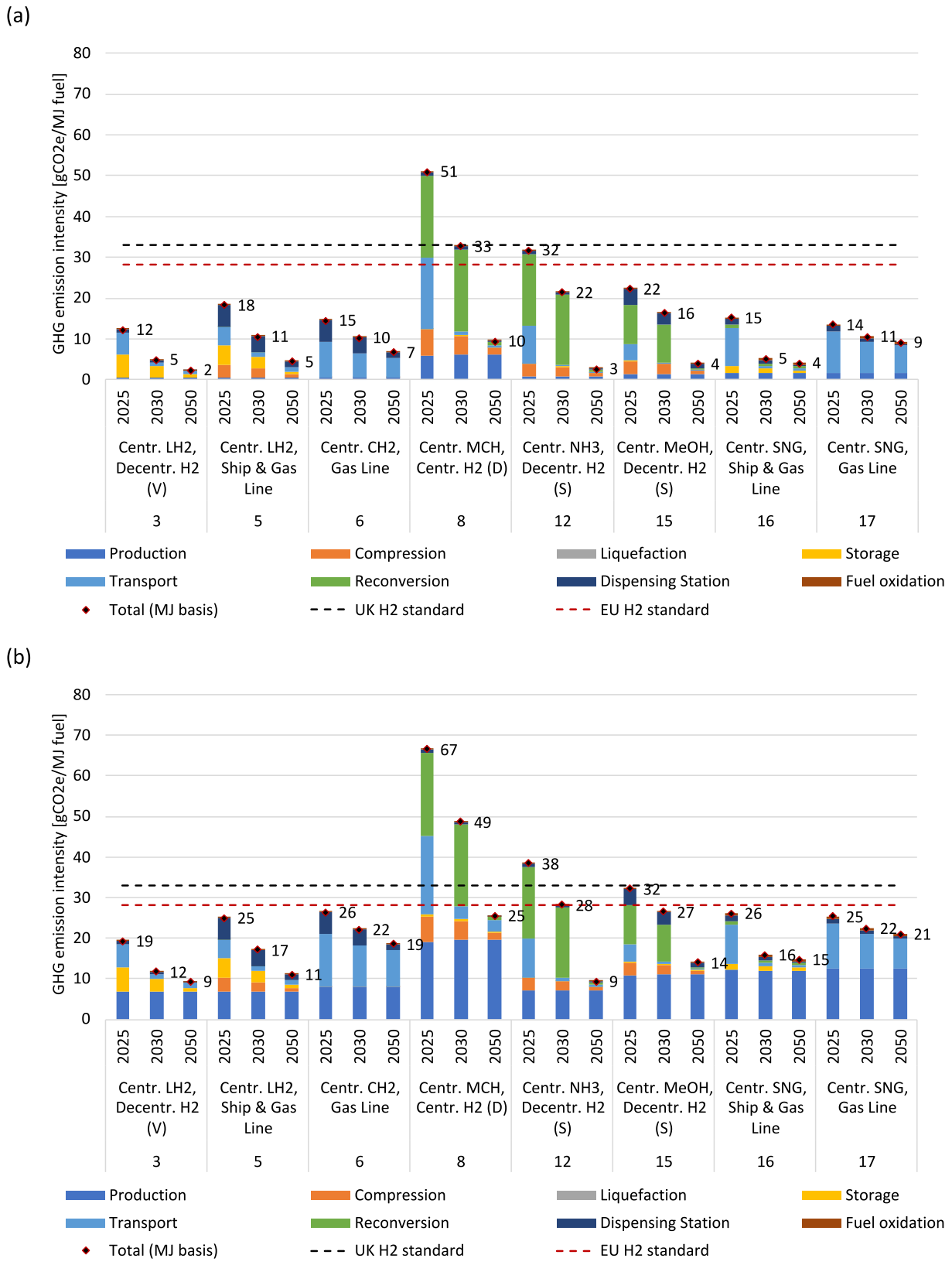

Fig. 3. Overall emissions of key green H_2 supply chains over time for SA to the UK (a) Excluding infrastructure embodied emissions and (b) Including infrastructure embodied emissions. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

scenarios that exclude them.

3.4. Projected future greenhouse gas emissions

Over time, the total life cycle GHG emission of the delivered H_2 is expected to decline, reflecting technological improvements and the gradual economy-wide decarbonisation. To demonstrate this point, Fig. 3*a–b* shows the total GHG emissions of green H_2 produced in SA and exported to the UK over 3 time horizons: 2025, 2030, and 2050 (other scenarios are available in SI 2 & 3). As highlighted in Section 3.3, GHG emissions from any activity in the supply chains are driven primarily by fuel/carrier production methods, H_2/CH_4 losses, and fuel and electricity emissions factors. Hence, from 2025 to 2050, even when the energy demand of H_2 supply chains remains largely unchanged and different approaches are used upstream or downstream of the plant gate, the GHG emissions from the different supply chains decline significantly with time. Scenario 3 [Centr. LH2, Decentr. H_2 (V)] is estimated to possess the lowest emission intensity, partly, driven by the marginal impacts of its lower energy demand in 2050. Furthermore, the GHG emission range in 2050 is significantly reduced compared to 2025. Generally, the GHG emissions of green H_2 supply chains in 2050 ranged from 2–17 gCO_2e/MJ without embodied emissions and from 9–41 gCO_2e/MJ with

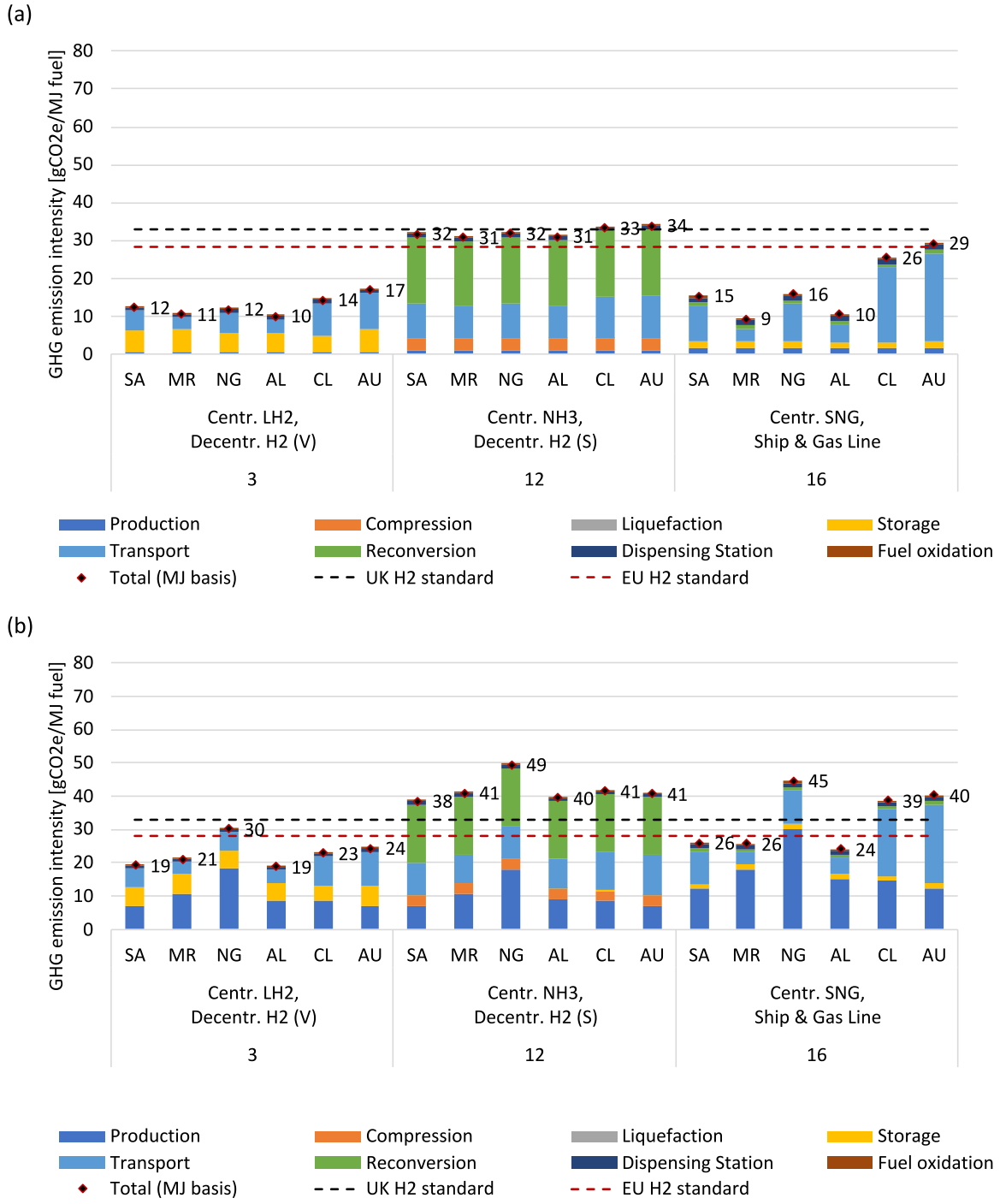

Fig. 4. Overall emissions of the best green H_2 states, carriers and SNG for key fuel production locations to the UK in 2025 (a) Excluding infrastructure embodied emissions and (b) Including infrastructure embodied emissions. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

embodied emissions, based on the IEA's ambitious Sustainable Development scenario. The GHG emission estimates are higher when adopting the IEA's Stated Policies scenario because of its higher grid electricity emission factors, which only considers current national policies. The 2025 scenarios, which were significantly higher than the comparative 2030 and 2050 scenarios, assumed the use of fossil fuel-powered vehicles for H_2 transportation with no boil-off gas recovery in storage and transport systems. The analysis assumes that for 2030 and 2050 scenarios, boil-off gas recovery systems will be incorporated into storage facilities, and dual fuel engines will be in operation using onboard H_2, which would otherwise be vented. Furthermore, the 2050 scenarios performed better than their corresponding 2025 and 2030 scenarios because of the changes in technologies over time, including a switch from NG for heating to grid electricity, SNG, or H_2. These technological changes mean better fuel emission factors and H_2/CH_4 losses, even when the transport distance between countries is unchanged. In a way, these prospective scenarios also highlight what could be achieved under a more ambitious deployment of climate mitigation technologies. These long-term improvements mean that all green H_2 and SNG supply chains in 2050 could meet the EU RED and UK RTFO emissions thresholds, including scenarios where H_2 is delivered using MCH and NH_3. Despite the EU and UK policies being based on lifecycle emissions without embodied emissions, the overall emissions with embodied emissions in 2050, which are 1.8–9.0 times the corresponding emissions without embodied emissions, are generally still within the EU and UK regulatory limits (Fig. 3*b* and Fig. SI 2).

3.5. Emission impacts of hydrogen production and delivery locations

The overall GHG emissions in 2025 for delivering low-carbon gaseous fuel to Europe from different countries (e.g., SA, MR, NG, AL, CL and AU) can vary significantly, as shown in Fig. 4*a–b* for the UK market. Some promising supply chain options can be less attractive when produced and delivered from other locations. For example, the total life cycle emissions for pipeline deliveries of SNG are considerably more attractive from MR to the UK than from the other countries considered. Additionally, emissions of fuel delivery to the NL market were higher than those to the UK in 2025, but these differences in emissions diminished with time, leading to both markets having roughly the same emissions in 2050 (SI 2 & 3). The factors that played a significant role in these variations were transport distance, the emission factors of renewables used in gaseous fuel production in the production location, and the emission factors of grid electricity at the receiving locations. By 2050, grid electricity in the UK and NL will be comparable, resulting in both countries having roughly the same emissions. Generally, from the scenarios analysed (SI 2 & 3), most of the green H_2 and SNG supply chains from various countries could meet the thresholds in the H_2 standards except for a few scenarios in 2025. Therefore, it is important to conduct a detailed, market-specific analyses on the source and delivery of H_2, and its derivatives, to get a proper estimate of the total GHG emissions.

3.6. Emission impacts of hydrogen boil-off and recovery

As seen in Fig. 2 and Fig. 5 for the supply chain from SA to UK in 2025 to 2050, respectively, the boil-off of gaseous fuel is mostly associated with supply chains involving LH2. Boil-off in LH2 systems can be reduced by using boil-off gas recovery systems in storage facilities and dual fuel engines using onboard H_2 that would otherwise be vented. Incorporating boil-off gas recovery of H_2 in LH2 supply chains can reduce overall emissions (without embodied emissions) by 2–3 gCO_2e/MJ fuel. Consequently, LH2 systems incorporating boil-off gas recovery in 2050 have 30–50 % less total GHG emissions compared with those without boil-off gas recovery. Additionally, boil-off gas recovery avoids both the direct emission impacts of H_2 and SNG emissions as well as either increasing the share of product making it to market or providing fuel for their transportation.

3.7. Emission impacts of hydrogen sources

In the preceding sections, we focused on the supply chains of green H_2 deliveries from multiple locations into Europe as a means to demonstrate that emissions due to international trade could be significant, where in some cases, the overall emissions could exceed the regulatory limits. When embodied emissions are excluded, the plant gate production emission of electrolytic H_2 using renewable electricity is typically considered to be zero; however, the choice of H_2 carrier, conversion technology, and supply chains could add anywhere from less

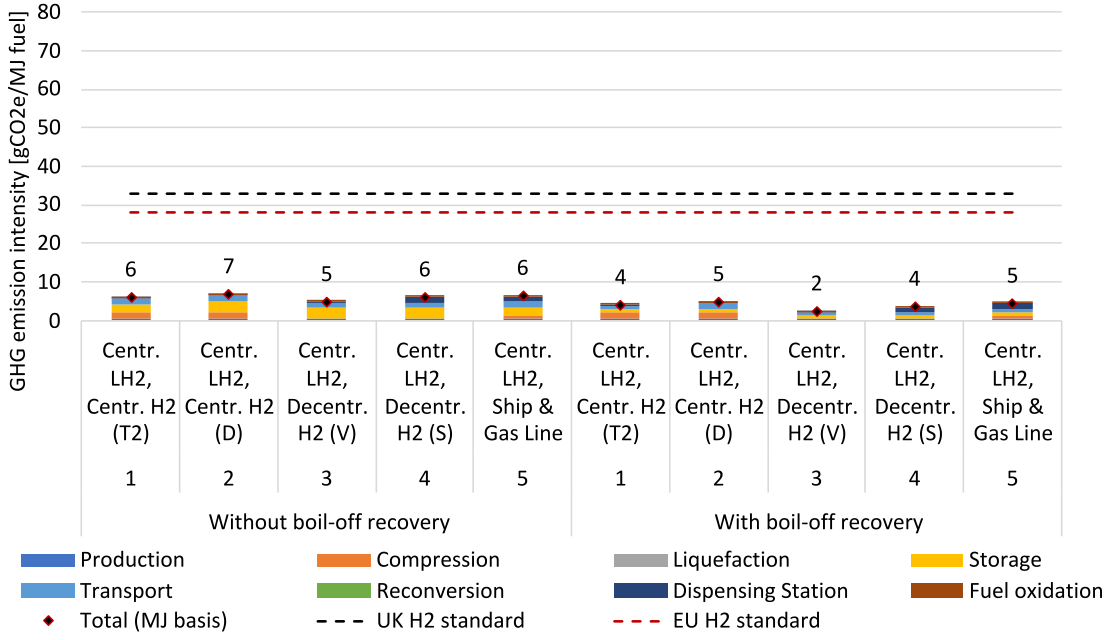

Fig. 5. The emissions impact of green H_2 systems with and without boil recovery for SA to UK route in 2050. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

than 10 to more than 50 gCO_2e/MJ to the overall life cycle emission. Such a broad range of supply chain emissions also raises the question of the impacts of international trade on other low-carbon H_2 sources. So, we conducted further analyses to assess the GHG impacts of delivering different H_2 types from 2025 to 2050, as shown in Fig. 6. Here, we considered 5 H_2 production types with plant gate carbon intensities of 10.6, 10.0, 2.5, 2.0, 1.5 and 0 $kgCO_2e/kg\ H_2$. These emissions represent the plant gate emission factors of grey H_2 in 2025–2030 based on Longden et al. [77], grey H_2 in 2050 based on the IEA [78], blue H_2 in 2025–2030 based on Longden et al. [77], blue H_2 in 2050 based on the IEA [78], blue H_2 in 2050 based on the IEA [78] best available technology (BAT), and green electrolytic H_2, respectively.

International supply chains can add significant variation to the overall life cycle GHG emissions of delivered H_2. As expected, green H_2 scenarios generally have the lowest emissions, followed by blue and grey H_2 scenarios. In some supply chain scenarios, the use of H_2 from NG without any CO_2 mitigation during its production, could lead to emissions that exceed 100 gCO_2e/MJ, well above the emissions from conventional fuels. Importantly, the GHG emissions range in Fig. 6 demonstrates that supply chain considerations can have a considerable impact on the overall life cycle emissions. Even when starting with H_2 with a low carbon intensity at the plant gate, the emissions associated with the supply chain can drive the emissions above the regulatory limits. For H_2 production carbon intensity of 2.0 $kgCO_2e/kg\ H_2$ at the plant gate, i.e., the average carbon intensity estimates for blue H_2 in 2050 based on IEA [78], most of the H_2 supply chain scenarios assessed could still be within regulatory thresholds. However, this would limit blue H_2 and blue SNG pipelines to distances within 6,000 km and 2,800 km in 2050 (SI 1 Table S21), respectively. If the H_2 production carbon intensity at the plant gate exceeds 3.0 $kgCO_2e/kg\ H_2$, it would be challenging for the H_2 supply chain scenarios assessed to meet the EU limit of 28.2 gCO_2e/MJ. In the case of blue H_2 productions, this suggests the need for minimising CH_4 leaks from the NG supply chain as well as enabling more than 90 % effective CCS capture rate.

4. Discussions on study perimeter and study results within policy frameworks

As with any prospective modelling exercises, we have had to make several assumptions on future technological progress, as well as supply chain performances that could have an impact on the overall findings reported. Given the complexity of the supply chains involved, and the lack of actual measurement data, uncertainties were associated with the analyses presented here. In order to take into account the variability of the parameters and their repercussion on the results, the study evaluated the impacts of changes in several supply chain assumptions, including concurrent variations of multiple parameters. Key parameters that were varied systematically include: (a) Grid electricity emission factors in Section 3.4, (b) producing/destination markets (transportation distance between countries) in Section 3.5, (c) inclusion/exclusion of boil-off gas recovery in Section 3.6, and (d) H_2 production efficiency and associated production emissions for green, blue, and grey H_2 in Section 3.7. Overall, over 10,000 key H_2 supply chain scenarios and sensitivities were assessed in this work and, throughout the paper, we offered critical discourses on the sensitivity of our findings to these key parameters. The primary sources of uncertainty in the emission estimates were found to be fuel/carrier production methods, H_2/CH_4 losses, and fuel and electricity emissions factors.

Furthermore, the scope of this work is limited to low-carbon gaseous synthetic fuels. Low-carbon gaseous fuels from biomass sources and nuclear power plants were excluded from this analysis. However, these could be important niche pathways for some countries and the downstream processes assessed in this study could be applicable to other low-carbon gaseous fuel production approaches too. Our findings reveal that technologies could help mitigate a large part of these supply chain emissions. Therefore, it isn't prudent to generalise the CO_2 attributes of H_2 purely on the basis of feedstock, as both blue and green H_2 pathways can be above and below the regulatory thresholds. Moreover, while this study demonstrates that the GHG emissions for delivered H_2 is expected to decline with time, it is premature to suggest a more stringent emissions threshold as it is unclear how much cross-border H_2 value chains will actually be realised. Considering the low success rates of prior green H_2 and some climate change mitigation projects [79–82], it is advisable

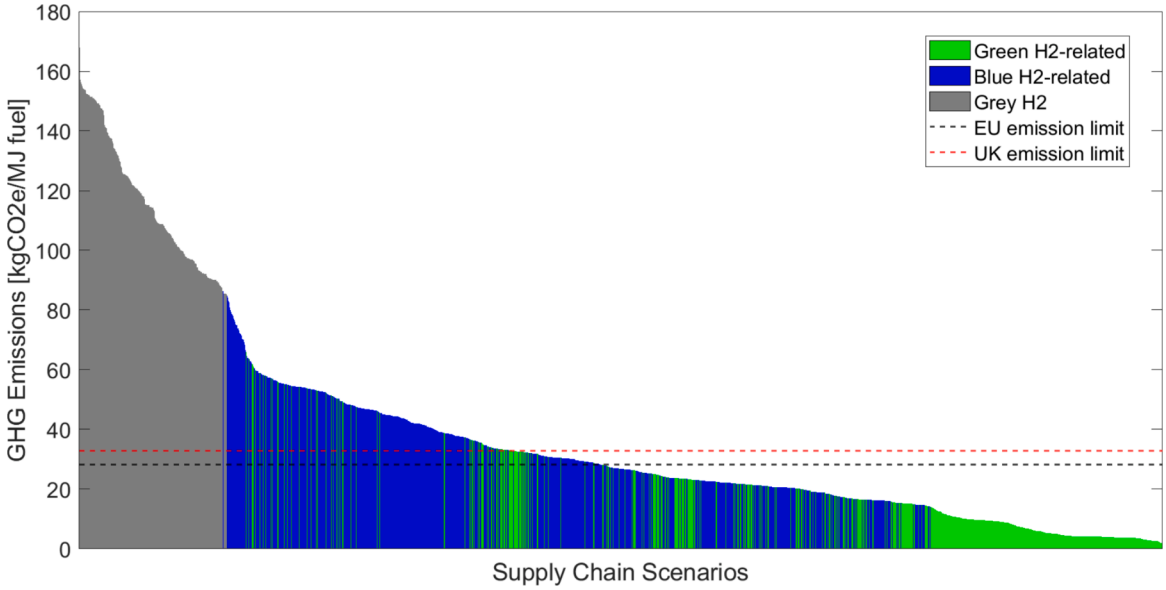

Fig. 6. Overall GHG emissions (without embodied emissions) from H_2 production technologies drawn from over 2000 key transport and heating supply chain scenarios in 2025, 2030 and 2050. Note: Two blue H_2 production emission scenarios were analysed for 2050 (a) Average blue H_2 production emission factor of 2.0 $kgCO_2e/kg\ H_2$ at the plant gate and (b) IEA BAT production emission factor of 1.5 $kgCO_2e/kg\ H_2$ at the plant gate without embodied emissions, based on IEA [78] and Longden et al. [77]. See SI 2 & 3 for additional information. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

for regulations to allow a broad range of solutions – including fossil fuel-based LCFs – to narrow the implementation gap.

Crucially, this underscores the need for LCA-based certification that is asset-specific and supply chain-specific for demonstrating compliance against regulatory limits or H_2 standards globally. LCA-based certificates that are asset-specific and supply chain-specific are beyond the scope of our work and will require further research and development. Amongst others, tools such as radio frequency identification (RFID) and a universal database of approvals could emerge as potential approaches for improving supply chain traceability. However, a key requirement would be the need for mutual acceptance and recognition of supply chain certificates by respective jurisdictions worldwide. More efforts will be required to accelerate progress towards a mutual recognition of certification schemes for H_2 and its derivatives, consistent with the COP28 declaration of intent in 2023 [83]. Without mutual recognition, the proliferation of H_2 standards worldwide could risk increasing the cost of certifications and compliances. This is on top of the already high anticipated levelised cost of H_2 delivered [84], especially when considering cross-border value chains. Recent regulatory trend towards a more prescriptive H_2 policy, such as the adoption of the principle of additionality and hourly time-matching requirements for green H_2, will likely increase the green premium for H_2 use [85]. H_2 economy, in its nascent stage, will require policies that are less complex, lower uncertainty, and less restrictive to support its production, delivery, and uses worldwide.

5. Conclusion

This paper addresses several pertinent questions relating to the global supply chains of H_2 and H_2-based fuels by summarizing insights from 17 key pathways drawn from over 10,000 scenarios and sensitivity cases. The analyses focused on H_2 productions from key renewables-rich regions [Saudi Arabia (SA), Nigeria (NG), Chile (CL), Morocco (MR), Algeria (AL), and Australia (AU)] and transporting it via different modes to European markets, using a variety of chemical carriers and physical states including compressed H_2 (CH2), liquefied H_2 (LH2), SNG, methylcyclohexane (MCH), ammonia (NH_3), and methanol (MeOH). We discussed the implications on the overall energy efficiency, product losses throughout the supply chains, and life cycle GHG emissions from temporal, geospatial, and technological perspectives.

The losses of H_2 and SNG throughout the supply chains are estimated to be in the range of 0.8–11.0 % per kg of gaseous fuel delivered at the station, with the AU to NL route having the highest loss rates due to the longest transport distance involved. For the scenarios assessed, the highest gaseous fuel leakage is obtained in LH2 systems without boil-off recovery technologies due to the boil-off of H_2 during storage and transportation. Typically, losses primarily arise from fuel production, boil-off in storage and transport facilities, and leakage in pipeline and equipment casing. However, we showed that the mitigation of boil-off losses through the use of dual fuel and liquefaction technologies could lead to significant GHG reductions. Other sources of loss which do not go into the environment include by-product formation.

The total energy consumption in delivering H_2 and SNG is in the range of 1.8–3.6 MJ per MJ of fuel product. Supply chains delivering H_2 as LH2 and CH2 had the lowest energy consumption, while those using chemical carriers, especially MeOH and SNG, had the highest energy consumption due to the energy losses in producing and reconverting the carriers.

The life cycle GHG emissions of the H_2 delivered to Europe can vary between 2 and 40 gCO_2e/MJ in 2050, and when embodied emissions are included, this can add up to 9–45 gCO_2e/MJ. The GHG emissions of H_2 vary significantly due to technological, design and operational factors, which are primarily driven by fuel/carrier production methods, H_2/CH_4 losses, and fuel and electricity emissions factors. Matching producer and consumer locations could significantly impact GHG emissions of H_2 and SNG, causing emissions from the same supply chain type to even double or triple in some cases due to the transport distances involved, renewable electricity generation capacity factors, and the emissions profile of the domestic grid electricity. Technologies can also have a large impact on the overall GHG emissions: the implementation of boil-off gas recovery systems in storage facilities and using dual fuel engines that utilise synthetic fuel along with onboard H_2 or SNG, which would otherwise be vented, can reduce GHG emissions considerably. Supply chain considerations, including the creation of a centralised/decentralised reconversion facility, whether at import terminals, distribution centres, or fuel dispensing stations, were found to affect the overall GHG emissions, which presents an opportunity for overall network design optimisation. The use of chemical carriers had the highest GHG emissions, primarily due to the grid electricity emission factors from the reconversion (or H_2 liberation) step. However, delivering H_2 in the form of MCH, in particular, could be more GHG intensive due to the return trip of the toluene carrier back to the production plant for it to be reused, thus increasing the total transport emissions. Over time, the overall GHG emissions associated with the delivery of low-carbon H_2 are expected to decline due to technological improvements and grid decarbonisations.

Our analyses found that supply chain emissions can be significant: even when starting with H_2 with a low carbon intensity at the plant gate, the emissions associated with the supply chain can drive the emissions above the EU and UK regulatory limits. Still, it isn't prudent to generalise the CO_2 attributes of H_2 purely on the basis of feedstock, as both blue and green H_2 pathways can be above and below the regulatory thresholds. This paper further adds to the body of evidence pointing to the need for LCA-based certification that is asset-specific and supply chain-specific for demonstrating compliance against regulatory limits or H_2 standards globally. Lastly, the results of this study should be used with a wholistic assessment of emissions mitigation strategies to find the best emission limits for achieving climate targets.

CRediT authorship contribution statement

Sylvanus Lilonfe: Writing – original draft, Visualization, Validation, Software, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization, Writing – review & editing. **Carlos A Jimenez Cortes:** Writing – review & editing, Validation, Resources, Methodology, Conceptualization. **Madeleine Mitschler:** Writing – review & editing, Validation, Supervision, Resources, Methodology, Conceptualization. **Victor Gordillo Zavaleta:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Methodology, Conceptualization. **Amir F.N. Abdul-Manan:** Writing – review & editing, Validation, Supervision, Project administration, Methodology, Funding acquisition, Conceptualization. **Ioanna Dimitriou:** Writing – review & editing, Validation, Supervision, Methodology, Conceptualization. **Jon McKechnie:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Methodology, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: [Sylvanus Lilonfe reports financial support was provided by Engineering and Physical Sciences Research Council (EPSRC). Sylvanus Lilonfe reports financial support was provided by Saudi Aramco. If there are other authors, they declare that the research was funded jointly by the EPSRC, the University of Nottingham and Saudi Aramco Technologies Company through the Centre for Doctoral Training in Resilient Decarbonised Fuel Energy Systems (Grant Code EP/S022996/1)].

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Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.enconman.2025.119803.

Data availability

The data supporting this article have been included in the supplementary documents – SI 1, 2 and 3.

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8 Life cycle assessments of liquid electro-fuels technologies

This chapter contributes to the overall thesis aim of assessing low-carbon fuel and chemical technologies by examining the life cycle environmental impacts of liquid electro-fuels and chemicals supply chains, including ammonia, methanol, gasoline, diesel and kerosene, across different policy, technical, geographical and temporal perspectives. The paper is the most comprehensive study to date on the life cycle greenhouse gas emissions impacts of liquid electro-fuels and chemicals.

The manuscript summarises key insights drawn from over 10,000 cases, analysing the supply and delivery of liquid electro-fuels and chemicals using different production and delivery approaches. It delivers important and original contributions in many ways, including 1) creating innovative and integrated methodologies for liquid electro-fuels productions and life cycle assessment, including with and without embodied infrastructure emissions; 2) assessing the use of key centralised and decentralised production approaches for electro-fuels life cycle energy demand and greenhouse gas emissions minimisation 3) analysing a set of H_2-related supply chain options, including renewable and grid electricity-based H_2 for electro-fuels, over different continents to determine the impacts of international trade on the life cycle environmental impacts of low-carbon liquid fuels. It incorporates the impact of location factors to offer specific insights, especially for renewable energy sources; 4) assessing the dynamic impacts of low-carbon liquid fuel emissions over 3-time horizons [2025, 2030, and 2050] and 5) assessing key energy policies and their implications on low-carbon fuels. As a result, insights were drawn from over 10,000 cases, as the manuscript reports that the life cycle greenhouse gas emissions (excluding embodied emissions) of 100% renewable electro-fuel supply chains typically range from 1–21 gCO_2e/MJ in 2025, and this could reduce to 1–10 gCO_2e/MJ in 2050.

The work is under internal review before its submission for publication with the title “Life cycle assessment of global liquid electro-fuels and chemicals supply chains from technological, geospatial, and temporal perspectives.” It is presented as Chapter 8 in this work. The main supplementary information for the work, SI 1, is reprinted in Appendix A5. Other supplementary information, which provides specific details on the various scenarios assessed, SI 2, totalling approximately 290 pages, will be provided in the online version of the published work or upon request if the work is not published.

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Life cycle assessment of global liquid electro-fuels and chemicals supply chains from technological, geospatial, and temporal perspectives

Abstract

Using low-carbon intensity synthetic fuels instead of fossil fuels, particularly in hard-to-abate areas of transportation and industry, can help achieve net zero emissions and mitigate climate change. Due to the different production and downstream operations that could be used in synthetic fuels supply chains, it is important to understand their life cycle greenhouse gas emissions. This study assesses the life cycle H_2 losses, energy efficiencies, water consumptions and greenhouse gas emissions of liquid low-carbon electro-fuels supply chains in transport and manufacturing applications using a dynamic Excel-based tool that analyses over 10,000 supply chain scenarios. The total loss of H_2 to the environment, energy efficiencies and water consumptions in liquid electro-fuel supply chains typically ranged from 0.2–2.6% H_2 per kg fuel, 1.9–4.0 MJ per MJ fuel and 0.41–5.04 kg H_2O per kg fuel delivered, respectively. The greenhouse gas emissions (excluding embodied emissions) of renewable electricity-based liquid electro-fuel supply chains typically ranged from 1–21 gCO_2e per MJ in 2025, and could reduce to 1–10 gCO_2e per MJ in 2050, due to technological, design and operational factors. Using approaches that minimise the impact of fuel/carrier production methods, H_2 losses and fuel emissions factors by combining centralised and decentralised processes efficiently offered the lowest greenhouse gas emissions estimates with liquid electro-fuels, making the scenarios using centralised fuel production approaches to perform well due to the high mass and energy density of the liquid electro-fuels which favours both short and long supply chain distances. Overall, the greenhouse gas emissions of all the renewable electricity-based liquid electro-fuels assessed were within EU/UK emission limits for transportation, which exclude embodied emissions. Furthermore, our analysis also indicates that existing policy definitions of low-carbon fuels are restrictive, potentially excluding viable production pathways that could significantly contribute to emission reductions and broader decarbonisation goals.

Keywords: Life cycle assessment, Greenhouse gas emissions, Low-carbon electro-fuels, Supply chains, Energy policies

Abbreviations

AL: Algeria

AU: Australia

BAT: Best available technology

BEV: Battery electric vehicle

CL: Chile

DAC: Direct air capture

E-fuel: electro-fuels

FT: Fischer-Tropsch

FTS: Fischer-Tropsch synthesis

FU: Functional unit

GHG: Greenhouse gas

LCA: Life cycle assessment

LCF: Low-carbon fuel

LH2: Liquid hydrogen

MeOH: Methanol

MR: Morocco

MTG: Methanol-to-gasoline

MTK: Methanol-to-kerosene

NG: Nigeria/natural gas (depending on context)

NL: Netherlands

NOx: Nitrous oxides

RFBO: Renewable fuels from biological origin

RFID: Radio Frequency Identification

RFNBO: Renewable fuels from non-biological origin

SA: Saudi Arabia

SAF: Sustainable aviation fuel

SNG: Synthetic natural gas

1 Introduction

Currently, approximately 50 $GtCO_2e$ are emitted annually into the atmosphere by anthropogenic activities, mostly arising from the transport and industrial sectors [1]. There is no silver bullet for reducing the emissions of greenhouse gases (GHGs) from industrial and transport sectors globally, though there are several promising low-carbon technologies that are gaining momentum amongst policymakers and industry players worldwide. For instance, decarbonising the transport sector will require a diverse set of solutions, including battery-electric vehicles (BEVs), advanced hybrid vehicles, sustainable biofuels, and electro-fuels (e-fuels).

E-fuels, often referred to as renewable fuels of non-biological origin (RFNBOs), are typically derived from (i) electrolysis using (renewable) electricity in the case of e-H_2 or (ii) the combination of (renewable) e-H_2 with another (renewable) feedstock (e.g., green CO_2 or N_2) in the case of other e-fuels (e.g., e-gasoline and e-NH_3). However, renewable fuels are defined differently between regions, increasing complexity when fuels are supplied to more than one destination. For example, the regulations by the UK RTFO, which are backed by law in the UK, defined RFNBOs to have 100% renewable energy from non-biological renewable origin [2], [3]. In contrast, EU policy definitions do not strictly specify the renewable energy source composition of feedstocks [4], [5], [6], [7]. Consequently, UK RTFO gives rise to other fuel classifications such as partial RFNBOs, partial renewable fuels of biological origin (RFBOs or biofuels), etc. Partial RFNBOs are defined by the UK RTFO to be fuels that have 1–99% of their energy content from renewable energy of non-biological origin [2], [3]. It is thus very important to define the source and process of e-fuel production properly, as definitions differ from one location to another, especially in international supply chains, and when emission limits vary by fuel classification. Additionally, the UK definition makes it operationally challenging for renewable fuel supply chains 1) due to the different possible combinations of energy sources that could be used in LCFs production 2) current approaches for mitigation of transient plant operational difficulties, e.g.,

plant start-ups and process disruptions and 3) mitigating the issue of electricity congestions that have seen around 3% of renewable electricity curtailment globally [8], [9]. The EU definition and regulation [4], [6], [7], which does not emphasise the final fuel's energy content and also allows for grid electricity to be used in stabilising process upsets, places more emphasis on the requirement of satisfying the emission limits of 28.2 gCO_2e/MJ fuel. This offers a more operationally friendly approach that could quickly drive up actions towards achieving emissions targets. However, the EU regulation also does not address the different possible approaches that can be used to produce LCFs, such as MeOH that could be produced from a mix of renewable and blue H_2 reacting with biogenic/DAC CO_2. Some of these approaches can help mitigate the variability of renewable electricity with low emission implications. Therefore, it is crucial to develop LCFs policies that encompass various production approaches and promote the optimal use of resources, as this can facilitate the achievement of climate targets and circular economy goals.

Currently, e-fuels have emerged as a promising complement to BEVs and biofuels because of their advantages. These advantages include compatibility with existing technologies, the ability to be integrated into current fossil fuel systems, and their potential as chemicals for long-term renewable energy storage. It is these recognitions and advantages that have led policymakers, including the EU [4], [5] and the UK [2], to introduce policies supporting e-fuels utilisation in transport. The EU regulations require that RFNBOs (e-fuels) achieve a minimum 70% reduction in GHG emissions compared to the fossil fuel benchmark of 94 gCO_2e/MJ [4], [5], [6]. This means that the life cycle GHG emissions of an RFNBO-qualified fuel must not exceed 28.2 gCO_2e/MJ. Similarly, the UK RTFO requires RFNBOs to achieve a minimum 65% GHG reduction, equivalent to a maximum emission threshold of 32.9 gCO_2e/MJ [2], [3]. In contrast, the UK SAF (Sustainable Aviation Fuel) mandate allows a higher emission limit of 53.4 gCO2e/MJ, representing a 40% reduction compared to conventional jet fuel, for RFNBOs used as SAFs [10]. However, currently, there is no policy regulating GHG emissions from fuels and chemicals in the manufacturing sector and its associated downstream sectors.

Like other low-carbon technologies, e-fuels face numerous challenges. E-fuels are generally still more expensive to produce than conventional fuels, and their production in renewable-scarce regions in some parts of Europe may not be cost-competitive compared to other global locations [11], [12]. Furthermore, local demand in the EU will likely outstrip the domestic production capacity of renewable energy [4], [11], [13]. Hence, producing LCFs in regions with higher renewable energy generation potential and with lower cost of production, for example, in the Middle East and North Africa, and transporting them to Europe, is considered a potential cost-competitive approach [11], [12]. However, since complex and multinational supply chains are involved, with variable geography-specific factors that could significantly affect renewable electricity generation potential, it is crucial to understand the efficiency and GHG emissions of producing and transporting different liquid e-fuels across various locations, especially within the context of regulatory limits for well-to-user emissions. Hence, this work aims to assess the emissions from these different supply chains.

2 Limitations of existing literature and research aims

The life cycle GHG emissions of synthetic fuels can range from as low as -175 gCO_2e/MJ for renewables with carbon capture & storage to more than 50 gCO_2e/MJ in some scenarios (e.g., H_2 carriers scenarios) [11], [14], [15], [16]. Generally, the GHG emissions of synthetic fuels can differ substantially, particularly given the varied design and operational factors, namely: H_2 production method, transformations for transport and storage, transportation modes and distances, and the form of fuel and dispensing method at the point of delivery to the user. Our previous paper demonstrated the wide range of GHG emissions arising from the production and supply of gaseous synthetic fuels under several scenarios, both including and excluding the embodied GHG emissions associated with the infrastructure [16]. While our previous study is limited to gaseous synthetic fuels – H_2 and synthetic natural gas (SNG) – for transport, heating and manufacturing applications, their supply chains could differ significantly from those of liquid synthetic fuels, which is the focus of this study. Additionally, while there are many existing studies on liquid synthetic fuels, there are

several important limitations with these prior works, for example: (i) A lack of details or limited assessments of geography-specific factors, e.g., renewable resource intensity [17], [18], [19] and national or generic market distances [19], [20], [21], which are particularly crucial for modelling renewable energy systems and (ii) the underlying fuel production assumptions [11], [15], [20], [22], which may not reflect the more pragmatic synthetic fuel production approaches, such as the use of synthetic fuels obtained from both renewable and grid electricity, that have the potential to shape fuel production pathways and policies significantly. A combination of grid and renewable electricity could be used in e-fuels production for several reasons, including marginally to stabilise process operations and in a significant portion to manage demand. Additionally, some fuel production approaches that utilise biogenic CO_2, like MeOH produced by combining renewable electricity H_2 with renewable biogenic CO_2, have received limited attention in the existing literature despite their potential and the global demand for MeOH of 170 MT in 2022. Almost 100% of the supply volumes of MeOH currently come from traditional pathways [23]. Nevertheless, significant volumes of biogenic CO_2 from fermentation plants – at least 69 $MtCO_2$ per annum from the bioethanol plant alone – are released into the atmosphere despite having a high purity of 99% CO_2 volume fraction [24], [25], [26]. This CO_2 could instead be utilised to produce low-carbon synthetic fuels and chemicals, which could improve circularity and sustainability, as well as reduce emissions.

Furthermore, fuel production and reconversion approaches, such as centralised and decentralised approaches, can have significant impacts on GHG emissions and costs, as identified in our previous publications [16], [27], [28]. Using centralised liquid fuel production approaches, which involve producing the fuel in one location and distributing it, is widely investigated in the literature [11], [29], [30], [31], [32]. However, decentralised fuel production approaches where H_2 is produced and transported from another location and combined with local CO_2 (e.g., biogenic CO_2 from bioethanol and biogas plants) to produce the final fuel in the local market have not been widely studied. The high purity of biogenic CO_2 streams, especially those from bioethanol fermentation plants with a CO_2 volume fraction of 99%, means that the energy demand for their CO_2 capture is almost zero compared to other CO_2 capture processes [24], [25], [26]. Hence, decentralised fuel production approaches could find strong application in a diverse range of environments, especially given the current sustainability goal of a circular economy. Therefore, understanding the emissions associated with using centralised and decentralised approaches could help to drive down GHG emissions.

Here, we report the insights drawn from an extensive life cycle assessment (LCA) of a variety of low-carbon, liquid-based, e-fuel supply chains. We explore the life cycle H_2 losses to the environment, energy efficiencies, water consumptions and GHG emission intensities from production to final use of different liquid e-fuel supply chains. The study considers multiple parameters that are technology and location-specific, as well as different production approaches and the impacts of embodied infrastructure emissions. We cover a wide range of e-fuels, including NH_3, MeOH, gasoline, diesel and kerosene, whereby, to the best of our knowledge, some of these fuels have received little attention in the existing literature. Our assessment also assesses their effects across 3 time horizons, i.e., 2025, 2030, and 2050. Overall, we present here the insights drawn from over 10,000 cases covering diverse scenarios and parametric sensitivities related to the production and supply of low-carbon, liquid-based e-fuels. These findings aim to inform the development and discussions of a nascent industry that is increasingly recognised as a key enabler for the energy transition.

3 Methodology

The methods employed in the LCA were derived from ISO 14 040 and 14 044, which include goal and scope definition, inventory analysis, impact assessment and interpretation [33], [34], [35]. The study aims to assess the supply chain of liquid low-carbon e-fuels and estimate the key life cycle environmental impacts associated with their production, delivery, and use. The boundary of the study starts at the renewable electricity generation plant and terminates at the transport vehicle where the fuel is oxidised or the manufacturing industry plant gate where NH_3/MeOH is transformed into other, non-fuel products. A Microsoft Excel-based

tool was developed for this analysis, which was used to analyse tens of thousands of liquid low-carbon e-fuels supply chains, as summarised in Figure 1 and Table 1. The LCA analysis performed in this paper incorporates both geospatial and temporal dimensions, assessing the impacts of location-specific variables, technological factors, and changes in technology and emissions factors over time. Moreover, GHG emissions were calculated both with and without accounting for the embodied emissions from infrastructure, including delivery trucks and plant equipment. The GHG emissions factors used were based on 100-year global warming potentials (GWPs) obtained from the existing literature, including Ecoinvent (version 3.7.1), IEA [36] and DESNZ [37]. The study's functional unit (FU) is 1 kg of fuel at the fuel station or manufacturing industry, where the GHG emission intensities are reported in gCO_2e per MJ fuel and tCO_2e per t chemical. Additional methodologies used in this work can be found in Lilonfe et al. [16].

In total, this study presents 9 key scenarios summarising more than 10,000 scenarios and parametric sensitivities that were evaluated, see Table 1 for details. Figure 1 presents a graphic summary of the approaches used in the analysis, considering numerous scenarios to assess the impacts of:

(1) Technological factors and process improvements over time – 2025, 2030, and 2050. Key technological factors assessed included the use of either conventional fuels or LCFs in delivery vehicles in 2025, LCFs in vehicles in 2030 to 2050, improvement in electrolyser efficiency in 2050, and switching from NG heating to grid electricity, e-H_2 or SNG in 2050;

(2) Geography-specific location factors like solar intensity for fuel production and grid electricity in terminals. This study considered the production and transportation of liquid low-carbon e-fuel across global locations. We also assessed with more comprehensive details the delivery of fuels into Europe (UK and NL [Netherlands]) from various markets, namely: Saudi Arabia (SA), Nigeria (NG), Chile (CL), Morocco (MR), Algeria (AL), and Australia (AU). Additionally, the production, delivery and consumption of e-fuels within Europe (UK and NL) were assessed for comparison with those from international locations;

(3) Green H_2 sources with different electrolyser efficiencies. The electrolysis of H_2 using alkaline electrolysers at efficiencies of 65.4% in 2025 and 2030 and 75% in 2050 was evaluated to account for improvements in efficiency over time. Additional cases where both renewable and grid electricity could be used for fuel production were also assessed;

(4) Different final delivered fuel products: NH_3, MeOH, gasoline, diesel and kerosene;

(5) Different fuel production approaches, such as CO_2 hydrogenation to MeOH, methanol-to-gasoline (MTG), methanol-to-kerosene (MTK), and Fischer-Tropsch synthesis (FTS). Additionally, centralised and decentralised fuel production approaches where feedstock to final fuel conversion take place in single and multiple locations, respectively, were also assessed. Please see Sections 3.1 and 3.2 for additional details;

(6) Different transport modes including ships, pipelines, rails and trucks (see Section 3.3 for details);

Table 1: The summary of key scenarios assessed in this work

Scenario	**Fuel production approach**	**Transmission mode**	**Distribution mode**	**Additional description**
1	Centr. NH_3	Ship (as NH_3)	Rail/trucks	H_2, N_2 and final fuel (NH_3) production in a central location before transportation to the end-user
2	Centr. MeOH	Ship (as MeOH)	Rail/trucks	H_2, CO_2 and final fuel (MeOH) production in a central

Scenario	Fuel production approach	Transmission mode	Distribution mode	Additional description
				location before transportation to the end-user
3	Decentr. MeOH	Ship (as LH2)	Rail/trucks	Final fuel (MeOH) production in decentralised markets (e.g., bio-CO_2 to fuel) after LH2 transportation
4	Centr. MTG	Ship (as gasoline)	Rail/trucks	H_2, CO_2 and final fuel (gasoline) production in a central location before transportation to the end-user
5	Decentr. MTG	Ship (as LH2)	Rail/trucks	Final fuel (gasoline) production in decentralised markets (e.g., bio-CO_2 to fuel) after LH2 transportation
6	Centr. MTK	Ship (as kerosene)	Rail/trucks	H_2, CO_2 and final fuel (SAF) production in a central location before transportation to the end-user
7	Decentr. MTK	Ship (as LH2)	Rail/trucks	Final fuel (SAF) production in decentralised markets (e.g., bio-CO_2 to fuel) after LH2 transportation
8	Centr. FTS	Ship (as FT-liquids)	Rail/trucks	H_2, CO_2 and final fuel (FT-liquids) production in a central international location before transportation to the end-user
9	Decentr. FTS	Ship (as LH2)	Rail/trucks	Final fuel production (FT-liquids) in decentralised markets (e.g., bio-CO_2 to fuel) after LH2 transportation
Note: LH2 for liquid H_2 and FT for Fischer-Tropsch				

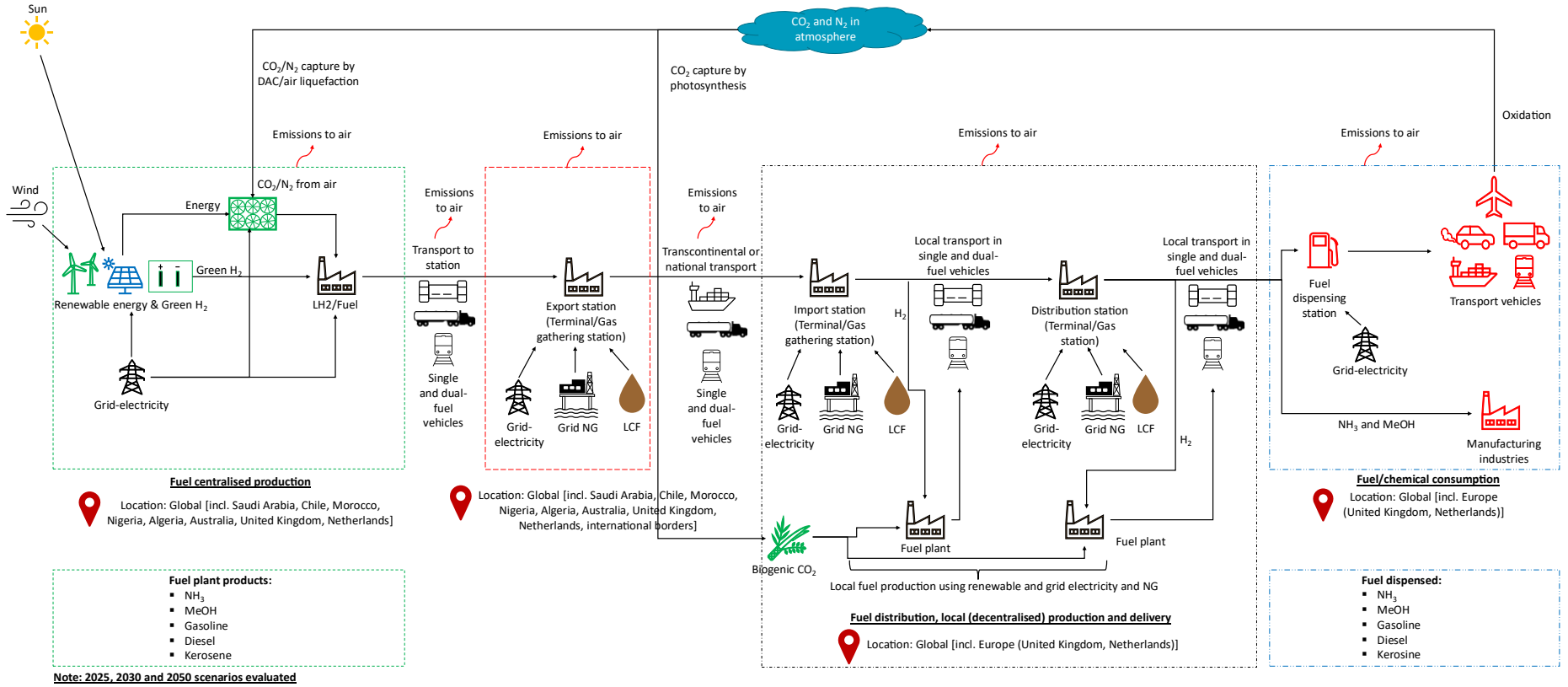


Figure 1: Summary of liquid low-carbon e-fuel supply chains analysed.

3.1 Fuel

This paper evaluates electricity-based NH_3, MeOH, gasoline, diesel and kerosene, which are produced using approaches, such as CO_2 hydrogenation to MeOH, MTG, MTK, and FT-liquids. The methods and assumptions for the H_2 production stage were based on Lilonfe et al. [16]. The reaction equation of green H_2 via electrolysis is shown in Equation (1) [11]. Emissions released from catalysts used in the fuel production are estimated to be less than 0.2 gCO_2e/MJ fuel [28], and are considered negligible, consistent with the UK Low Carbon Hydrogen Standard materiality threshold of 0.2 gCO_2e/MJ H_2 [38]. The CO_2 scenarios assessed included CO_2 capture via DAC using renewables in the centralised cases, and waste CO_2 in the decentralised cases, e.g., waste biogenic CO_2 from bioethanol and biomethane plants. The energy demand and emission factors of DAC CO_2 are presented in supplementary information (SI) 1 Table S3. Biogenic CO_2 were assumed to be sourced from bioethanol and biomethane plants, where CO_2 can be obtained as a waste product at 99% by volume purity, with a negligible capture energy requirement [24], [25], [26]. These assumptions relating to biogenic CO_2 can also be applied to flue gas CO_2 under certain conditions. Fuels produced by combining waste CO_2 and renewable electricity H_2 were regarded as e-fuels (RFNBOs), since the CO_2 is a waste that is often vented to the atmosphere and has zero energy content, consistent with both UK RTFO and EU policies [2], [3], [39]. N_2 used for NH_3 production was assumed to be obtained by air liquefaction, based on current commercial operations for N_2 production [11]. Table 2 shows the process, material, energy, and emission factor data used in the analysis. The process yields and other key process data are shown in SI 1 Table S2 and Table S3. Figure 1 and Table 1 present the supply chain scenarios of the liquid e-fuels evaluated. Additional methods and assumptions related to this work can be found in Lilonfe et al. [16].

Electrolysis: $2\ H_2O \rightarrow 2\ H_2 + O_2 \qquad \Delta H = +286\ kJ/mol$ (1)

Table 2: Key material, energy, and embodied emission factor data for fuel production.

Technology	Process conditions	Casing leaks/direct H_2 losses during fuel production		Electricity demand		Fuel/Heat demand		Embodied emissions		Reference
		Value	Units	Value	Units	Value	Units	Value	Units	
Electrolysis 65.4% (green) – basis H_2 at plant gate	T: 50–80 °C, P: Up to 30 bar	0.52%	per kg H_2	50.95	kWh/kg H_2	-	MJ/kg H_2	0.7167	$kgCO_2e/kg\ H_2$	[11], [14], [16], [40]
Electrolysis 75% (green) – basis H_2 at plant gate	T: 50–80 °C, P: Up to 30 bar	0.52%	per kg H_2	44.43	kWh/kg H_2	-	MJ/kg H_2	0.6249	$kgCO_2e/kg\ H_2$	[11], [14], [40]
Haber-Bosch process (traditional): NH_3	T: 400–500 °C, P: 150– 250 bar	0.09%	per kg fuel	0.60	kWh/kg fuel		MJ/kg fuel	Based on MeOH plant data on Ecoinvent	$kgCO_2e/kg$ fuel	[11], [40], [41]
Haber-Bosch process (electrochemical): NH_3	T: 25–250 °C, P: 1–10 bar	0.09%	per kg fuel	0.46	kWh/kg fuel		MJ/kg fuel	Based on MeOH plant data on Ecoinvent	$kgCO_2e/kg$ fuel	[40], [42], [43]
CO_2 hydrogenation: MeOH	T: 200–300 °C, P: 10–100 bar	0.15%	per kg fuel	0.28	kWh/kg fuel	-	MJ/kg fuel	Based on MeOH plant data on Ecoinvent	$kgCO_2e/kg$ fuel	[11], [40], [44]
Gasoline via MTG	T: 300–400 °C, P: 15–20 bar	0.44%	per kg fuel	0.83	kWh/kg fuel		MJ/kg fuel	Based on MeOH plant data on Ecoinvent	$kgCO_2e/kg$ fuel	[11], [44]
Kerosene via MTK	T: 300–400 °C, P: 15–20 bar	0.46%	per kg fuel	0.84	kWh/kg fuel		MJ/kg fuel	Based on MeOH plant data on Ecoinvent	$kgCO_2e/kg$ fuel	[11], [44]
FT-liquids via FTS	T: 190–350 °C, P: 1–50 bar	0.50%	per kg fuel	0.53	kWh/kg fuel	0.12	MJ/kg fuel	Based on MeOH plant data on Ecoinvent	$kgCO_2e/kg$ fuel	[11], [45]

Key: T- temperature, P- pressure

Note: The energy demands for Haber-Bosch process, CO_2 hydrogenation to MeOH, MTG, MTK and FTS presented in this table are the energy demands for the process (excluding other processes such as H_2 production, N_2 liquefaction and CO_2 capture via DAC). For details on other processes such as H_2 production, N_2 liquefaction and CO_2 capture via DAC, see H_2 production in this table and CO_2 and N_2 capture in SI Table S3.

MeOH is an important industrial feedstock for producing a wide range of products e.g., plastic and hydrocarbon fuel. Due to its high-octane rating of 114, it can also be used directly as a transport fuel in blended ratios of up to 100% MeOH by volume [46], [47]. However, the scenarios for MeOH usage as fuel in this work are limited to ship transportation and industrial applications due to MeOH's poisonous nature. The model for CO_2 hydrogenation to MeOH in Equation (2) and Table 2 was based on Concawe [11].

MeOH synthesis: $CO_2 + 3\,H_2 \leftrightarrow CH_3OH + H_2O \qquad \Delta H = -49.4\ kJ/mol$ (2)

NH_3 can be used directly as a transport fuel in ICEVs such as ships. However, its combustion poses some technical challenges, such as the slow combustion rate [48], [49] and nitrous oxides (NOx) emissions [50], which can result in lower engine performance and NH_3 slip. In the future, these issues are expected to be resolved as ongoing research has shown promising development [51], [52]. Hence, only scenarios for NH_3 applications in ship transportation and industrial applications were modelled in this work due to ammonia's toxicity. It was also assumed that ships would have space to mitigate NH_3 that slipped during combustion if engine mitigation approaches could not be achieved. Currently, NH_3 is mainly produced via the Haber-Bosch process, as shown in Equation (3). Other scenarios evaluated here include the electrochemical-driven Haber-Bosch process. Table 2 shows the material, energy, and emissions data used for NH_3 production.

NH_3 synthesis: $N_2 + 3\,H_2 \leftrightarrow 2\,NH_3 \qquad \Delta H = -92\ kJ/mol$ (3)

Synthetic "drop-in" fuels, such as gasoline, diesel and kerosene, can be produced via MTG, MTK, and FTS. In MTG and MTK, the CO_2 stream is first hydrogenated into MeOH and then further hydrogenated from MeOH to gasoline or kerosene via multiple reactions, as shown in Equations (4–6) [11], [53], [54]. In FTS, the CO_2 stream is first reduced to carbon monoxide before hydrogenation into long paraffins (Fischer-Tropsch reaction) and further hydrotreated and hydrocracked into FT-liquids (hydrocarbons), which include gasoline, diesel, and kerosene. The overall FTS reaction is shown in Equation (7) [11]. The data used for evaluating the production of synthetic gasoline, diesel, and kerosene is provided in Table 2.

Dimethyl ether synthesis: $2n\ CH_3OH \leftrightarrow n\ CH_3OCH_3 + n\ H_2O \qquad \Delta H = -10\ kJ/mol$ (4)

Olefin oligomerisation: $n\ CH_3OCH_3 \rightarrow 2\ (CH_2)_n, olefins + n\ H_2O \qquad \Delta H = -18.7\ kJ/mol$ (5)

Hydrocarbon synthesis: $2\ (CH_2)_{n,olefins} \rightarrow C_{2n}H_{4n,hydrocarbons} \qquad \Delta H = -16\ kJ/mol$ (6)

FTS: $n\ CO + (2n+1)\ H_2 \rightarrow H(CH_2)_nH + n\ H_2O \qquad \Delta H = -152\ kJ/mol$ (7)

3.2 Centralised and decentralised production approaches

The use of different fuel production approaches, such as centralised and decentralised fuel production approaches, has been reported to provide significant benefits in biofuel production [27], [28]. Here, we evaluated the impacts of centralised and decentralised fuel production approaches on the supply chains of e-fuels to determine the options with the lowest GHG emissions. The centralised fuel production approach scenarios assumed that fuel production (from feedstocks to fuel products) occurred in a single location (overseas or within Europe) and that the fuel was then transported and consumed in European markets. The decentralised fuel production approach scenarios assumed that feedstock conversion to fuel products took place in multiple locations, such as the production of fuel products (within Europe) using H_2 [from another location (either overseas or within Europe in this work)] and CO_2 from fermentation plants (within Europe). Here, the final fuel production plants in the decentralised cases were assumed to be co-located with waste CO_2 sources, e.g., fermentation plants. Practically, decentralised fuel production approaches may find strong applications in small to medium-scale and remote applications, such as biomass, biogenic and flue gas CO_2 conversion into fuel and chemical products. It was estimated that 69 $MtCO_2$ per annum of biogenic CO_2 is

emitted globally at 99% purity during ethanol production by fermentation [26]. Hence, this paper analysed various approaches, including e-fuel production by DAC and biomass/biogenic CO_2 hydrogenation.

3.3 Transportation

The transportation of e-fuels using various modes such as trucks, rails, pipelines, and ships was also assessed. Ships were used for the long-distance, intercontinental transportation of e-fuels, while trucks, rails, and pipelines were used for local and regional fuel transportation. Intercontinental shipping distances were obtained from Port.com. The use of fossil fuels and LCFs in fuel delivery vehicles were analysed to understand the impact of switching to low-carbon solutions. Moreover, LCFs like synthetic gasoline, diesel and kerosene are compatible with existing engines, enabling relatively easy deployment once produced at scale. The transport parameters used in the analysis are given in Table 3 and SI 1 Table S4 to Table S8. The embodied emissions for vehicles used in fuel delivery were based on data obtained from Ecoinvent. Figure 1, Table 1, Table 3, and SI 1 Tables S4 to S8 provide a summary of the transport scenarios analysed.

Table 3: Truck/trailer transportation parameters.

Trucks	**Units**	**as NH_3**	**as MeOH**	**as gasoline/diesel/kerosene**	**Data based on ref.**
Truck life	years	15	15	15	
Truck capacity	t (cargo)	31.5	35.7	36.6	[55]
Product stored pressure	bar	1	1	1	[56], [57]
Speed (loaded)	km/h	60	60	60	[44], [58]
Speed (unloaded)	km/h	70	70	70	
Delivery distance	km	400	400	400	
Travel time (loaded)	h	6.67	6.67	6.67	
Travel time (unloaded)	h	5.71	5.71	5.71	
Loading/unloading time	h	1.75	1.75	1.75	[44], [59], [60]
Total time	h	8.42	8.42	8.42	
Total time with empty return	h	14.13	14.13	14.13	
Total time with toluene return	h	15.88	15.88	15.88	
Energy consumption	MJ/kg fuel product/km	0.00107	0.00083	0.00081	[11]
Energy consumption with empty return	MJ/kg fuel product/km	0.00132	0.00105	0.00102	
Embodied emissions (single trip basis)	$kgCO_2e$/kg fuel product	0.00013	0.00011	0.00011	Trailer, Ecoinvent

3.4 Electricity

Both renewable and grid electricity were employed depending on the location and the type of process. Processes at the fuel production plant location used green electricity, while downstream processes used the grid electricity in that location, taking into consideration a decrease in the emissions of grid electricity between 2025 and 2050 (SI Table S17). For a hybrid of renewable and grid electricity used in the plant for fuel production, the grid electricity emission factors of that location were used in combination with those of renewable electricity. The emissions factors for renewable electricity without embodied emissions were

taken as zero, based on the UK Low Carbon H_2 Standard [38]. However, embodied emissions factors included emissions from infrastructures for wind turbines and solar panels used solely for fuel production (local power plants) and were calculated using Equations (8)–(10) and the methodology developed by Lilonfe et al. [16]. Grid electricity emissions factors for 2025 across the locations were obtained from the IEA's Stated Policies scenarios. The 2030 and 2050 grid scenarios were obtained from the IEA's Sustainable Development and Stated Policies scenarios. The grid electricity emissions factors for countries not found in the IEA report were determined based on the data outlined in the IEA's report and the region to which the countries belong; see SI 1 Table S11 for details. The embodied emissions associated with grid electricity were set to zero, consistent with existing LCA principles for public infrastructure, such as grid pipelines, roads, and airports, which are used for numerous purposes that usually make co-allocated emissions immaterial. SI 1 Table S11 to Table S17 summarise the electricity emission factors used in the study.

Local power plant embodied emissions factor: $EF = \frac{Emissions\ from\ constructing\ power\ plant}{Annual\ power\ generated \times life\ time\ of\ power\ plant}$ (8)

Wind turbine design equation: $P_T = 0.5 \cdot \rho \cdot A_T \cdot C_P \cdot v^3$ (9)

Where, P_T is the power generated by the turbine in W, ρ is the air density at the hub height in kg/m^3, A_T is the rotor swept area in m^2, C_P is the overall efficiency coefficient (power coefficient) that changes with both wind speed and turbine rotational speed in %, and v is the wind speed in m/s. The design parameters of the turbine are shown in SI 1 Table S14.

Solar PV design equation: $E_{PV} = A_{PV} \cdot E_{sun} \cdot \eta_{PV} \cdot PR$ (10)

Where, E_{PV} is the energy produced by the solar PV in kWh, A_{PV} is the area of the solar PV in m^2, E_{sun} is the Global Horizontal Irradiation (GHI) in kWh/m^2, η_{PV} is the solar PV efficiency, and $PR = (1 - system\ loss)$ is the performance ratio, the coefficient for losses. The design parameters of the solar PV are shown in SI 1 Table S15.

3.5 Fuel use

The assessment of the fuel use stage assumed that the oxidation of 1 kg of fuel in any burner or engine type produces the same oxidation products (emissions), whether the engine is stationary or mobile. The emissions factors for the combustion of gasoline, diesel and kerosene were obtained from DESNZ and BEIS [61], which assumes negligible variation in emissions by engine type. This approach further assumes that fuel combustion returns the CO_2 initially captured at the initial fuel production stage and only accounts for other emissions, such as CH_4 and N_2O emissions, from the combustion of these fuels. The oxidation of NH_3 is taken to emit zero GHG by emitting 100% H_2O and N_2. However, NOx are emitted during NH_3 combustion in practice. As reported in the literature [62], [63], [64], NH_3 combustion emits between 25 and 5000 ppm of NOx, compared to 50 to 1000 ppm from diesel combustion. Based on DESNZ and BEIS [61] emission factors, this corresponds to a maximum of 0.0001 kgCO_2e per kg of NH_3 (0.005 gCO_2e/MJ). This emission figure is immaterial, based on the UK Low Carbon Hydrogen Standard materiality threshold of 0.2 gCO_2e/MJ [38]. Furthermore, NH_3 combustion engines can be equipped with selective catalytic reduction units to mitigate NOx emissions, which was considered in this work. Using data from Ecoinvent, the emissions for constructing delivery vehicles were considered when estimating GHG emissions with embodied emissions [SI 1 Table S20]. Transportation via road, rail, water, and air involves trucks, trains, ships and aircraft, respectively.

4 Results and discussions

4.1 Present day emissions

The life cycle GHG emissions for all key scenarios assessed in this study are provided in SI 2. In sections 4.1 to 4.3, we present only the scenarios for 100% renewable electricity-based liquid e-fuels supply chains. The

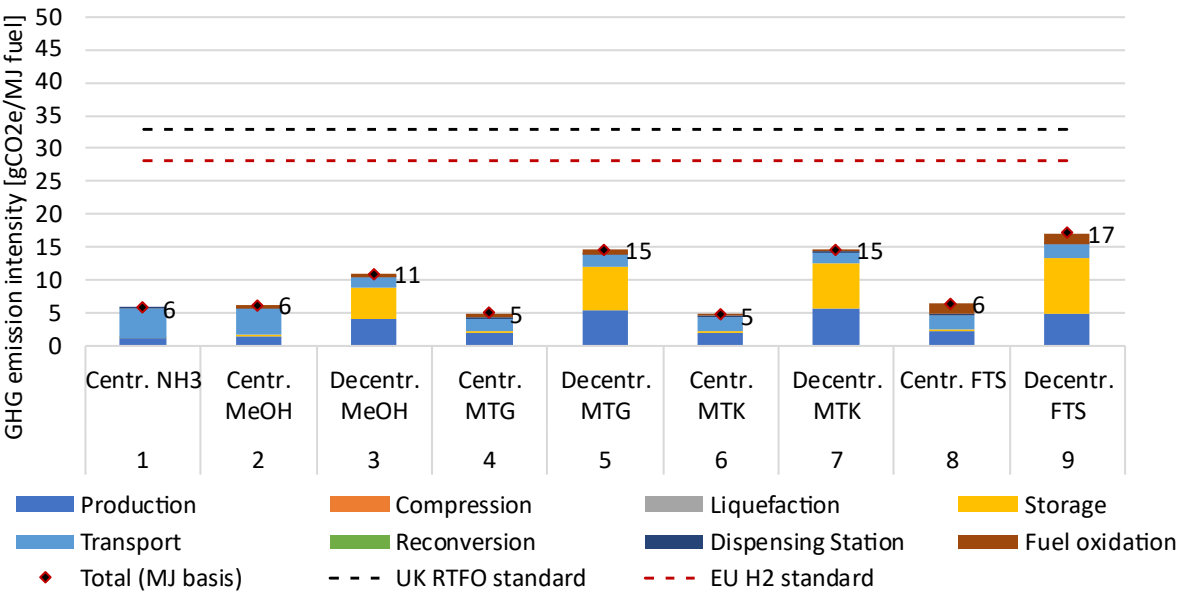
findings on GHG emissions for the remaining scenarios are available in Sections 4.4 and SI 2. The general insights discussed here apply to these scenarios as well.

Figure 2 and SI 2 shows that GHG emissions from liquid e-fuel supply chains are strongly influenced by technology factors (design and operation), including fuel production method and centralised and decentralised production approaches, as well as LCA methodology (with or without embodied emissions).

For centralised approaches – where H_2, N_2 or CO_2, and final fuel are produced on a large scale in a single location – the main emissions sources are fuel production (1–2 gCO_2e/MJ) and transportation (0–7 gCO_2e/MJ). For decentralised approaches – where H_2 and CO_2 are produced in multiple locations with the final fuel produced inside the final market (e.g., in bio-CO_2 to fuel) – the main emissions sources are fuel production (4–7 gCO_2e/MJ), transport (0–5 gCO_2e/MJ) and (H_2) storage (0–10 gCO_2e/MJ) [Figure 2 and SI 2]. These emission categories are primarily driven by fuel/carrier production methods, H_2 losses and fuel emissions factors. It is important to note that in the decentralised cases, the final fuel plants were assumed to be co-located with the source of biogenic CO_2, e.g., bioethanol and biomethane plants; therefore, emissions from transportation of biomass or biogenic CO_2 were taken as zero (see Section 3.2 for details).

From all the scenarios assessed, the centralised liquid e-fuels scenarios had the least GHG emissions, with emissions for green liquid e-fuel scenarios of Scenario 1 [Centr. NH_3], Scenario 2 [Centr. MeOH], Scenario 6 [Centr. MTK], Scenario 4 [Centr. MTG] and Scenario 8 [Centr. FTS] being the lowest, ranging from 1–9 gCO_2e/MJ without embodied emissions and from 9–33 gCO_2e/MJ with embodied emissions. The centralised approaches for liquid fuel production offer an optimal solution for two major reasons. First, the high mass and energy density of the final liquid e-fuels produced at central plant locations helps minimise GHG emissions associated with transporting the fuels, even when the life cycle energy consumptions of the fuels from the decentralised approaches were lower than the corresponding scenarios from centralised approaches in this study (Section 4.5 and SI 1 Figures S10–S18). This also enables emissions of liquid e-fuels to be generally lower than those of gaseous synthetic fuels [16] despite the higher energy demand for their production. Second, centralised approaches exhibit significantly lower H_2 leakage (0.2–0.9% H_2 per kg fuel) compared to decentralised approaches (incl. those using H_2 from overseas) (0.3–2.6% H_2 per kg fuel) and gaseous fuel supply chains [16], as the main source of leakage in centralised approaches is the H_2 production stage (SI 1 Figures S1–S9). The main sources of leakage in the decentralised approaches are the H_2 production stage and the H_2 transport distance associated with the final fuel. Since H_2 has a higher GWP than CO_2, even small leakages can substantially increase the total GHG emissions of a supply chain. Hence, by using high-mass and energy-density fuels and avoiding H_2 losses along downstream supply chains, the centralised approaches performed better. Currently, there are no emission limits for NH_3 and MeOH in industrial applications; however, several policies exist for e-fuel applications in the transport sector. Without embodied emissions, which is the methodology currently adopted by EU and UK RTFO regulations for transport fuels, the emissions (ranging from 1–21 gCO_2e/MJ) in 2025 from all 100% renewable electricity-based, liquid e-fuel supply chains could meet the GHG emissions limits in the EU and UK.

(a)



(b)

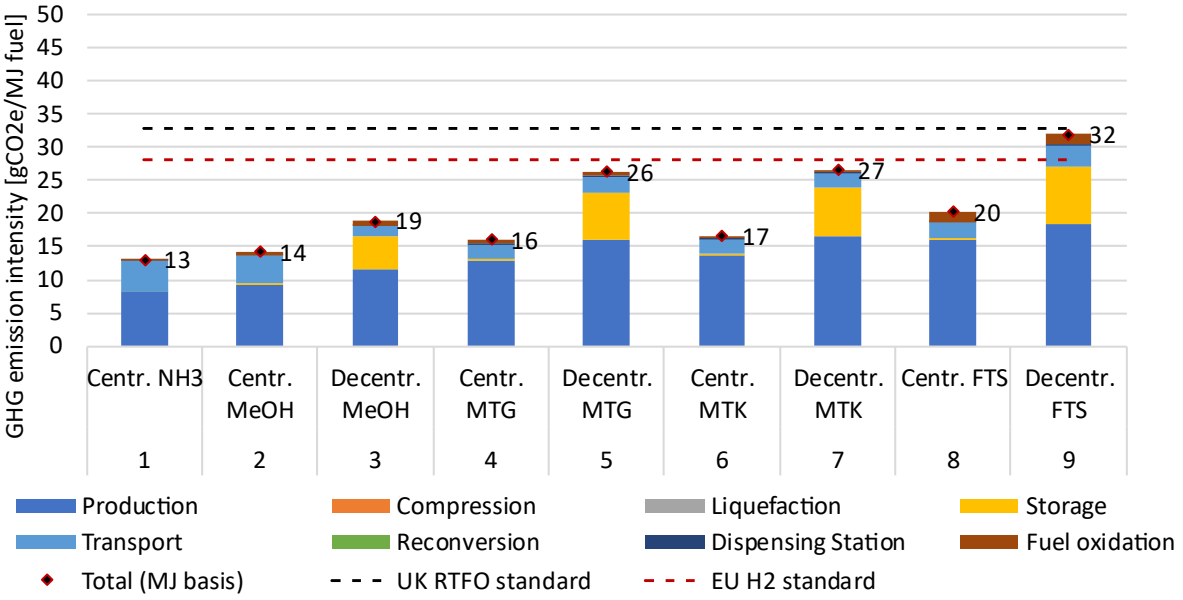


Figure 2: GHG emissions of key 100% renewable electricity-based liquid e-fuels supply chains for the SA to UK in 2025 (a) Excluding infrastructure embodied emissions and (b) Including infrastructure embodied emissions. Despite the higher energy demand of the liquid synthetic fuels compared to gaseous synthetic fuels, their emissions are less than those of gaseous synthetic fuels [16] due to their higher mass and energy densities and avoidance of downstream H_2 and CH_4 losses, which minimise their downstream and overall emissions. Hence, assessing other factors such as cost, infrastructure, and demand for liquid and gaseous fuels/chemicals across different industries and locations is crucial in establishing an effective and efficient fuel deployment strategy. The 2025 scenarios presented here were based on fossil fuel use by delivery vehicles. For additional details on delivery vehicles that use LCFs in their engines in 2025, see SI 2. Note: The UK RTFO emission limit for SAF in aviation is higher than that in non-aviation transport, and it is currently set at 53.4 gCO_2e/MJ.

The total life cycle emissions, when accounting for embodied emissions, are 1.9 to 10.3 times higher than those of corresponding scenarios that exclude them, ranging from 9–33 gCO_2e/MJ (Figure 2 and SI 2). These estimates exclude embodied emissions of the decentralised scenarios, in line with ISO standards, since the scenarios are parallel scenarios where H_2 will be produced for the general market for any application. The leading cause of these differences is the embodied emissions from wind and solar PV infrastructures. But the methodologies of EU and UK regulations do not include embodied emissions from infrastructure. Generally, the supply chains assessed would meet the EU and UK RTFO regulatory emission limits of 28.2 gCO_2e/MJ and 32.9 gCO_2e/MJ, respectively, in 2025. However, a few of the scenarios from FTS may not meet EU regulations. This further demonstrates the importance of liquid fuels over gaseous fuels, as gaseous fuels' embodied emissions, even for green cases, could exceed 80 gCO_2e/MJ [16].

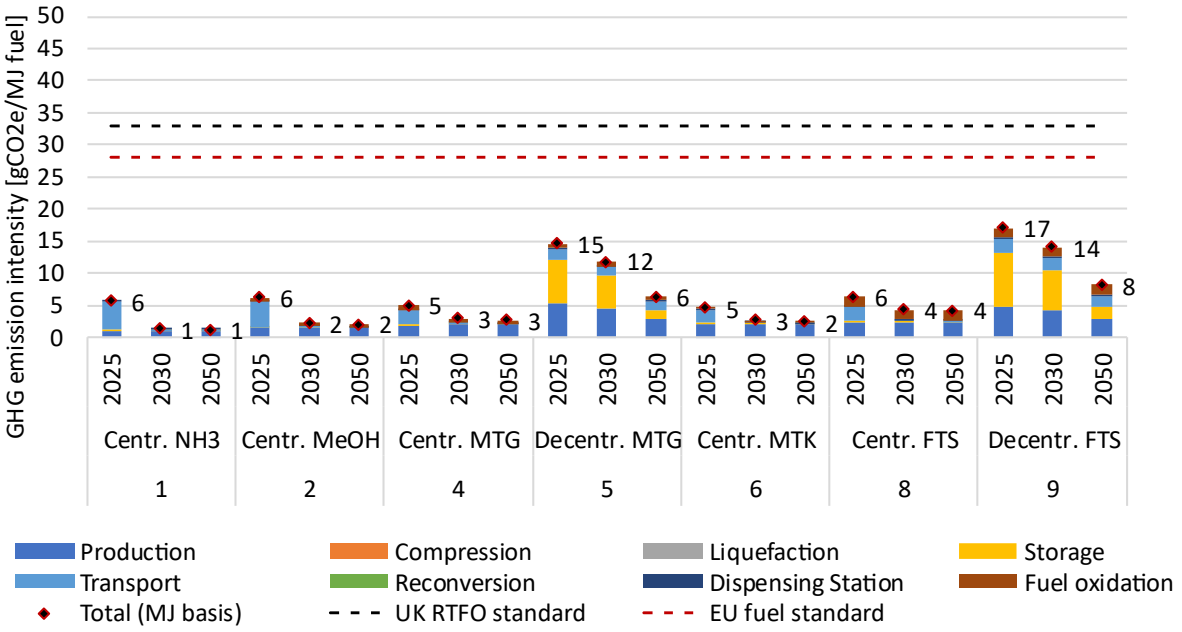
Furthermore, comparing this study's estimates with the literature, other studies reported the GHG emissions (without embodied emissions) of renewable electricity-based liquid e-fuels from centralised production approaches ranging from 0.1–25 gCO_2e/MJ [11], [32], [65]. Hence, this study's estimates (without embodied emissions) of 1–21 gCO_2e/MJ align well with existing literature. However, direct qualitative comparisons should be made with caution due to the diverse methodologies and assumptions adopted by existing studies. For example, Concawe [11] reported well-to-tank emissions (without embodied emissions) for centralised fuel production approaches of 1–2 gCO_2e/MJ in 2020 for NH_3, MeOH, MTG, MTK and FT-liquids. In addition to the Concawe study's boundary of well-to-tank vs entire life cycle in this study, the study does not account for H_2 losses to the environment during H_2 production in e-fuel supply chains. Although H_2 losses may be small, typically 0.52% per kg H_2 produced [40], H_2 is an indirect GHG with a GWP much higher than CO_2 [66]. These factors partly drive emissions from corresponding centralised scenarios in this study to be slightly higher than Concawe's estimates, ranging from 1–9 gCO_2e/MJ in 2025. Other studies, such as the study by IEA [65], reported NH_3, MeOH and FT-liquids GHG emissions of 2–25 gCO_2e/MJ. Apart from only electricity-based emissions being considered in the IEA [52] analysis, little information is provided on the LCA methodology, such as the type of production approach (centralised or decentralised) and location factors, which can have a significant impact on emissions. The decentralised fuel production approach for green H_2 derivatives here showed estimates in the range of 5–21 gCO_2e/MJ.

4.2 Projected future emissions

Figure 3 and SI 2 show that the lifecycle GHG emissions of 100% renewable electricity-based liquid e-fuels decline by corresponding scenarios over time (from 2025 to 2050), with overall emissions in 2050 ranging from 1–10 gCO_2e/MJ without embodied emissions and from 9–30 gCO_2e/MJ with embodied emissions, based on the IEA's ambitious Sustainable Development scenario. The reductions in emissions from 2025 to 2050 were mainly driven by the switch to LCFs in fuel delivery systems. The 2025 scenarios, when conventional fuel is used in delivery vehicles, have slightly higher emissions than the comparative 2030 and 2050 scenarios, however, this difference cancels out when synthetic fuels are used in delivery vehicles in 2025 (SI 2). Additionally, in decentralised approaches, there is a further reduction in emissions between 2030 and 2050 from storage and transportation (of H_2) due to the incorporation of boil-off gas recovery systems into storage facilities, and dual-fuel engines using onboard H_2, which would otherwise be vented. Unlike gaseous synthetic fuel supply chains [16], there is negligible variation in the GHG emission estimates when adopting the IEA's Stated Policies scenario, which only considers current national policies in the electricity emission factor estimates. This is due to the higher mass and energy density of liquid synthetic fuels compared to gaseous synthetic fuels, which significantly reduces downstream fuel and electricity consumption and GHG emissions. These insights further confirm those in Section 4.1 that the GHG emissions from liquid fuel supply chains are primarily driven by fuel/carrier production methods, H_2 losses and fuel emissions factors. Furthermore, from a regulatory perspective of transport fuels, all 100% renewable electricity-based liquid e-fuels supply chains could meet the EU RED and UK RTFO emissions limits from 2025 to 2050. Despite the EU and UK policies

being based on overall emissions without embodied emissions, the overall emissions with embodied emissions in 2050, which are 4.4–12.0 times higher than the corresponding emissions without embodied emissions, are generally within the EU and UK regulatory limits (Figure 3b and SI 2).

(a)



(b)

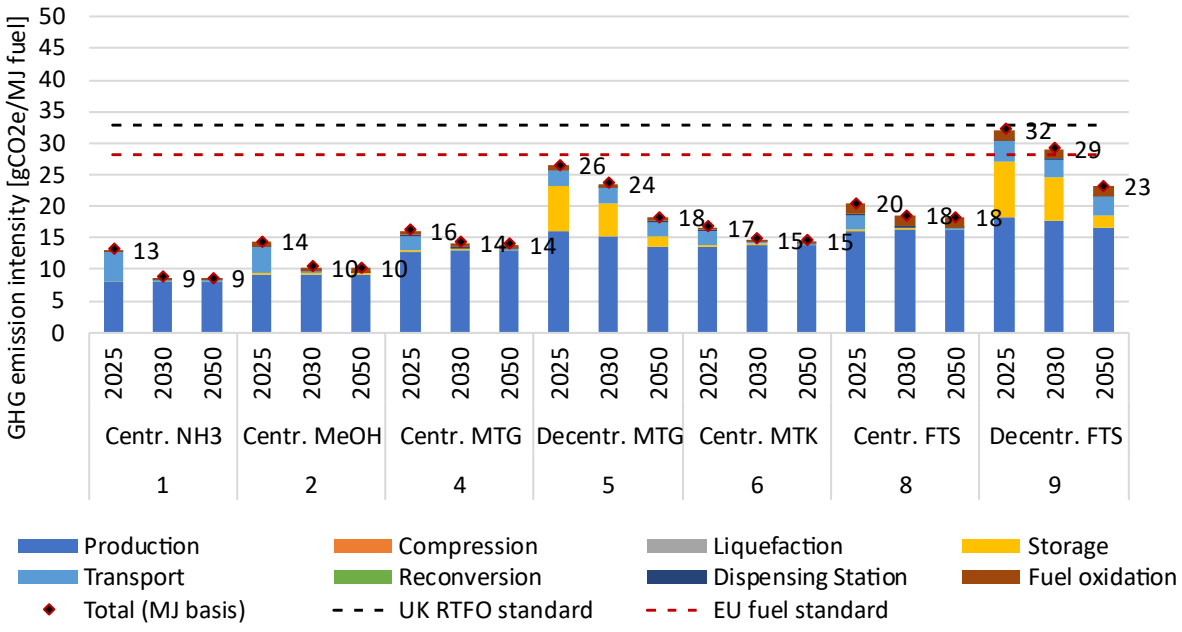
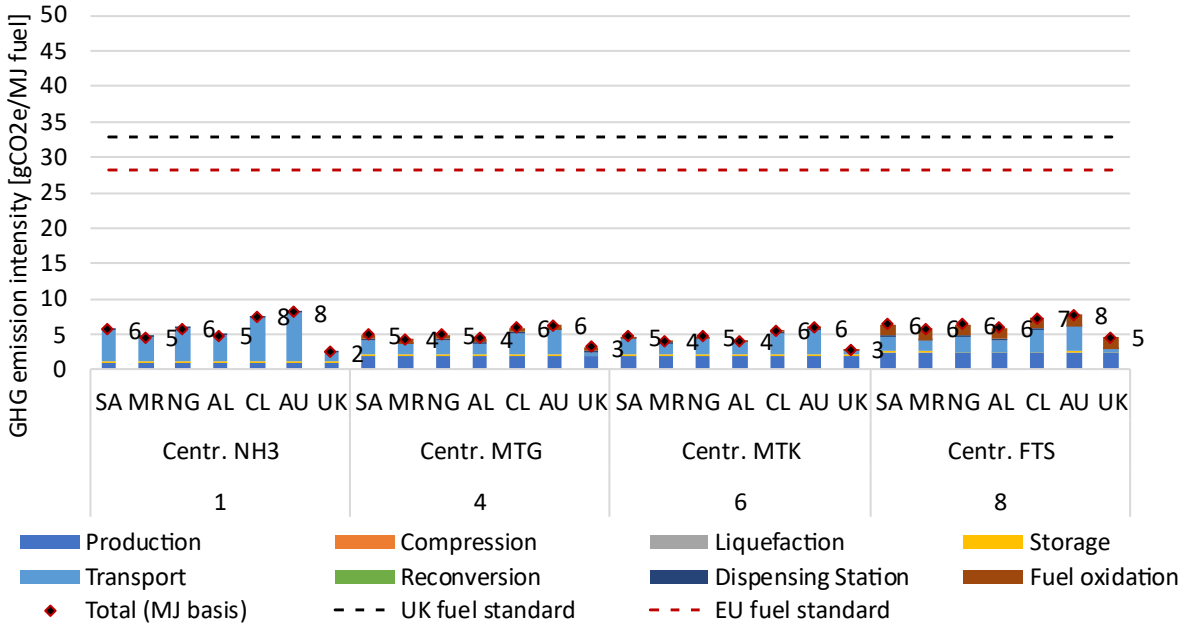


Figure 3: Overall emissions of key 100% renewable electricity-based liquid e-fuels supply chains over time for SA to the UK (a) Excluding infrastructure embodied emissions and (b) Including infrastructure embodied emissions. Compared with gaseous LCFs supply chains [16], the emissions from liquid LCFs supply chains are fairly stable with time, especially for the centralised scenarios. The 2025 scenarios presented here were based on fossil fuel use by delivery vehicles. For additional details on the use of LCFs in delivery vehicles in 2025, see SI 2. Note: The UK RTFO emission limit for SAF in aviation is higher than that in non-aviation transport, and it is currently set at 53.4 gCO_2e/MJ.

4.3 Emission impacts of fuel production locations

The overall GHG emissions in 2025 for delivering 100% renewable electricity-based liquid e-fuels to Europe (UK and NL) from the countries considered (SA, MR, NG, AL, CL and AU) varied marginally for centralised approaches excluding embodied emissions (with less than ±8 gCO_2e/MJ uncertainty), as shown in Figure 4a and SI 2. Additionally, there is a marginal difference in emissions when these international supply chains are compared to producing and consuming these fuels within European markets using centralised approaches (1–9 gCO_2e/MJ for international to Europe vs 1–5 gCO_2e/MJ for within European markets). However, the emissions differences could become significant when using decentralised approaches, from 9–21 gCO_2e/MJ for international locations to Europe vs 5–9 gCO_2e/MJ within European markets, due to emissions along H_2 supply chains. Furthermore, the overall emissions (with embodied emissions) can vary significantly due to location factors, such as wind power plant infrastructure emission factors and capacity factors, leading to more than ±20 gCO_2e/MJ uncertainty (Figure 4b and SI 2). When comparing liquid and gaseous synthetic fuels, the overall GHG emissions (without embodied emissions) of liquid synthetic fuels vary marginally with location factors in centralised approaches, whereas emissions from gaseous synthetic fuels supply chains can differ significantly with location factors. The authors' previous paper on gaseous synthetic fuels highlights market-specific analyses on the source and delivery of H_2, and its gaseous derivatives, to get a proper estimate of the total GHG emissions due to the significant variation of GHG emissions with location factors (e.g., transport distances) [16]. Nevertheless, due to the high mass and energy density of liquid fuels, market-specific analyses on liquid H_2 derivatives showed negligible variation in the total GHG emissions for most scenarios. Hence, liquid low-carbon synthetic fuels can open doors to new production routes towards meeting the EU's/UK's regulatory mandates, which are based on overall emissions (without embodied emissions), because of their GHG emissions' low sensitivity to changes in location factors.

(a)



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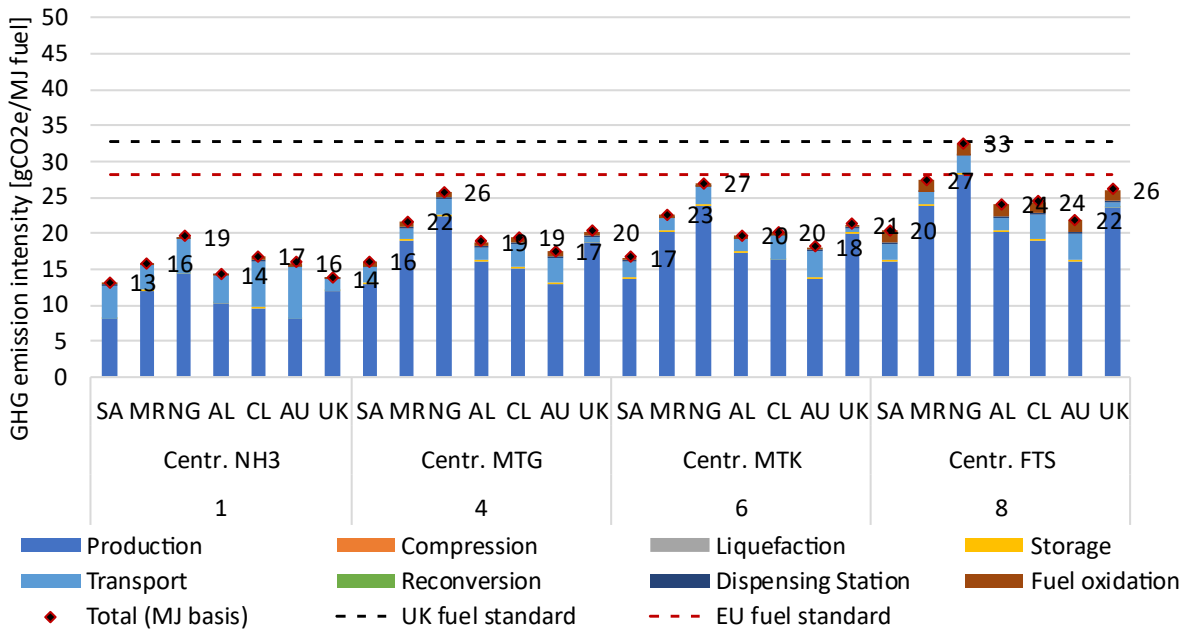


Figure 4: Overall emissions of key 100% renewable electricity-based liquid e-fuels supply chains from key fuel production locations, including the UK, with fuel delivery to the UK in 2025 when fossil fuel is used in delivery vehicles (a) Excluding infrastructure embodied emissions and (b) Including infrastructure embodied emissions. Note: The UK RTFO emission limit for SAF in aviation is higher than that in non-aviation transport, and it is currently set at 53.4 gCO_2e/MJ.

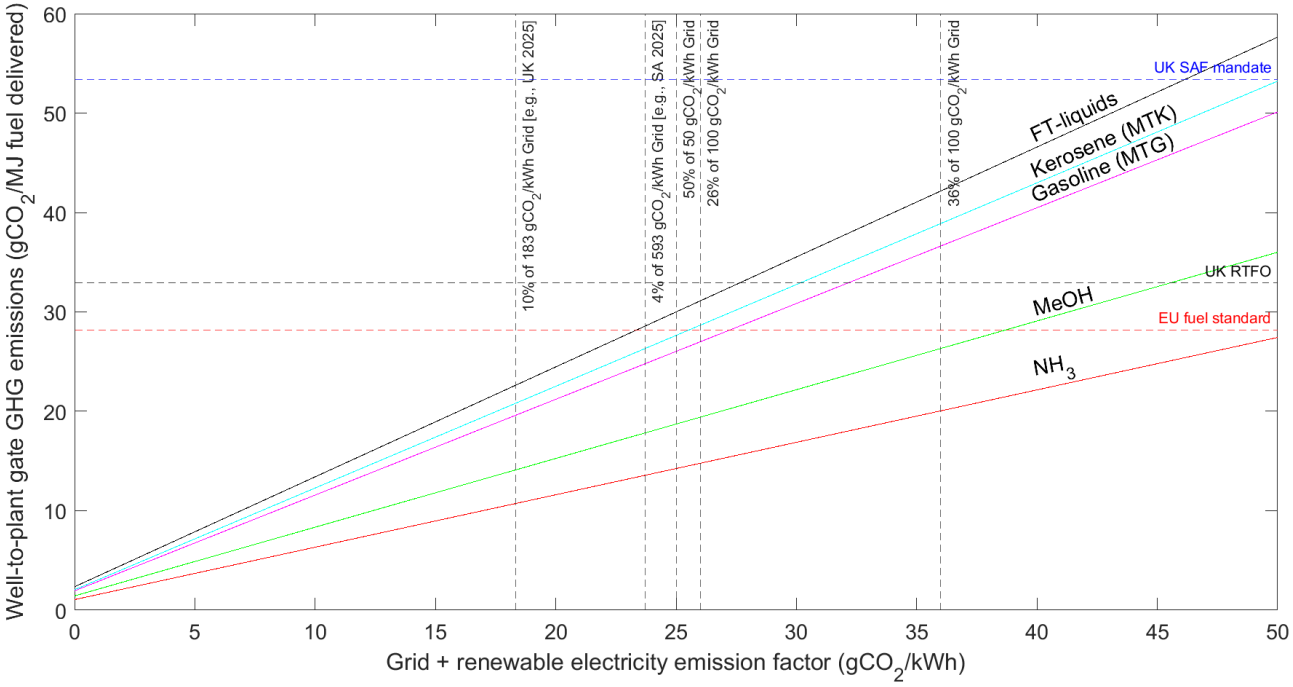
4.4 Emission impact of renewable and grid electricity hydrogen sources

In the preceding sections (Sections 4.1 to 4.3), we focused on fuel production from 100% renewable electricity. However, it is very possible that a hybrid of renewable and grid electricity will be used in producing e-fuels. This could be driven by several factors, such as economic considerations, stabilising the transient nature of renewable electricity, and managing process disruptions (including electricity curtailment from renewable electricity supply in the grid electricity system). For example, in the UK alone, renewable electricity curtailment of 3.5 TWh in 2022 had a financial impact of £750 million, and this is projected to grow to £3.5 billion by 2030 [67], [68]. Hence, we assessed the GHG emissions impacts of producing and delivering e-fuels that are produced from a combination of renewable and grid electricity here. This analysis could help provide information on the best operating points associated with GHG emissions of e-fuels when combining renewable and grid electricity. Additionally, we assessed the impact of improving electrolysis efficiencies up to 75%, in anticipation of the electrolysers performance outlook.

As shown in Figure 5 and SI 2, all scenarios of 100% renewable electricity-based liquid e-fuels meet the regulations from 2025 to 2050 for transport applications when excluding embodied emissions. Renewable electricity, such as wind power and Solar PV, has a zero electricity emission factor when excluding embodied emissions. However, some GHG emissions are associated with renewable e-fuels, even at the fuel production plant, due to fugitive H_2 losses into the environment, which causes GHG effects. There is no tangible change in GHG emissions (0.00%) due to the increase in H_2 electrolyser efficiency from 65.4% to 75%. For a mix of renewable and grid electricity, which is most suitable for centralised fuel production approaches, most (more than 80%, 95% and 99%) of the centralised scenarios from global locations will meet even the stricter EU emission limit of 28.2 gCO_2e/MJ in 2025, 2030 and 2050 for a grid electricity fraction of 4%, 5% and 17%, respectively, based on the IEA Sustainable Development scenario. In some locations, such as the UK and Belgium, with a grid electricity emission factor of ca. 200 gCO_2/kWh, up to 10% grid electricity fraction can

be used in the fuel production, while the emissions from most fuel options remain within 28.2 gCO_2e/MJ. For a grid electricity fraction above 26% in the fuels of countries (e.g., SA and MR) whose grid electricity emissions factors were expected to exceed 100 gCO_2/kWh in 2050, the emissions from the fuels (excluding NH_3 and MeOH) would not be within 28.2 gCO_2e/MJ. However, countries (e.g., the UK, NL and CL) that could decarbonise their grid electricity emissions to about 50 gCO_2/kWh in 2050 could have grid electricity fractions exceeding 50% in the fuels, while staying within the EU emission limits. Therefore, grid electricity should be used with caution, and in the near term, it would be mostly suitable for stabilising process operations of renewables rather than enhancing production cost and volumes. Additionally, policies should be developed in a way that encourages the optimal use of resources and allows for the use of different approaches, including contingencies, while achieving the required climate targets.

(a)



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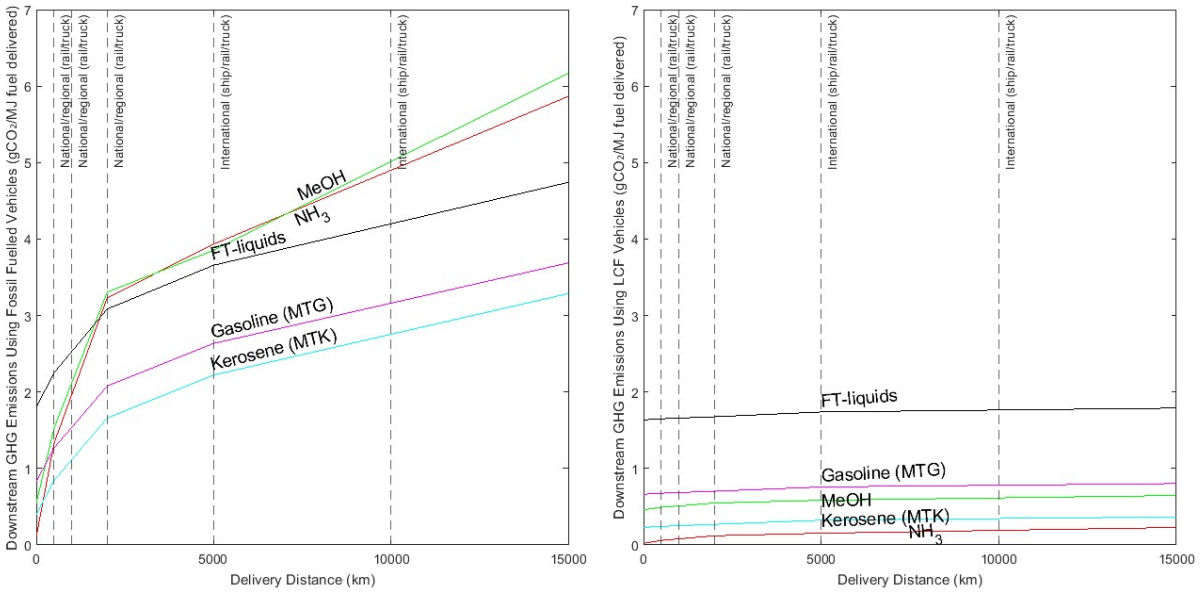

Figure 5: Upstream and downstream GHG emissions of liquid electricity-based fuels and chemicals from different H_2 production technologies for global supply chains, based on the centralised production approach. Note 1: Total life cycle GHG emissions equal well-to-plant gate GHG emissions + downstream GHG emissions. 1 kg of liquid fuel at the plant gate is approximately equivalent to 1 kg of the fuel at the fuel station, since negligible loss is experienced in downstream supply chains during product distribution. Note 2: Some regulations, e.g., the EU, are not strict on the energy content of e-fuels (RFNBOs) and fuels produced by combining renewable and non-renewable electricity are regulated by RFNBOs regulations accordingly [4], [5], [6], [7]. In contrast, the UK RTFO is very strict on the energy content of RFNBOs and refers to fuels produced by combining renewable and non-renewable electricity as partial RFNBOs, with only the portion of fuel from renewable electricity considered in RFNBOs-associated certificates, emission limits, and benefits [2], [3]. Consequently, some LCFs may be classified differently under various regulations; see Section 1 for additional information. The authors suggest that the energy content requirements of fuels in emission limits, along with the associated benefits and incentives of RFNBOs, should be relaxed at production facilities, up to a certain level of non-renewable energy at the plant gate. However, downstream of the production plants, fuels obtained through blending should be considered by their individual components.

4.5 Energy and water consumptions

The total energy consumption of practical e-fuels supply chains varied from 1.9–4.0 MJ per MJ fuel delivered, with at least 85% of this consumption occurring during the fuel production stage, as shown in Figure 6 and SI 1 Figures S10–S18. There are no significant changes in energy consumption up to 2050, which were based on current operations. The total energy consumption of the fuels from the decentralised approaches were lower than those from centralised approaches due to the energy savings achieved by using biogenic CO_2 from fermentation plants, which is captured at negligible energy demand, thereby avoiding the energy-intensive DAC used in the centralised approaches. Synthetic gasoline, diesel and kerosene produced via FTS have the highest energy consumption due to the energy-intensive conversion steps. Additionally, up to 70 wt% of the H_2 feed is lost as water during their formation [see Equations (2–7) for additional details]. It should also be noted that the yield of FTS is lower than that of the other fuel production processes. However, as water is produced as a by-product in e-fuel production, carbon is added to H_2 in the chemical structure of synthetic gasoline, diesel and kerosene. For every 1 kg of H_2 used, 2.0–5.5 kg of H_2 derivatives could be produced, with a corresponding decrease in energy content (from 120 MJ/kg H_2 to 19 MJ/kg NH_3) and an increase in fuel and energy density. Hence, these improvements in fuel yield, as well as fuel and energy densities, favour even long-distance transportation of the fuels and their use in sectors that require energy-dense fuels.

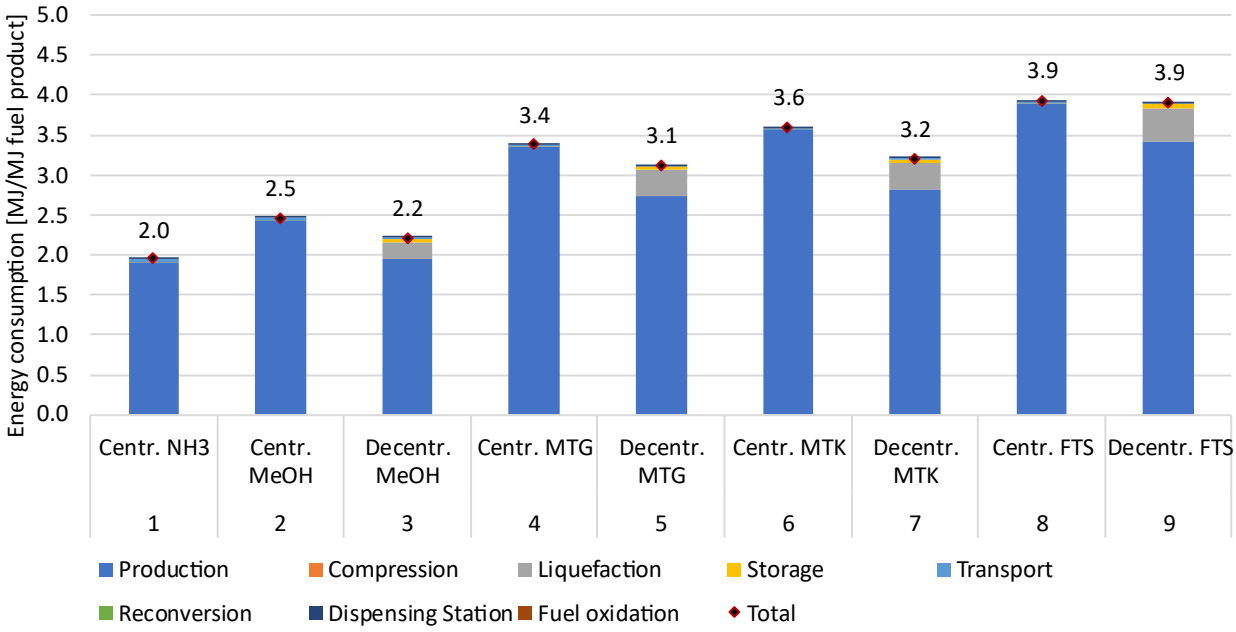

Figure 6: The energy consumption of liquid e-fuel supply chains from the SA to UK. The centralised scenarios were based on DAC CO_2, while the decentralised scenarios were based on (waste) biogenic CO_2.

The life cycle water consumption of e-fuels mainly arises from the water consumed in H_2 production by water electrolysis, with at least 9 kg H_2O consumed per kg H_2 produced. Moreover, the water produced as a by-product of e-fuel (MeOH, gasoline, kerosene and FT-liquids) production, up to 0.7 kg water per kg H_2, can be used as a starting material for water electrolysis, thereby reducing the water footprint of electrolytic H_2. Additionally, the water adsorbed alongside CO_2 in DAC (up to 0.9 kg H_2O per kg CO_2 [69], [70]) can be recovered and used in the plant for water electrolysis. Hence, the life cycle water consumption of liquid e-fuels typically ranged from 0.41 kg H_2O/kg fuel (0.016 kg H_2O/MJ) to 5.04 kg H_2O/kg fuel delivered (0.118 kg H_2O/MJ) [Figure 7 and SI 1 Table S22]. This finding highlights the importance of integrating electrolytic H_2 and H_2 derivatives plants to recover and reuse energy and water, thereby minimising energy and water demands. This could be vital for offshore renewable electrolytic H_2-based fuel and chemical plants where freshwater availability for electrolysis is critical. The water consumption of e-fuels is significantly lower compared to other alternative low-carbon technologies, such as biofuels and lithium (used in BEVs) (Figure 7). This finding highlights the importance of life cycle assessment and energy policy that covers different environmental factors. Energy and water consumption analysis are crucial for evaluating the efficiency of technologies and the sustainability of systems, and they should be combined with other assessment approaches. It is recommended that other assessments, such as resource availability, economic, environmental (see Sections 4.1–4.4) and social factors, be made when developing energy policies and deploying low-carbon solutions.

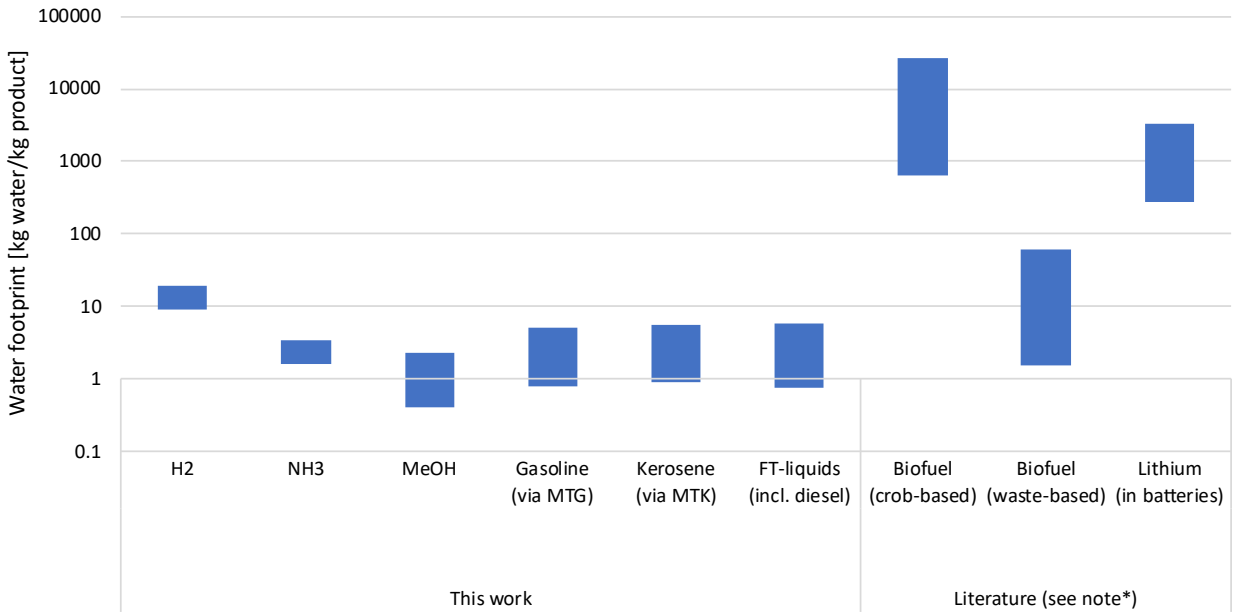

Figure 7: Water footprint of liquid e-fuels in comparison with alternative technologies, showing significant variation in water footprint with technology type. E-fuels require significantly less water per kg of product compared to alternative low-carbon technologies like biofuels and lithium (used in BEVs). *Note: Data for biofuels from [71], [72], [73], [74], [75] and lithium from [76], [77], [78], [79].

4.6 Discussion on study's boundaries and study results within policy frameworks

As discussed in Sections 1 and 2, the scope of this study is limited to liquid low-carbon e-fuels. Like any modelling project, we needed to make various assumptions about future technological advancements and supply chain performances, which could influence the overall findings reported. Due to the complexity of the supply chains involved and the absence of concrete measurement data, uncertainties were linked to the analyses presented here. To account for the variability of the parameters and their impact on the results, the study assessed the effects of changes in various supply chain assumptions, including concurrent variations of multiple parameters. Key parameters that were systematically varied include: Electricity emission factors (renewable electricity and IEA's grid electricity scenarios) in Sections 4.2 to 4.4, (b) producing/destination markets (transportation distance between countries) in Sections 4.3 and 4.4 and (c) H_2 production efficiency and production emissions for renewable and grid electricity-based H_2 in Section 4.4. This work assessed over 10,000 key liquid H_2 derivatives supply chains and discussed the sensitivity of key parameters throughout the discussion of the respective results. The primary sources of uncertainty in the emission estimates were found to be fuel/carrier production methods, H_2 losses, and fuel and electricity emissions factors.

Furthermore, while GHG emissions of 100% renewable electricity-based liquid e-fuels are low, often less than 25 gCO_2e/MJ, the authors recommend that adequate assessments be made before reducing or increasing emission limits, now or in the future. Policies on emission limits can be relatively static (e.g., EU [14] and the UK RTFO [2]), dynamic over different purposes, time or locations (e.g., the UK RTFO [2] vs SAF mandate [10] and California Low Carbon Fuel Standard [80]) and in other cases, no emission limits (e.g., domestic heating and industrial use of NH_3). But considering the low success rates of prior green H_2 and some climate change mitigation projects [81], [82], [83], [84], [85], [86], it is advisable for policies to allow a broad range of solutions, to narrow the implementation gap and enable emission reductions. Additionally, there would be a need for mutual acceptance and recognition of supply chain certificates for H_2 and its derivatives by respective jurisdictions globally, consistent with the COP28 declaration of intent in 2023 [87]. Utilising LCA-based, asset-based certification, radio frequency identification (RFID), and a database of approvals, among

other methods, can aid in managing LCFs' emissions and fraud [13]. Furthermore, for a successful energy policy, it is crucial that it is based on an assessment of resource availability, technology design and operations, environmental, costs and social impacts. This will help avoid concerns such as unmet targets, delays or cancellations of policies, fraud, slowdowns of technological innovation and social inequalities [81], [82], [83], [84].

5 Conclusion

Synthetic fuels from low-carbon technologies can provide low-carbon solutions for transport and manufacturing applications. However, because of the different production approaches that could be used for synthetic fuels and the series of transforming processes that take place from the fuel production plant to the point of fuel consumption, it is important to understand the lifecycle GHG emissions of synthetic fuels along their supply chains. This paper assessed the impact of H_2 losses, energy efficiencies, water consumptions and GHG emissions of thousands of liquid e-fuel supply chains across 3 time horizons. It was found that both renewable electricity-based and hybrid of renewable and grid electricity-based liquid e-fuels can have low life cycle emissions that are within the current UK and EU emission limits for transportation.

The losses of H_2 throughout practical liquid e-fuel supply chains are estimated to be in the range of 0.2–2.6% H_2 per kg of fuel delivered, with the decentralised approaches of biomass or bio-CO_2 to fuel routes having the highest loss rates due to the longest H_2 transport distance involved in the fuel production.

The total energy consumption in delivering liquid e-fuels is typically in the range of 1.9–4.0 MJ per MJ of fuel delivered. Supply chains based on e-fuels from NH_3 had the lowest energy consumption due to the high selectivity and yield of the Haber-Bosch process, while those using e-fuels from FTS had the highest energy consumption due to the low selectivity and yield of the process.

The life cycle water consumption of liquid e-fuels typically ranged from 0.41 kg H_2O/kg fuel (0.016 kg H_2O/MJ) to 5.04 kg H_2O/kg fuel delivered (0.118 kg H_2O/MJ). This is also due to the nature, yield and selectivity of e-fuel production processes, with NH_3 having the highest water consumption.

The life cycle GHG emissions of liquid e-fuels vary significantly due to technological, design and operational factors, as well as LCA methodologies. These factors are primarily driven by fuel/carrier production methods, H_2 losses, and fuel and electricity emissions factors. It was found that approaches that minimise the impact of fuel/carrier production methods, H_2 losses and fuel emissions factors by combining centralised and decentralised processes efficiently offered the best GHG emissions estimates with e-fuels. Scenarios using centralised synthetic fuel production approaches performed the best due to the liquid state and high mass and energy density of the e-fuels, which minimises H_2 losses along downstream supply chains and favours both short and long supply chain distances. Hence, the life cycle GHG emissions of 100% renewable electricity-based liquid e-fuels ranged from 1–21 gCO_2e/MJ in 2025, and when embodied emissions are included, this can add up, ranging from 9–33 gCO_2e/MJ. Hence, the justification for excluding embodied emissions from infrastructure in current regulations is valid for liquid e-fuels, since the upper range of their emissions (including embodied emissions) is just above the EU and UK emission limits. However, there may be a need to consider the impact of embodied emissions in gaseous synthetic fuels supply chains. By 2050, the emissions from 100% renewable electricity-based liquid e-fuels would reduce to 1–10 gCO_2e/MJ and 9–30 gCO_2e/MJ, excluding and including embodied emissions, respectively. This implies that all supply chains of 100% renewable electricity-based liquid e-fuels would meet the EU and UK emission limits, which excludes embodied emissions. This could open doors to new production routes for meeting the EU's and UK's mandates, given the low sensitivity of liquid e-fuel GHG emissions to changes in location factors. Additionally, it was found that grid electricity could be used to stabilise the process operations of e-fuels in the near-term, up to a 10% fraction, while the fuel emissions would typically remain within 28.2 gCO_2e/MJ (EU emission

limit). In the long-term, grid decarbonisation would allow a higher fraction, more than 25% of grid electricity fractions in e-fuels, while the fuel emissions still stay within 28.2 gCO_2e/MJ.

Lastly, because of the different production approaches that could be used to produce LCFs, it is crucial for policy definitions of LCFs to adequately reflect various LCF production approaches, as this could drive efforts towards achieving climate targets. In defining and regulating fuels, it is important to note that the emission benefits of the fuels are better than the share of the energy content from which the fuels arise from.

CRediT authorship contribution statement

Sylvanus Lilonfe: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Validation, Project administration, Software, Visualization, Writing – original draft, Writing – review & editing.

Carlos A Jimenez Cortes: Conceptualization, Resources, Methodology, Validation, Writing – review & editing.

Madeleine Mitschler: Conceptualization, Resources, Methodology, Supervision, Validation, Writing – review & editing.

Victor Gordillo Zavaleta: Conceptualization, Resources, Methodology, Project administration, Supervision, Validation, Writing – review & editing.

Amir F.N. Abdul-Manan: Conceptualization, Funding acquisition, Methodology, Validation, Supervision, Validation, Writing - review & editing.

Ioanna Dimitriou: Conceptualization, Methodology, Supervision, Validation, Writing – review & editing.

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Data availability

The data supporting this article have been included in the supplementary documents – SI 1 and 2.

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9 Conclusions and recommendations

The study aims to perform technical, economic and life cycle assessments for low-carbon fuel and chemical technologies, including biomass-to-liquids, direct air capture and power-to-X systems, has been achieved. The findings from this study showed that several factors, including design and operations, as well as techno-economic and life cycle assessment methodologies, can influence the economics and life cycle environmental impacts of low-carbon fuel and chemical technologies.

The design and operation of various technologies were found to significantly influence the cost and environmental impact of low-carbon technologies. Advanced biofuels were found to have lower production costs compared to renewable electro-fuels due to the cost and availability of feedstocks (e.g., biomass), as well as technology development. However, their environmental impacts could vary widely depending on consequential factors, such as land use, avoided emissions and foregone benefits. Additionally, direct air capture technologies could provide significant benefits that would not be achieved with biofuels and electro-fuels, by offsetting CO_2 emissions through permanent storage, thus enabling them to have net negative emissions. Therefore, different low-carbon technologies could be combined adequately to address the complex challenge of climate change mitigation.

Furthermore, the use of centralised and decentralised production and reconversion configurations influences low-carbon technologies differently. This is due to technological factors, such as raw materials, intermediates, and product states, as well as location-specific factors, including transport distances, costs, and emission factors. Generally, centralised and decentralised production and reconversion configurations have minimal impact on the greenhouse gas (GHG) emissions of liquid-based supply chains, such as advanced “drop-in” biofuels and liquid electro-fuels, because of their high mass and energy densities, which favour even long-distance transportation. However, GHG emissions from gas-based or low-density product supply chains could vary considerably depending on whether a centralised or decentralised approach is employed. Additionally, production costs could differ significantly between centralised and decentralised approaches. Therefore, it is important to map low-carbon technologies' supply chains adequately to manage cost and environmental emissions.

Even when starting with low-cost, low-environmental-impact materials and energy, the overall product cost and environmental impacts throughout a product's life cycle can exceed the limits generally considered low-cost and low-carbon. Additionally, a product, e.g., gaseous synthetic fuels, can perform better in one environmental impact category, such as energy consumption, while another alternative product, e.g., liquid synthetic fuels, which have higher energy consumption, can perform better in another environmental impact category, such as GHG emissions. These insights can also be extended to other low-carbon technologies, including direct air capture systems and battery electric vehicles. Hence, these underscore the need to develop robust low-cost solutions and supply chain-specific policies to demonstrate compliance with regulations. Energy policies should allow a broad range of low-carbon solutions to address climate change, given that there is no silver bullet to global warming. Additionally, current EU and UK energy policies, which exclude embodied emissions from infrastructure, should consider the significance of embodied emissions to climate targets, given that the findings in this work indicate overall emissions including embodied emissions from many supply chains could be well above current regulatory limits. Furthermore, it is advisable that energy policies should be based on comprehensive assessments of resource availability, technology design and operation, economic, environmental and social factors, considering the current challenges associated with low-carbon technologies. Additional information, including the specific conclusions and recommendations drawn from the study, is further shown in the following sections.

9.1 Dry and wet biomass-to-liquids technologies assessment

Concerns over climate change, energy security, food price inflation, and forest degradation have led to rising interest in the development and use of advanced biofuels, particularly for hard-to-abate sectors such as freight and aviation transport. Advanced "drop-in" biofuels can be produced from a variety of sources, including second- to fourth-generation biomass feedstocks, which utilise waste and residual biomass products with potentially lower environmental impacts. This work covers both the review and analysis of thermochemical methods for producing advanced biofuels.

The findings from this review indicate that thermochemical methods for producing advanced biofuels, such as gasification with Fischer-Tropsch synthesis and pyrolysis with upgrading, can enable the use of a wide variety of biomass feedstocks, ranging from agricultural residues to high moisture content wastes like food waste. The performance indicators of thermochemical processes, such as product prices and emissions, are highly dependent on energy and material consumption, as well as other process operation factors, such as production approach. Hence, several design and operational considerations, such as heat integration, H_2 sources, and centralised and decentralised operations, are key to the profitability and sustainability of thermochemical routes. The review of the literature found that the prices of advanced biofuels range from $0.60–3.88 per gasoline litre equivalent (GLE) [$17.14–110.82 per GJ]. The lower range of these prices showed that, in some cases, advanced biofuels can be competitive with the wholesale price of fossil diesel of $1.22 per GLE ($38.57 per GJ). Additionally, the review of life cycle assessment on advanced biofuels highlights the low-carbon potential of these pathways, which, when produced sustainably, the GHG emissions of advanced biofuels can be much lower than those of fossil fuels. The emissions from these fuels range from -122 to 98 gCO_2e per MJ. However, several key factors could impact the GHG emissions of advanced biofuels, including the types of renewable feedstocks and energy sources, land use change and indirect land use change, life cycle assessment methodologies, and foregone emissions.

The findings from the analysis of this work indicate that the availability of feedstocks is an important factor for the successful operation of any process or production plant. Biomass is available in various regions in the UK; however, its availability is limited and also subject to many competing uses such as bioenergy generation in biomass plants, panelboard and anaerobic digestion. However, some biomass feedstocks, such as wet feedstocks like biogenic municipal waste (BMW) and food wastes, are in excess, even after deducting for other competing uses, and are often disposed of without energy recovery. The production of non-food UK-origin biomass feedstocks is estimated at 167–205 Mtpa (wet) [839–1033 PJ per year], with high moisture content feedstocks, such as manure and sewage sludge (SS), accounting for most of the estimates. Furthermore, it is estimated that a total of up to 563 PJ per year and up to 269 PJ per year can be produced from UK-origin biomass feedstocks, based on 100% feedstock availability and competing cases, respectively, which represent 38.2% and 18.3% of the 2021 road transport fuel consumption. Producing biofuel from waste resources could provide an alternative method for waste management, thus, partly addressing the challenges accompanying current waste management systems. The total GHG emissions savings from the use of non-food biomass feedstocks as advanced biofuels in internal combustion engines can significantly reduce the UK transport sector's GHG emissions. The initial estimates in this work indicate that the emissions savings from using advanced biofuels in the UK could reach up to 64.7% of the UK's total road transport GHG emissions in 2021. Thus, there is strong potential for the use of biomass-to-liquids in the UK.

Importantly, this study highlights the potential of sustainable biofuels in general as an option for GHG mitigation for the UK's transport sector. More broadly, based on the insights of this review, it would be recommended that policymakers also consider encouraging rapid developments and uptake of a wide range of advanced, low-carbon fuels (LCFs) as a complementary strategy to decarbonise transport sectors. Life cycle assessment and other techno-environmental assessment tools should be used to guide policy decisions towards achieving a decarbonised transport future.

9.2 Wet biomass-to-liquids technology assessment

This study demonstrates the potential for economically viable production of advanced biofuels from wet waste feedstocks, capable of achieving low and even negative life cycle GHG emissions. The hydrothermal liquefaction (HTL) of digestates, food waste, BMW, and SS into advanced biofuels using various production approaches, such as plant configurations and H_2 sources, were studied using techno-economic and life cycle assessment methodologies.

It was found that several key elements, such as plant configuration (e.g., centralised and decentralised operations), feedstocks, fuel production and supply chain factors, can have a significant influence on the minimum fuel selling price and life cycle GHG emissions of biofuels. The use of either a centralised or a decentralised approach for the optimal processing of wet biomass is highly dependent on the availability, distribution and transportation of the wet biomass feedstocks, as both approaches can be beneficial. For the wet biomass feedstocks studied, when the local availability of feedstocks is less than 6000 kg/h of dry feed, the use of a centralised approach has significant cost advantages over the use of a decentralised approach. However, when the local availability of the feedstocks is above 6000 kg/h (dry), a decentralised approach provides better cost advantages over a centralised approach. The choice of centralised or decentralised configurations requires an optimal balancing between plant scaling and feed transportation distance, as both factors play important roles in the economics of fuel production from wet biomass feedstocks. On the other hand, in terms of GHG emissions, the choice between a decentralised and a centralised approach has a marginal impact on the overall life cycle emissions of biofuels. Similarly, the choice of H_2 production methods can influence the cost and CO_2 impacts of the drop-in fuel, demonstrating the trade-off between the CO_2 benefit of utilising a low-carbon H_2 supply and its higher cost of production and supply. An additional production cost of up to \$7.29 per GJ can be added due to the high costs of low-carbon H_2; however, a GHG emissions reduction of up to 40% relative to the corresponding grey H_2 scenarios can be achieved using low-carbon H_2. Hence, this analysis estimated the minimum fuel selling price of advanced biofuels produced via HTL in the range of \$19.92–36.59 per GJ (\$0.63–1.16 per GLE), which is lower than the current fuel prices in the UK. From a CO_2 perspective, biofuel emissions could vary according to life cycle assessment methodologies, as well as design and operational factors, such as H_2, electricity and thermal energy emission factors. Based on consequential and attributional life cycle assessment methods, the GHG emissions from biofuels from wet biomass feedstocks are estimated to range from -82.0 to 59.7 $kgCO_2e$ per GJ and 5.1–36.1 $kgCO_2e$ per GJ, respectively. Consequential life cycle assessment methods cover broader market-mediated effects beyond the typical fuel's production boundary.

There are significant opportunities for the production of advanced biofuels by diverting the UK's wet waste feedstocks from conventional waste treatments into transport fuels as a means to increase renewable energy penetration and mitigate transport emissions. However, this study estimated that the UK's wet biomass feedstocks could supply only about 4.5–6.8% of the total gasoline and diesel consumption in 2021, potentially resulting in a 3.4–7.3% reduction in the UK's total road transport emissions. While they can contribute to the current UK fuel mix on top of the existing biofuel volumes of 5%, this study also highlights the need for other complementary LCF alternatives to close the supply gap in the mid and long-term towards achieving a net zero future. As a complementary measure, the UK could consider other synthetic fuel pathways, for example, the production of drop-in fuel from green H_2 and CO_2 captured from existing, CO_2-intensive industries in the UK. This is an emerging technology that could potentially be scaled up. Synthetic electro-fuel has gained regulatory attention in the EU, which has recently allowed internal combustion engine vehicles to be sold after the 2035 ban as long as the vehicles operate exclusively on low-carbon, synthetic electro-fuel. This is a technology area that is worth considering for the UK and is further investigated in this thesis.

9.3 Direct air capture technologies assessment

Direct air capture (DAC) is crucial for the production of synthetic fuels and chemicals, as well as for permanent carbon storage. Therefore, this study provides a comprehensive evaluation of the cost and GHG implications of solid sorbent DAC technologies with emphasis on the technical, geographical, and temporal perspectives. This assessment incorporated the effects of different solid sorbent chemistries, their adsorption kinetics, types of energy used, location-specific parameters including capacity factors across two countries, the end-use fate of captured CO_2, and their evolution over time.

The technical and economic performances of DAC technologies are found to be heavily influenced by: (i) economic factors (e.g., capital expenses and energy costs), (ii) design elements (e.g., plant scale and energy capacity factors) and (iii) operational parameters (e.g., sorbent's adsorption rate and time). Conversely, the GHG emissions of DAC are mostly determined by the source of energy. Hence, the cost and GHG emissions of sorbents ranged from \$1,200–40,400/t sorbent and 3.1–12.3 tCO_2e/t sorbent in 2024, respectively, which are mainly driven by raw materials used in their manufacturing. However, they contribute ca. 0.2% and 0–10% to the overall cost and GHG emissions of DAC, given that sorbent consumption in DAC is relatively small compared to other parameters, including the cost and emissions associated with energy use. From an LCA perspective, the GHG emissions of DAC could vary from 0.01 to 0.37 tCO_2e/tCO_2 captured, with wind energy resulting in the lowest emissions, while the 2025 US grid electricity producing the highest carbon intensity. Consistent with earlier studies, the source of energy used is a key determining factor in the total life cycle GHG emissions of DAC, accounting for about 49–99% of the overall emissions. On the other hand, key factors influencing the cost of DAC include capital expenses, fixed operating costs, energy costs, monolith costs, and sorbent costs. Consequently, DAC levelized cost of capture ($LCOC_{net}$) ranged from $\$_{2024}148–623/tCO_2$ captured in 2025, which can be reduced to $\$93–523/tCO_2$ captured in 2050, with the best-performing DAC scenarios by country in 2050 being US Wind & Grid and UK Wind. Importantly, though, these analyses also highlight the importance of chemical kinetics, specifically the adsorption rate and time, on the costs and CO_2 emissions of DAC. This work demonstrated the opportunity to identify and develop an optimal adsorption rate and time to minimise the cost of DAC.

The costs of DAC from the best technological approaches assessed here are still generally above $LCOC_{net}$ of $\$_{2024}100/tCO_2$ captured. These cost estimates far exceed current CO_2 prices in the market, both, voluntary and compliance. Therefore, DAC is unlikely to be fully financed by the carbon market in its current form and, in the short term, will necessitate fiscal incentives to achieve gigaton-scale CDR buildouts. The US Inflation Reduction Act, for example, enhances the 45Q tax credit for DAC by increasing the incentives from $\$50/tCO_2$ to $\$180/tCO_2$ for geological sequestration of CO_2. While an engineered CDR like DAC is generally considered costly, it is important to situate this in the context of the social cost of carbon. The current US EPA's official cost of carbon is $\$51/tCO_2$, however, there is a growing recognition that this is a significant underestimate. Therefore, the latest EPA proposal is to increase it to $\$190/tCO_2$, based on a more recent scientific estimate (Rennert *et al.*, 2022). With this higher social cost of carbon, the high cost of DAC becomes even more justifiable. Furthermore, with carbon prices projected to increase from $\$40–100/tCO_2$ in 2023 to $\$140–240/tCO_2$ in 2030–2050, DAC could be a commercially profitable CDR option. Hence, well-designed policies encouraging investments in DAC are crucial for achieving gigaton-scale DAC buildouts.

9.4 Life cycle assessment of gaseous low-carbon fuels technologies

This paper addresses several pertinent questions relating to the global supply chains of H_2 and its gaseous derivatives by summarising insights from over 10,000 scenarios and sensitivity cases. The analyses focused on H_2 productions from key renewables-rich regions [Saudi Arabia (SA), Nigeria (NG),

Chile (CL), Morocco (MR), Algeria (AL), and Australia (AU)] and transporting it via different modes to European markets, using a variety of chemical carriers and physical states including compressed H_2 (CH2), liquefied H_2 (LH2), SNG, methylcyclohexane (MCH), ammonia (NH_3), and methanol (MeOH). The thesis discussed the implications on the overall energy efficiency, product losses throughout the supply chains, and life cycle GHG emissions from temporal, geospatial, and technological perspectives.

The overall H_2 and SNG losses, total energy consumption and GHG emissions throughout H_2 and SNG supply chains can vary considerably across different supply chains due to technology design and operational factors, as well as the life cycle assessment methodologies in the case of GHG emissions. The losses of H_2 and SNG throughout the supply chains can be significant, as they are estimated to be in the range of 0.8–11.0% per kg of gaseous fuel delivered at the station. For the scenarios assessed, the highest gaseous fuel leakage is obtained in LH2 systems without boil-off recovery technologies due to the boil-off of H_2 during storage and transportation. The mitigation of boil-off losses through the use of dual fuel and liquefaction technologies could lead to significant GHG reductions. The total energy consumption in delivering H_2 and SNG is in the range of 1.8–3.6 MJ per MJ of fuel product. Supply chains delivering H_2 as LH2 and CH2 had the lowest energy consumption, while those using chemical carriers, especially MeOH and SNG, had the highest energy consumption due to the energy losses in producing and reconverting the carriers. The life cycle GHG emissions (without embodied emissions) of the H_2 and SNG supply chains range from 5–86 gCO_2e/MJ in 2025, and this reduces significantly over time to those between 2 and 40 gCO_2e/MJ in 2050. When embodied emissions are included, the overall emissions can add up to 9–45 gCO_2e/MJ in 2050. Matching producer and consumer locations could significantly impact GHG emissions of H_2 and SNG, causing emissions from the same supply chain type to even double or triple in some cases due to the transport distances involved, renewable electricity generation capacity factors, and the emissions profile of the domestic grid electricity. Technologies, such as the implementation of boil-off gas recovery systems in storage facilities and using dual fuel engines that utilise synthetic fuel along with onboard H_2 or SNG, which would otherwise be vented, can reduce GHG emissions considerably. Supply chain considerations, including the creation of a centralised/decentralised reconversion facility, whether at import terminals, distribution centres, or fuel dispensing stations, were found to affect the overall GHG emissions, which presents an opportunity for overall network design optimisation. Over time, the overall GHG emissions of low-carbon H_2 are expected to decline due to technological advances.

These analyses found that supply chain emissions can be significant: Even when starting with H_2 with a low carbon intensity at the plant gate, the emissions associated with the supply chain can drive the emissions above the EU and UK regulatory limits. Still, it isn't prudent to generalise the CO_2 attributes of H_2 purely on the basis of feedstock, as both blue and green H_2 pathways can be above and below the regulatory thresholds. This paper contributes to the growing body of evidence highlighting the need for asset-specific and supply chain-specific life cycle assessment-based certification to demonstrate compliance with regulatory limits or H_2 standards globally. Lastly, the results of this study should be used with a wholistic assessment of emissions mitigation strategies to find the best emission limits for achieving climate targets.

9.5 Life cycle assessment of liquid electro-fuels technologies

This paper assessed the impact of H_2 losses, energy efficiencies, water consumptions and GHG emissions of liquid e-fuel supply chains across 3 time horizons, by summarising insights from over 10,000 scenarios and sensitivity cases. It was found that both renewable electricity-based and hybrid of renewable and grid electricity-based liquid e-fuels can have low life cycle GHG emissions that are within the current UK and EU emission limits for transport applications.

The losses of H_2 throughout practical liquid e-fuel supply chains are estimated to be in the range of 0.2–2.6% H_2 per kg of fuel delivered, with the decentralised approaches of biomass or bio-CO_2 to fuel routes having the highest loss rates due to the longest H_2 transport distance involved in the fuel production. The total energy consumption in delivering liquid e-fuels is typically in the range of 1.9–4.0 MJ per MJ of fuel delivered. Supply chains based on e-fuels from NH_3 had the lowest energy consumption due to the high selectivity and yield of the Haber-Bosch process, while those using e-fuels from FTS had the highest energy consumption due to the low selectivity and yield of the process. The life cycle water consumption of liquid e-fuels typically ranged from 0.41 kg H_2O/kg fuel (0.016 kg H_2O/MJ) to 5.04 kg H_2O/kg fuel delivered (0.118 kg H_2O/MJ). This is also due to the nature, yield and selectivity of e-fuel production processes, with NH_3 having the highest water consumption.

The life cycle GHG emissions of liquid e-fuels vary significantly due to technology design and operational factors, which are primarily driven by fuel/carrier production methods, H_2 losses, and fuel and electricity emissions factors. It was found that approaches that minimise the impact of fuel/carrier production methods, H_2 losses and fuel emissions factors by combining centralised and decentralised processes efficiently offered the best GHG emissions estimates with e-fuels. Scenarios using centralised synthetic fuel production approaches performed the best due to the liquid state and high mass and energy density of the e-fuels, which minimises H_2 losses along downstream supply chains and favours both short and long supply chain distances. Hence, the life cycle GHG emissions of 100% renewable electricity-based liquid e-fuels ranged from 1–21 gCO_2e/MJ in 2025, and when embodied emissions are included, this can add up, ranging from 9–33 gCO_2e/MJ. Hence, the justification for excluding embodied emissions from infrastructure in current regulations is valid for liquid e-fuels, since the upper range of their emissions (including embodied emissions) is just above the EU and UK emission limits. However, there may be a need to consider the impact of embodied emissions in gaseous synthetic fuels supply chains. By 2050, the emissions from 100% renewable electricity-based liquid e-fuels would reduce to 1–10 gCO_2e/MJ and 9–30 gCO_2e/MJ, excluding and including embodied emissions, respectively. This implies that all supply chains of 100% renewable electricity-based liquid e-fuels would meet the EU and UK emission limits, which excludes embodied emissions. This could open doors to new production routes for meeting the EU's and UK's mandates, given the low sensitivity of liquid e-fuel GHG emissions to changes in location factors. Additionally, it was found that grid electricity could be used to stabilise the process operations of e-fuels in the near-term, up to a 10% fraction, while the fuel emissions would typically remain within 28.2 gCO_2e/MJ. In the long-term, grid decarbonisation would allow a higher fraction, more than 25% of grid electricity fractions in e-fuels, while the fuel emissions still stay within 28.2 gCO_2e/MJ.

Lastly, different production approaches can be used to produce LCFs. Hence, it is crucial for energy policies to adequately reflect the various LCF production approaches, as this could drive efforts to achieve climate targets. In defining and regulating solutions, it is important to note that environmental benefits are better than the share of the energy content from which the fuels arise from.

9.6 Key limitations and future work

This section further highlights the key limitations of the current work and provides recommendations for future work, considering the limitations and broader implications of the current study.

Techno-economic assessments depend highly on location factors, technological advancements and time horizons. This study examined synthetic fuel and chemical supply chains across key locations, including the UK and the US. While we could consider all other countries, the aim here is not to evaluate every possible option but rather to focus on key representative supply chains. Nonetheless, the approaches and models developed in this work can be easily applied to other production and

consumption markets. Future work could look at matching production and consumption markets and optimising the demand and supply networks globally, since the demand and supply of synthetic fuels and chemicals could vary by location and time. Also, matching locations adequately could help minimise the cost of synthetic fuels and chemicals. Additionally, due to the scope of the study, the costs of electro-fuels and chemicals have not been presented here; however, the author's economic assessment of these fuels, which is associated with this thesis, is nearing completion, with preliminary results indicating promising reductions in the costs of electro-fuels compared to existing models. Future studies may investigate how the costs of electro-fuels fluctuate based on location factors and time, given that renewable electricity is highly variable and dependent on location factors and time.

Life cycle assessments can measure a range of environmental parameters, such as GHG emissions, water consumption, abiotic depletion and ozone layer depletion potential, which provide vital insights for sustainability. This work assessed limited environmental parameters – GHG emissions, energy consumption, H_2/CH_4 losses and water consumption – due to the project's scope, which was based on current energy policies regarding the deployment of low-carbon synthetic fuels and chemicals. Current policies regarding transport fuels are based on the implications of GHG emissions along fuel supply chains, and there is currently no regulation for the application of synthetic fuels and chemicals in manufacturing industries. Future work should examine other environmental parameters associated with synthetic fuels and chemicals to gain a comprehensive understanding of the environmental impacts of deploying synthetic fuels and chemicals. Since, for a successful energy policy, it is crucial that it is based on an assessment of resource availability, technology design and operations, environmental, costs and social impacts. This will help avoid concerns such as unmet targets, delays or cancellations of policies, fraud, slowdowns of technological innovation and social inequalities.

Although the technologies assessed in this work are similar and comparable – for example, solid sorbent direct air capture (i) using five different types of solid sorbents and (ii) for various applications including CO_2 storage in reservoirs and use in chemical industries – they are also different and often incomparable in many aspects. This is because they have different (i) technical designs and operations, (ii) markets (e.g., biofuels vs captured CO_2), and (iii) economic and life cycle assessment methodologies (e.g., selling price for fuel vs levelised cost of capture for CO_2). Hence, their technical and economic (techno-economic) assessments are also incomparable in many aspects. The thesis could compare technologies using other analyses, such as carbon abatement cost to have a common economic metric ($/t$CO_2$); however, these technologies are often complementary to each other, each with unique advantages. Carbon abatement costs would not address the complex systems associated with these technologies, e.g., limitations on biofuels volumes and the need to offset emissions from hard-to-abate sectors using direct air capture, as well as differences in supply chain types tailored to specific needs. Additionally, the extensive nature of this work required prioritising analyses, as many important analyses were moved to the supplementary information. Both the main work and the supplementary information were longer than those in average theses and journal articles. Future work can explore how low-carbon technologies complement one another and how common assessment frameworks can be used to tackle the complex challenge of mitigating climate change.

Lastly, the techno-economic and life cycle assessment methodologies used in this work covered different technologies, geographies, and time horizons. Like any modelling project, we needed to make various assumptions about future technological advancements and supply chain performances, which could influence the overall findings. Due to the complexity of the supply chains involved and the absence of concrete measurement data, uncertainties were linked to the analyses presented here. To account for parameter variability and its impact on the results, the study assessed the effects of changes in various supply chain assumptions, including concurrent variations in multiple parameters.

Key parameters were systematically varied to understand the uncertainties in results and their drivers. Future work could adapt other uncertainty analysis methods, such as stochastic approaches like Monte Carlo simulations, to show the range of probable outcomes for an uncertain scenario.

Appendices

Appendix A1: Supplementary information for Chapter 3: A review of techno-economic analyses and life cycle greenhouse gas emissions of biomass-to-hydrocarbon “drop-in” fuels

Appendix A2: Supplementary information for Chapter 5: Comparative techno-economic and life cycle analyses of synthetic “drop-in” fuel production from UK wet biomass

Appendix A3: Supplementary information for Chapter 6: Technical, economic and lifecycle greenhouse gas emissions analyses of solid sorbent direct air capture technologies

Appendix A4: Supplementary information for Chapter 7: Life cycle greenhouse gas implications of low-carbon gaseous fuel supply chains from technological, geospatial, and temporal perspectives

Appendix A5: Supplementary information for Chapter 8: Life cycle assessment of global liquid electro-fuels and chemicals supply chains from technological, geospatial, and temporal perspectives

Appendix A1: Supplementary information for Chapter 3: A review of techno-economic analyses and life cycle greenhouse gas emissions of biomass-to-hydrocarbon "drop-in" fuels

A review of techno-economic analyses and life cycle greenhouse gas emissions of biomass-to-hydrocarbon "drop-in" fuels

Supplementary Information

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1 Biomass resources

1.1 Municipal solid waste (biogenic fraction)

The competing uses for BMW are anticipated to be strong in the future, as more EfWs are commissioned. According to Defra (Defra, 2022), 70% of paper & cardboard and 44% of wood waste were recycled in 2020, which corresponds to 9.5 Mtpa and 2.2 Mtpa, respectively. Additionally, 2.1 Mtpa of food waste is recycled in the UK annually (Facchini *et al.*, 2018). Hence, the total volume of food waste recycled in the UK is 13.8 Mtpa. Applications such as composting and landspreading used 2.7 Mtpa. Furthermore, based on Defra, BMW sent to landfills in 2020 was 6.1 Mtpa (wet). Therefore, based on mass balance, the volume of BMW in energy applications is 11.8 Mtpa. Also, based on Tolvik (Tolvik, 2022), in 2021, an estimated total of 14.9 Mt of residual waste was used in the UK energy-from-waste (EfWs). The report further estimated an operational capacity of 16.4 Mt of EfWs used in 2020. IEA reported that up to 80% of MSW in EfWs is biomass-derived (IEA, 2003), thus this makes about 13.1 Mt of the 16.4 Mt of waste processed at EfWs to be biogenic. These numbers agree with each other with slight variations probably due to the fraction of biogenic waste in EfWs, which is based on an IEA publication in 2003.

There has been a reduction in landfilled BMW volumes over the past years, currently, there is about an 8% reduction in BMW sent to landfills compared to the 2019 levels. The amount of waste sent to landfill in the UK continued to reduce over the past few years and is expected to continue to reduce in the following years, as new EfWs are commissioned. According to Tolvik, there will be a total of 19.4 Mtpa operational capacity in 2026 (Tolvik, 2022). Extrapolating this, about 24.1 Mtpa will be available in 2030 for EfW. However, it is expected that there will be a shift away from some EfW processes like incineration to EfW processes like AD and BTL, as waste generators and collectors aim to avoid the high gates fees charged at incineration plants. Recycling rates in the UK are fairly constant between 44.4 – 46.0% over the last 5 years. Based on this data, close to no BMW will be landfilled in 2030, as all BMWs are used for recycling, composting, and energy.

1.2 Food waste

The distribution of food waste in the UK, based on data WRAP (WRAP, 2019, 2020), is shown in Table 1. Most of the UK food waste is from the household, which produces up to 60% of the UK's total food waste volumes.

Table 1: UK food waste arisings (in kt) summary, based on WRAP (WRAP, 2019, 2020).

Component	2018	2030
Pre-farm gate	**1600**	**1600**
Household	6646	5300
Suppy chain	2880	2300
Retail	277	200
Manufacture	1505	1300
Hospitality & food service	1098	800
Post-farm gate waste	**9525**	**7600**
Total	**11125**	**9200**

The competing use for food waste is high. According to NNFCC in 2021, 4.9 million tonnes of food wastes from pre-farm and post-farm gates were used in AD sites to produce biogas, which was used for heat and electricity generation or biomethane production (NNFCC, 2021). Other areas of utilisation of food waste are recycling (2.1 Mt), incineration (2.5 Mtpa), landspreading (0.9 Mt) and composting (0.4 Mt), based on data by Facchini et al. (Facchini *et al.*, 2018) and Defra (Defra, 2021). Unutilised food waste is often landfilled. Based on data from Defra in 2017 and 2021 for the fraction of food waste (Defra, 2017) and the volumes of MSW sent to landfills (Defra, 2022), 1.9 million tonnes of food waste were unutilised and sent to landfills in 2020.

1.3 Forest residues

Forest residues are by-products, such as branches, foliage, roots, distorted wood, stumps, tops, barks and brash, produced from forest management or harvesting. Not all forest residues can be removed, as some must be left for ecological benefits (NNFCC, 2014). The UK production capacity of forest residues is estimated at 1.4 Mtpa on a dry basis (2.70 Mtpa wet, 50% moisture), based on estimates by NNFCC in 2014 (NNFCC, 2014). Most of the generation volumes arise from softwood cultivation, which is about 1.3 Mtpa. NNFCC estimate is based on woodland areas in the UK. UK forest residue generation is forecasted to grow slightly up to 1.7 Mtpa in 2031, before experiencing a slight drop to 1.6 Mtpa in 2036. The supply of forest residue in the UK is mostly from Scotland, supplying nearly 1 Mtpa of forest residues (NNFCC, 2014).

The utilisation of forest residues is similar to sawmill products and recycled wood. Forest residues are used to produce wood pellets and briquettes for use in bioenergy production. In 2021, the Forestry Commission reported that a total of 0.3 Mt of forest residues was used for wood pellets and briquettes (Forestry Commission, 2021). Forest residues have a high moisture content of about 50% and an LHV in the range of 15.8 – 21.4 MJ/kg on a dry basis (Thörnqvist, 1985; Nurek, Gendek and Roman, 2019). The GHG emissions of bioenergy applications of forest residues are reported to be 8.3 – 17.9 g CO_2eq per MJ of wood burned (28.6 – 61.7 g CO_2eq per MJ of electricity based on a net electricity efficiency of 29%) (Sgarbossa *et al.*, 2020). Assuming only 65% of forest residues can be assessed due to the low distribution of forest residues over wider geographical regions, about 2.2 Mtpa of forest residues can be available in the competing use case.

1.4 Other feedstocks

Other biomass feedstocks produced marginally or in insufficient quantities in the UK include virgin wood [10.8 Mtpa wet basis (Forestry Commission, 2021), LHV of 15.8 – 21.4 MJ/kg on dry basis (Thörnqvist, 1985; Nurek, Gendek and Roman, 2019)], miscanthus [0.08 – 0.13 Mtpa wet basis (Defra, 2019), LHV of 17 MJ/kg dry basis (Defra, 2001)], short rotation coppice [0.02 – 0.042 Mtpa wet basis

(Defra, 2019), LHV of 16.5 – 19.0 MJ/kg dry basis (AFBI, 2015; Hammar, Hansson and Sundberg, 2017)], used cooking oil [0.25 – 0.40 Mtpa wet basis (Toop *et al.*, 2013), LHV of 37 MJ/kg dry basis (Mehta and Anand, 2009)], black and brown liquor [0.28 Mtpa wet basis (E4tech, 2014), LHV of 9.0 – 13 MJ/kg dry basis (Vakkilainen, 2017; Bajpai, 2018)], tallow also referred to as animal fat [0.08 – 0.12 Mtpa wet basis (E4tech, 2014), LHV of 37.0 – 38.4 MJ/kg dry basis (Mehta and Anand, 2009; Gautam and Kumar, 2020)], and crude glycerine [0.03 Mtpa wet basis (E4tech, 2014), LHV of 14.0 – 20 MJ/kg dry basis (Kerr *et al.*, 2009; Yang, Hanna and Sun, 2012; Bala-Litwiniak and Radomiak, 2019)]. Despite UK virgin wood production volumes, the UK is strongly a net importer of virgin wood resources and imported a total of 20.6 Mt of wood in 2020 (Forestry Commission, 2021).

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Appendix A2: Supplementary information for Chapter 5: Comparative techno-economic and life cycle analyses of synthetic "drop-in" fuel production from UK wet biomass

Comparative techno-economic and life cycle analyses of synthetic "drop-in" fuel production from UK wet biomass

Supplementary Information

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1 General

1.1 Analysis scenarios

The analysis considers various scenarios where feedstock types, plant configurations and hydrogen sources are employed for fuel production. The feedstock types considered are wet biomass feedstocks- digestates, food waste, landfilled BMW and SS- distributed across the UK. The plant configurations used in the study are centralised and decentralised production approaches, adopting various scales. Also, various hydrogen sources- grey, blue and green hydrogen- were considered in biocrude hydroprocessing into drop-in fuels. In summary, the different feedstocks were studied based on six key scenarios, as shown in Table 1.

Table 1: Plant scenarios considered used for the various feedstocks in the analysis

Scenario	Title
Centralised, Grey H2	Centralised fuel production using grey hydrogen
Decentralised, Grey H2	Decentralised fuel production using grey hydrogen
Centralised, Blue H2	Centralised fuel production using blue hydrogen
Decentralised, Blue H2	Decentralised fuel production using blue hydrogen
Centralised, Green H2	Centralised fuel production using green hydrogen
Decentralised, Green H2	Decentralised fuel production using green hydrogen

(1) Centralised approach: In the centralised scenarios, the feedstocks from various regions in the UK are processed directly into drop-in fuels at central facilities located in the respective regions of the UK. The processing of biomass to drop-in fuels takes place within a single location, see Figure 1.

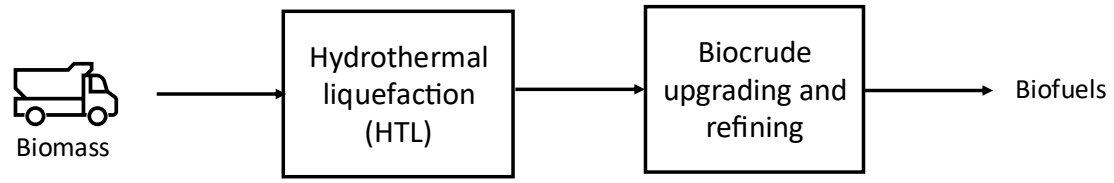


Figure 1: Centralised approach network representation

(2) Decentralised approach: In the decentralised scenarios, the biocrude produced in localised plants from various regions in the UK are transported to central facilities and processed into drop-in fuels, as shown in Figure 2.

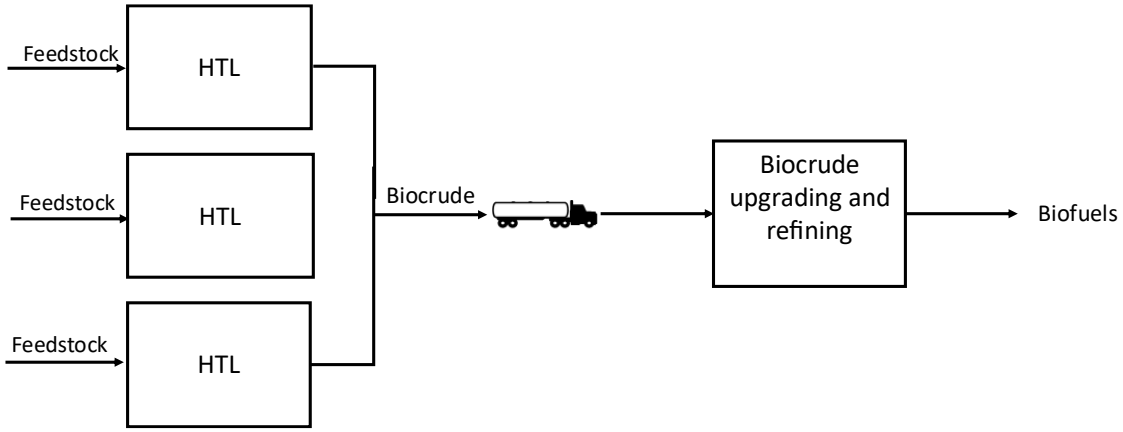


Figure 2: Decentralised approach network representation

1.2 Material and energy flow diagram

1.2.1 Feedstocks collection

1.2.1.1 Digestates

The digestate volumes in various regions of the UK were determined based on the volumes of anaerobic digestion (AD) feedstocks and the composition of digestates published by NNFCC [1], [2]. NNFCC reported a total of 15.4 Mtpa of biomass feedstocks were processed in AD facilities in 2021. NNFCC volumes arise from various feedstocks sent to AD plants such as food waste, manure, crop, and crop waste, which are processed at various AD plants in the UK. Based on NNFCC, which reported digestates yield of 90–95% and moisture content of 90–95%, the analysis assumed a digestate yield of 92.5% of input feedstocks and a moisture content of 90% [1], [2]. The digestates produced are assumed to be further dewatered mechanically to a moisture content of 75% before processing in the HTL reactor, in accordance with data produced by NNFCC [3].

The plant scales were chosen based on the 75% utilisation of digestates produced across the UK, which assumed some digestates will be inaccessible for fuel production due to wide geographical distribution, very small nature of capacities and marginal competing energy use. Table 2 gives the digestates feedstock volumes utilised in the various scenarios. The centralised cases assumed that digestates are transported to central facilities located in each of the various regions of the UK where the digestates are converted into drop-in fuels. In the decentralised case, for the localised processing of digestates into biocrude, the biocrude plants were assumed to be co-located with AD facilities which have capacities that are more than 30,000 tpa. It is further assumed that some digestates from nearby AD plants which have a capacity within 30,000 tpa are collected at the nearest biocrude plants so that the average biocrude plant capacity in any region is the total digestates volumes in the region

divided by the number of AD plant which had a capacity of more than 30,000 tpa. For more details on the transportation distance assumptions, see Section 2.4 in the main work and Section 1.2.2 ahead.

Table 2: Dewatered digestate distribution, based on data by NNFCC and plant utilisation of 75% [1], [2]

Location	**Centralised scenarios**		**Decentralised scenarios**			
	Distance (km)	**Digestate, wet (tpa)**	**Distance (km)**	**Digestate, wet (tpa)**	**Distance (km)**	**Biocrude, wet (kg/h)**
East England	52	635,272	0	23,529	52	7,425
East Midlands	47	461,492	0	25,638	47	5,394
London	15	52,753	0	52,753	15	617
North East	35	143,426	0	23,904	35	1,676
N. Ireland	45	328,692	0	97,396	45	3,842
North West	45	277,741	0	27,774	45	3,246
Scotland	105	650,713	0	27,113	105	7,605
South East	52	325,953	0	18,109	52	3,810
South West	58	519,206	0	24,724	58	6,068
Wales	54	182,647	0	30,441	54	2,135
W. Midlands	43	368,306	0	30,692	43	4,305
Yorkshire	41	348,959	0	24,926	41	4,078
Total		**4,295,160**		**406,999**		**50,200**

1.2.1.2 Food waste

The volume of food waste generated in the UK is reported to be 13.1 Mtpa [4]. It was assumed 6.06 Mtpa (46%) of food waste is available for fuel production, based on the availability of food waste after competing uses by recycling (2.1 Mtpa) and AD (4.9 Mtpa). The moisture content of the food waste was assumed to be 75%, based on Selvam [5]. As Jeswani et al. [4] and WRAP [6], [7] report did not include the distribution of food waste across the various region of the UK, the distribution of the food waste across the regions of the UK was estimated based on the population distributions of these regions, as food waste generation is heavily linked to population density. The population distribution data used were based on the 2020 UK population data reported in Statista by Clark [8].

The plant scales for the food waste case were chosen based on the availability of food waste after competing uses by recycling and AD. Table 3 gives the distribution of food waste feedstock volumes. The centralised cases assumed that food wastes are transported to central facilities located in each of the various regions of the UK where the food wastes are converted into biocrude and drop-in fuels. In the decentralised cases, for the localised processing of food waste into biocrude, each biocrude plant was assumed to be in locations which have a population of roughly 200,000 people or more, so that the individual local plant capacity is the regional food waste volumes divided by the number of plants. This favours the processing of a reasonable scale of feedstocks locally considering the population distribution of the UK over counties and cities. The produced biocrude is further processed into drop-in fuel at a central fuel production plant located in that region.

Table 3: Food waste distribution, based on data by WRAP [6], [7] and Clark [8]

Location	Centralised scenarios		Decentralised scenarios			
	Distance (km)	**Food waste, wet (tpa)**	**Distance (km)**	**Food waste, wet (tpa)**	**Distance (km)**	**Biocrude, wet (kg/h)**
East England	52	566,345	0	62,927	52	7,009
East Midlands	47	439,548	0	48,839	47	5,439
London	15	813,269	0	203,317	15	10,064
North East	35	242,175	0	80,725	35	2,997
N. Ireland	45	171,237	0	85,619	45	2,119
North West	45	665,563	0	95,080	45	8,236
Scotland	105	493,789	0	61,724	105	6,111
South East	52	832,671	0	69,389	52	10,304
South West	58	511,237	0	42,603	58	6,327
Wales	54	286,335	0	95,445	54	3,543
W. Midlands	43	538,590	0	89,765	43	6,665
Yorkshire	41	499,241	0	83,207	41	6,178
Total		**6,060,000**		**1,018,640**		**74,993**

1.2.1.3 Biodegradable municipal waste (BMW)

The volumes of BMW landfilled were based on volumes reported by Defra [9] in 2022, and the distribution of these volumes across the regions of the UK was based on BMW landfilled 2019 data published by Waste Interrogator [10]. The moisture content of BMW was assumed to be 50% and was adjusted to 75% at the HTL plants to meet pumping requirements.

The BMW MFSP analysis assumes that only 30% of landfilled BMW is used in liquid drop-in fuel production, as strong competing uses may arise for landfilled BMW from increasing AD plant capacity and other potential new energy uses. Table 4 gives the BMW feedstock volumes (with 75% moisture content) as utilised in the analysis. The centralised cases assumed that landfilled BMW volumes are transported to central facilities located in each of the various regions of the UK where the BMW are converted into biocrude and drop-in fuels. The volume distribution was based on regional landfill numbers from Waste Interrogator [10] and a BMW fraction of 48% was applied based on Defra [9] BMW fractions of landfill MSW. In the decentralised cases, for the localised processing of landfilled BMW into biocrude, each biocrude plant was assumed to be in locations which have a population of roughly 200,000 people or more, so that the individual local plant capacity is the regional landfilled BMW volumes divided by the number of plants.

Table 4: BMW distribution, based on data by Waste Interrogator [10] and Defra [9] and 30% BMW utilisation in HTL plants

Location	Centralised scenarios		Decentralised scenarios			
	Distance (km)	Landfilled BMW, wet (tpa)	Distance (km)	Landfilled BMW, wet (tpa)	Distance (km)	Biocrude, wet (kg/h)
East England	52	619,951	0	68,883	52	7,672
East Midlands	47	326,975	0	36,331	47	4,046
London	15	157,917	0	39,479	15	1,954
North East	35	166,182	0	55,394	35	2,057
N. Ireland	45	123,065	0	61,533	45	1,523
North West	45	321,235	0	45,891	45	3,975
Scotland	105	364,910	0	45,614	105	4,516
South East	52	648,774	0	54,065	52	8,029
South West	58	319,585	0	26,632	58	3,955
Wales	54	138,283	0	46,094	54	1,711
W. Midlands	43	378,224	0	63,037	43	4,681
Yorkshire	41	394,900	0	65,817	41	4,887
Total		**3,960,000**		**608,769**		**49,005**

1.2.1.4 Sewage sludge (SS)

Based on Nuamah et al. (2012), SS production was estimated to be 1.5 Mtpa (dry) in the UK, which is about 30 Mtpa (wet) for raw SS with a moisture content of 95% [11]. It is assumed that the SS is dewatered mechanically at SS plants prior to transportation and utilisation in HTL. It is dewatered to a moisture content of 75%, which is the minimum moisture content that is considered to be attainable with conventional dewatering technology while still enabling effective pumping in the HTL plant [12]. The distribution of the SS across the regions of the UK was estimated using the population distribution of the UK at various regions, based on the 2020 UK population data reported in Statista by Clark [8].

The plant scales for the SS case were chosen based on the 100% utilisation of the SS produced in the UK, as this process seeks to avoid the expensive conventional SS treatment process. The cost of treating raw SS is reported to be £200 per dry tonne of sludge treated [13]. Table 5 gives the SS feedstock volumes utilised in the scenarios. The centralised cases assumed that SS are transported to central facilities located in each of the various regions of the UK where the SS are converted into biocrude and drop-in fuels. In the decentralised cases, for the localised processing of SS into biocrude, each biocrude plant was assumed to be in locations which have a population of at least 200,000 people, so that the individual local plant capacity is the regional SS volumes divided by the number of plants. The produced biocrude is further processed into drop-in fuel at a central fuel production plant located in that region.

Table 5: Dewatered SS distribution, based on data by Nuamah et al. [11], Clark [8] and 100% SS utilisation.

Location	Centralised scenarios		Decentralised scenarios			
	Distance (km)	**SS, wet (tpa)**	**Distance (km)**	**SS, wet (tpa)**	**Distance (km)**	**Biocrude, wet (kg/h)**
East England	52	560,738	0	62,304	52	5,706
East Midlands	47	435,196	0	48,355	47	4,428
London	15	805,217	0	201,304	15	8,193
North East	35	239,778	0	79,926	35	2,440
N. Ireland	45	169,542	0	84,771	45	1,725
North West	45	658,973	0	94,139	45	6,705
Scotland	105	488,900	0	61,112	105	4,975
South East	52	824,427	0	68,702	52	8,389
South West	58	506,175	0	42,181	58	5,150
Wales	54	283,500	0	94,500	54	2,885
W. Midlands	43	533,258	0	88,876	43	5,426
Yorkshire	41	494,298	0	82,383	41	5,029
Total		**6,000,000**		**1,008,554**		**61,050**

1.2.1.5 Co-processing of the feedstocks

In the co-processing of the feedstocks, the various feedstocks were assumed to be processed together based on their respective individual volumes. Hence, the average moisture content of 75% and biocrude yield of 37.1 wt% per dry feedstock were used (see SI Section 1.2.4.1 for details). Table 6 gives the input flow stream of the co-processing scenario.

Table 6: Feedstocks distribution in the co-processing of various wet biomass together

Location	Centralised scenarios		Decentralised scenarios			
	Distance (km)	**Feedstocks, wet (tpa)**	**Distance (km)**	**Feedstocks, wet (tpa)**	**Distance (km)**	**Biocrude, wet (kg/h)**
East England	52	2,382,306	0	248,627	52	27,811
East Midlands	47	1,663,211	0	204,446	47	19,308
London	15	1,829,155	0	354,531	15	20,828
North East	35	791,561	0	183,442	35	9,169
N. Ireland	45	792,536	0	441,375	45	9,209
North West	45	1,923,511	0	224,420	45	22,163
Scotland	105	1,998,311	0	194,104	105	23,206
South East	52	2,631,826	0	264,252	52	30,531
South West	58	1,856,203	0	147,116	58	21,500

Location	Centralised scenarios		Decentralised scenarios			
	Distance (km)	**Feedstocks, wet (tpa)**	**Distance (km)**	**Feedstocks, wet (tpa)**	**Distance (km)**	**Biocrude, wet (kg/h)**
Wales	54	890,765	0	199,669	54	10,274
W. Midlands	43	1,818,377	0	245,304	43	21,076
Yorkshire	41	1,737,397	0	284,668	41	20,173
Total		**20,315,160**		**2,991,953**		**235,247**

1.2.2 Transportation

The transportation distances used in the TEA, with key assumptions as highlighted in the main work in Section 2.4, were estimated based on the area-weighted average radius (two-thirds of the radius) of the circle is the average transport distance and are shown in Table 7.

Table 7: Average feed transport distance in various regions of the UK

Region	Area (km^2)	Average transport distance (km)
East England	19120	52.0
East Midlands	15627	47.0
London	1527	14.7
North East	8592	34.9
Northern Ireland	14130	44.7
North West	14165	44.8
Scotland	77933	105.0
South East	19096	52.0
South West	23800	58.0
Wales	20779	54.2
West Midlands	12998	42.9
Yorkshire	11903	41.0

In the LCA, transportation of the biomass feedstocks was assumed to be done using a truck (14-20 t) with a payload of 12 t. The national average distance over the regions of 50 km, for the transportation of the feedstocks to central facilities, while the average distance of 0 km was used in the decentralised movement of feedstocks for biocrude production at local sites. Local biocrude plants are assumed to be co-located with the waste generation/collection sites. The transportation emissions factor was obtained from the GaBi [14].

1.2.3 Feedstock dewatering

The moisture contents of digestates and SS are significantly high, up to 95%, and this requires water removal prior to processing in HTL reactors, to optimise the plant capital and operating cost. Dewatering usually consumes saves energy in HTL than when sludge or digestates are treated by HTL without reducing their moisture content [15]. The dewatering of these wet feedstocks is usually done to a moisture content of about 75%, which is the target considered the maximum attainable with

conventional dewatering technologies while still enabling effective pumping of the wet feedstocks. In this analysis, the dewatering of the feedstocks was assumed to be done at the local plants where they are generated, that is in AD and SS plants, due to the ease of integration of dewatering systems to these plants, as some AD plants often dewater digestates, according to WRAP [16]. Also, dewatering at AD and SS sites will provide savings on the cost of transportation.

In dewatering systems, the performance and power consumption of sludge dewatering depends on the sludge type and the technology used [15]. Conventional mechanical dewatering technologies, such as screw presses have low power consumption and can easily be maintained by operators. Huber [15] reported the power consumption of belt and screw press machines in the range of 10–30 kWh/t, while Zebra Tube [17] reported a power consumption of 30 kWh/t. These reported data have good agreement with each other, and hence, the analysis assumed an average of 30 kWh/t power consumption.

1.2.4 Feedstock processing

The process flow of the HTL plant was based on simulation approaches by Zhu [18], Snowden-Swan et al. [12] and Jones et al. [19], as shown in Figure 3. The fuel production processes can be divided into biocrude production and upgrading.

1.2.4.1 Biocrude production

Based on Snowden-Swan et al. [12], the feed, which is the waste material is pumped and preheated in the pre-treatment unit of the plant. The heat from the reactor liquid product (biocrude/aqueous mixture) is used for the preheating of the feed, prior to further heating to the reaction temperature of 347°C in a fired heater using a hot oil system. Also, other activities are done in this unit such as salt removal. The heated and pressurized feedstock is fed to the HTL reactor where the HTL of the feedstock into biocrude is done. Some side products are produced in the HTL reactor which include aqueous solution, solids (char) and some amount of gases, which are separated from the biocrude downstream of the reactor. The solids in the reactor effluent are separated using a hot filter. After solids separation, the biocrude-aqueous-gas mixture is cooled and passed through a three-phase separator where it is separated into biocrude, aqueous and gas streams. The biocrude is then stored and sent for further processing into biofuels in the biocrude upgrading plant. The aqueous stream, which contains effluent water and any remaining soluble organics, metal salts, and ammonia, is channelled to the HTL aqueous phase treatment for wastewater treatment. The gas stream is utilised in a fired heater for the final heating of the feedstock to the reactor operating temperature. Additional heating is supplied by natural gas to supplement the energy demand of HTL. The HTL biocrude yields for digestates, food waste, BMW and SS used in the analysis were 37.4%, 39.6, 39.6% and 32.6%, respectively, based on data from Snowden-Swan et al. [20] and Chen et al. [21]**.** The yield reported by Snowden-Swan et al. [20] for sludge conversion was assumed to also represent digestates conversion since both feedstocks are produced from the same process of AD. The biocrude yields of digestates and SS were adjusted to the dry basis of the feedstocks by using digestates ash content of 15% from Taufer [22] and Dziedzic [23] reported range and SS ash content of 26% from Snowden-Swan et al. [20]. See Table 8 for details.

Table 8: Product distribution of HTL of digestates

Component	**Yield, wt% per dry basis of feed**	**References**
Oil	37	[20]
Aqueous (water)	26	[20]
Gas	29	Material balance

Component	Yield, wt% per dry basis of feed	References
Solid	8	[20]

Table 9: Product distribution of HTL of food waste

Component	Yield, wt% per dry basis of feed	References
Oil	40	[21]
Aqueous (water)	31	[24], [25]
Gas	17	Material balance
Solid	12	[24], [25]

Table 10: Product distribution of HTL of BMW

Component	Yield, wt% per dry basis of feed	References
Oil	40	[21]
Aqueous (water)	31	[24], [25]
Gas	17	Material balance
Solid	12	[24], [25]

Table 11: Product distribution of HTL of SS

Component	Yield, wt% per dry basis of feed	References
Oil	33	[20]
Aqueous (water)	23	[20]
Gas	38	Material balance
Solid	7	[20]

Table 12: Product distribution of HTL in the co-processing case

Component	Yield, wt% per dry basis of feed	References
Oil	37	Material balance
Aqueous (water)	28	Material balance
Gas	26	Material balance
Solid	9	Material balance

In the TEA and LCA, side products produced during this process, which are gas and char, are assumed to be consumed in the plant, by combustion to generate the thermal energy requirements for the plants. These assumptions were based on similar assumptions taken in the TEA studies by several authors such as Snowden-Swan [12], Jones [19] and Zhu [18]. Energy is recovered from the burning of gases and char, which is used to pre-heat the feedstocks and provide heat to the HTL reactor. Additionally, a total of 6.54 scf per GLE (7.04 MJ/GLE) of biocrude is used in the HTL and wastewater treatment units, based on the model by Snowden-Swan [12]. The biocrude energy is recovered via heat exchangers, and this is used to provide most of the heating requirement for the preheating.

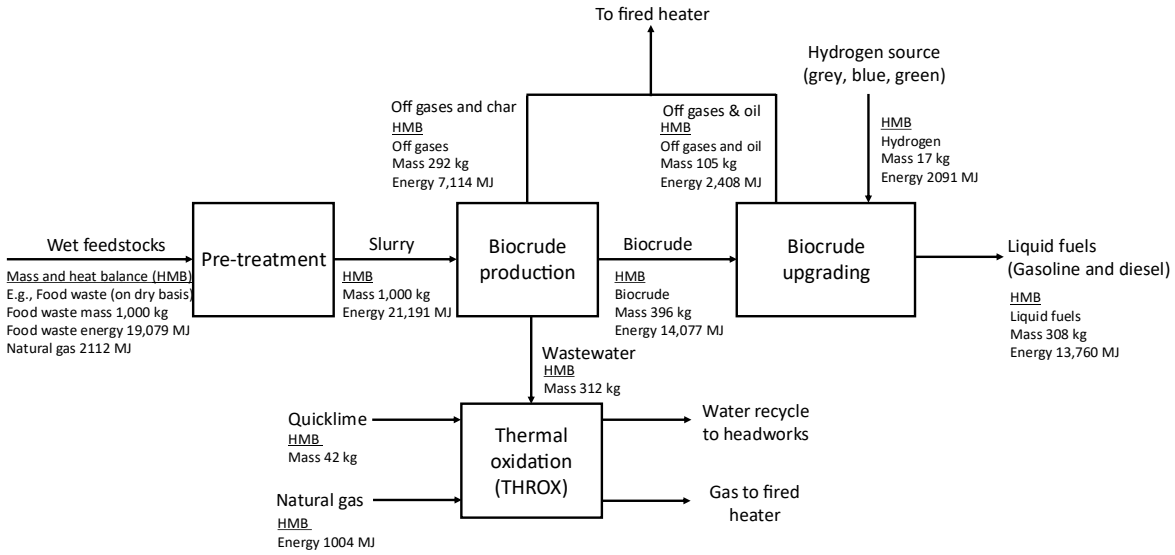


Figure 3: HTL biocrude production and upgrading flow diagram with material and energy balance of key processes

1.2.4.2 Biocrude upgrading

The biocrude upgrading stage converts the biocrude produced into renewable gasoline and diesel. This is done through hydroprocessing which uses hydrogen to de-oxygenate and other impurities such as nitrogen and sulphur from the biocrude, while cracking it into short-chain hydrocarbon fuels. The hydrocarbon fuels are separated in the product fractionating unit. The liquid fuels yield- gasoline and diesel- produced during hydroprocessing were estimated at 77.9% wt/wt biocrude, based on simulation results obtained by Snowden-Swan [12]. The amount of hydrogen used in hydroprocessing is dependent on the composition of the biocrude. The hydrogen required for the hydroprocessing stage was estimated to be about 0.039–0.049 kg/kg biocrude, based on analyses by Jones [19], Jiang [26] and Bennion [27]. Grey, blue and green hydrogen scenarios were analysed in this study. Other data such as the electricity emissions factor, hydrogen emissions factor and other material and energy emissions factors were obtained from the literature. No natural gas consumption is assumed to be done in the oil upgrading unit as off-gases and heavy fuel oil are used for heating, based on Snowden-Swan [12] model.

1.2.4.3 Material and energy balance

The summary of the mass and energy balance is shown in Figure 3 and Table 14. The mass balance of the fuel process is generated from the respective biocrude yield of the feedstocks and the hydrotreating yield. The energy balance is generated by using the energy efficiency of 57%, based on the simulated efficiency of 52–65% by Zhu et al. [18]. The energy efficiency is the ratio of the energy of the liquid fuels to the energy (of the feedstocks, natural gas and hydrogen) directly used in the plant. Using intermediates and final products LHV in Table 13, the LHV of the input feedstock materials are determined. The LHV of hydrogen was taken as 120 MJ/kg [28], [29]. It is worthwhile to note that this study only modelled the fuel production process and doesn't experimentally convert the biomass feedstocks to fuel nor directly measure the energy content of the feedstocks and products. Conversion from kg of fuel to L of fuel was done using a gasoline density of 0.737 kg/L and a diesel density of 0.798 kg/L, based on data from Snowden-Swan [12].

Table 13: Energy contents of key streams

Material	**Energy content, MJ/L**	**Reference**
Naphtha (gasoline) blendstock	32.0	[30]
Gasoline	31.8	[30]
Diesel blendstock	36.1	[30]
Biocrude	34.8	[12]

Table 14: Mass and energy balance of digestates to drop-in fuels

Component	**Value**	**Unit**
Biomass feed consumption	18021.0	MJ
H2 consumption	1974.7	MJ
Natural gas consumption	2943.1	MJ
Liquid HC fuels	12995.9	MJ
Biomass feed consumption, dry	1000	kg
H2 consumption	16.5	kg
Liquid HC fuels	291	kg
Diesel to gasoline ratio	3.25	kg/kg
Energy efficiency (biomass, H2 and natural gas to fuels)	57	%
Mass efficiency	29	%
Liquid HC fuel yield	97.9	gal/dry ton
Biomass (digestates) LHV	18.0	MJ/kg
Average fuel LHV	35.1	MJ/L

Table 15: Mass and energy balance of food waste to drop-in fuels

Component	**Value**	**Unit**
Biomass feed consumption	19079.3	MJ
H2 consumption	2090.9	MJ
Natural gas consumption	3116.2	MJ
Liquid HC fuels	13760.4	MJ
Biomass feed consumption, dry	1000	kg
H2 consumption	17.4	kg
Liquid HC fuels	308	kg
Diesel to gasoline ratio	3.25	kg/kg
Energy efficiency (biomass, H2 and natural gas to fuels)	57	%
Mass efficiency	30	%
Liquid HC fuel yield	103.6	gal/dry ton
Biomass (food waste) LHV	19.1	MJ/kg
Average fuel LHV	35.1	MJ/L

Table 16: Mass and energy balance of BMW to drop-in fuels

Component	**Value**	**Unit**
Biomass feed consumption	19077.1	MJ

H2 consumption	2090.9	MJ
Natural gas consumption	3116.2	MJ
Liquid HC fuels	13760.4	MJ
Biomass feed consumption, dry	1000	kg
H2 consumption	17.4	kg
Liquid HC fuels	308	kg
Diesel to gasoline ratio	3.25	kg/kg
Energy efficiency (biomass, H2 and natural gas to fuels)	57	%
Mass efficiency	30	%
Liquid HC fuel yield	103.6	gal/dry ton
Biomass (BMW) LHV	19.1	MJ/kg
Average fuel LHV	35.1	MJ/L

Table 17: Mass and energy balance of SS to drop-in fuels

Component	**Value**	**Unit**
Biomass feed consumption	15688.0	MJ
H2 consumption	1719.2	MJ
Natural gas consumption	2562.2	MJ
Liquid HC fuels	11314.1	MJ
Biomass feed consumption, dry	1000	kg
H2 consumption	14.3	kg
Liquid HC fuels	254	kg
Diesel to gasoline ratio	3.25	kg/kg
Energy efficiency (biomass, H2 and natural gas to fuels)	57	%
Mass efficiency	25	%
Liquid HC fuel yield	85.2	gal/dry ton
Biomass (SS) LHV	15.7	MJ/kg
Average fuel LHV	35.1	MJ/L

Table 18: Mass and energy balance of the co-processing of the various feedstocks to drop-in fuels

Component	**Value**	**Unit**
Biomass feed consumption	17840.8	MJ
H2 consumption	1956.5	MJ
Natural gas consumption	2562.2	MJ
Liquid HC fuels	12876.2	MJ
Biomass feed consumption, dry	1000	kg
H2 consumption	16.3	kg
Liquid HC fuels	289	kg
Diesel to gasoline ratio	3.25	kg/kg
Energy efficiency (biomass, H2 and natural gas to fuels)	57	%
Mass efficiency	28	%
Liquid HC fuel yield	97.0	gal/dry ton
Biomass (Coprocessing) LHV	17/8	MJ/kg

Average fuel LHV	35.1	MJ/L

1.2.5 Fuel transportation and distribution

The transportation and distribution of the fuels were assumed to be within an average distance of 50 km. A truck (14-20 t) with a payload of 12 t, which emits 0.06 g CO_2eq/kg cargo.km, was assumed to be used for the transportation and distribution of the fuels, based on a publication by GaBi [14].

2 Economic analysis

In the estimation of capital cost, equipment costs are used. The original equipment cost, the associated scaling factor (n) and the installation factors of various equipment are shown in Table 19. These factors were majorly based on values reported by Jones et al. [19] and Snowden-Swan et al. [12]. Adjustments using the chemical engineering plant cost indexes were made where necessary to account for any differences in equipment costing year.

1 Table 19: Plant equipment costing basis

Unit	Equipment name	New flow basis	Original equip. flow	Units	Original equip. cost	Base year	Cost: installed (i) or bare (b)	Scaling factor	Instal factor	Ref.
HTL	HTL system (reactor, heater, pump, cooling, product separation)	Feed rate	138,889	kg/h	£13,888,099	2011	b	0.77	2.1	[19]
	Solids filter, oil/water separat.	Feed rate	553,276	kg/h	£2,923,476	2011	b	0.68	1.9	[19]
	Hot oil system	Feed rate	138,889	kg/h	£3,460,679	2011	b	0.6	1.4	[19]
HTL water treatment	Water treatment system (lime, ammonia, THROX unit)	Feed rate	15,422	kg/h	£902,341	2014	b	0.65	2.4	[12]
Biocrude upgrading	Desalter	Biocrude flow rate	2,732	bpd	£569,458	2007	i	0.75	2.5	[12]
	Hydrotreater Fe Bed	Biocrude flow rate	15,472	bpd	£12,079,150	2014	i	0.75	1.5	[12]
	Hydrotreater Reactor, vessels, columns	Biocrude flow rate	15,472	bpd	£57,118,776	2014	i	0.75	1.5	[12]
	Hydrogen compressor	50% of biocrude flow	1,717	kg/h	£1,026,675	2014	b	0.6	1.4	[12]
	PSA for Hydrogen Recycle	Biocrude/H2 ratio	10	MMscfd	£1,296,680	2004	b	0.8	1.4	[12]
Hydrocracking	Hydrocracker Unit + auxiliaries	Biocrude flow rate	15,472	bpd	£37,684,338	2014	i	0.75	1.5	[12]
Cooling water system	Cooling tower and pump system	Circ./feed rate ratio	16,162,240	kg/h	£1,812,167	2009	b	0.6	2.95	[19]
OSBL	Plant air compressor	Feed rate (dry) × 3	119,047	kg/h	£65,147	2007	b	0.3	1.6	[12]
	Instrument air dryer	Feed rate (dry) × 3	119,047	kg/h	£6,186	2002	b	0.6	2.5	[12]
	Plant air receiver	Feed rate (dry) × 4	119,047	kg/h	£15,564	2007	b	0.65	5.4	[12]
	Firewater pump	Feed rate (dry) × 5	119,047	kg/h	£17,074	2007	b	0.3	3.7	[12]
	Firewater storage tank	Feed rate (dry) × 6	119,047	kg/h	£170,347	2007	b	0.65	1.5	[12]
	Feed storage tank- 3 day	Feed rate (wet) × 3	1,000,000	gal	£1,757,484	2010	b	0.7	1.4	[12]
	Product storage tank- 3 day	Product rate × 3	1,000,000	gal	£1,757,484	2010	b	0.7	1.4	[12]
	Product storage tank- 3 day	Product rate × 3	1,000,000	gal	£1,757,484	2010	b	0.7	1.4	[12]
	Product storage tank- 3 day	Product rate × 3	1,000,000	gal	£1,757,484	2010	b	0.7	1.4	[12]

2

3 Life-cycle analysis

The production of drop-in fuels via HTL consists of stages such as the raw material generation and the fuel production stage. Various inventory data and emission factors from the literature were used to estimate the life cycle emissions involving the fuel production and utilisation processes.

3.1 Current waste management

In the consequential approach, the emissions associated with the diversion of the wet waste feedstocks from current waste management systems are evaluated. The current waste management systems for food waste (excluding recycling) include AD, composting, incineration and landspreading. The volumes used in this waste treatment were based on data published by NNFCC [1], Defra [9], WRAP[7], [31], WRAP and Jeswani [4]. Digestates are usually applied on land, with a small portion being incinerated. Landfilled BMW volumes are reported by Defra [32], and these have been used for this analysis, while SS is mainly applied on land as fertiliser with a small fraction being incinerated.

3.1.1 Foregone fertiliser credits

The waste treatment processes of AD, compositing, landspreading and SS treatment yield valuable products. These products (digestates, compost and dry SS) are known for their nutrient content, especially their high nitrogen content when compared to livestock slurries and manure. The two other important nutrients that are present in digestates, compost and SS are phosphate and potash. These products are used as substitutes for synthetic fertilisers when they are applied to soils. The impact of these products on land applications is crucial in the evaluation of the impact of using these feedstocks for fuel production. According to WRAP [33] and Singh et al. [34], the use of digestates, SS and compost provides nutrient benefits shown in Table 20. Digestates and SS are assumed to have similar nutrients since both are produced via AD processes. These benefits are captured in the foregone fertiliser displacement credits, and the GHG emissions of producing these nutrients in synthetic fertilisers are accounted for in this analysis. The digestates were assumed to be stripped of methane during the first phase of their decomposition, as AD and SS plants aim to maximise biogas yield. Emission factors of N, P_2O_5, and K_2O from Ecoinvent were used in the analysis.

Table 20: Nutrient displacement credits from land application of digestates, compost and SS

Nitrogen content	kg N/ton fresh weight	kg P_2O_5/ton fresh weight	kg K_2O/ton fresh weight	Moisture content	Ref.
Digestate	5	0.5	2	96%	[33]
Compost	9.25	3	5.5	60%	[33]
SS	1.59	0.62	0.41	95%	[34]

3.1.2 Carbon sequestration

Furthermore, the application of some products like digestates, compost and SS are reported to offer some form of carbon locking into the soil. Digestates, compost and SS have significant amounts of carbon content, in which some fractions are eventually released to the environment as biogenic CO_2 while some are sequestered into the soil. According to Nyang'au et al. [35], 12–16% of the carbon in digestates is sequestered in the soil for the long-term, while the balance is oxidised into biogenic CO_2. The sequestered carbon from SS and compost were assumed to be of the same yield, as shown in Figure 4.

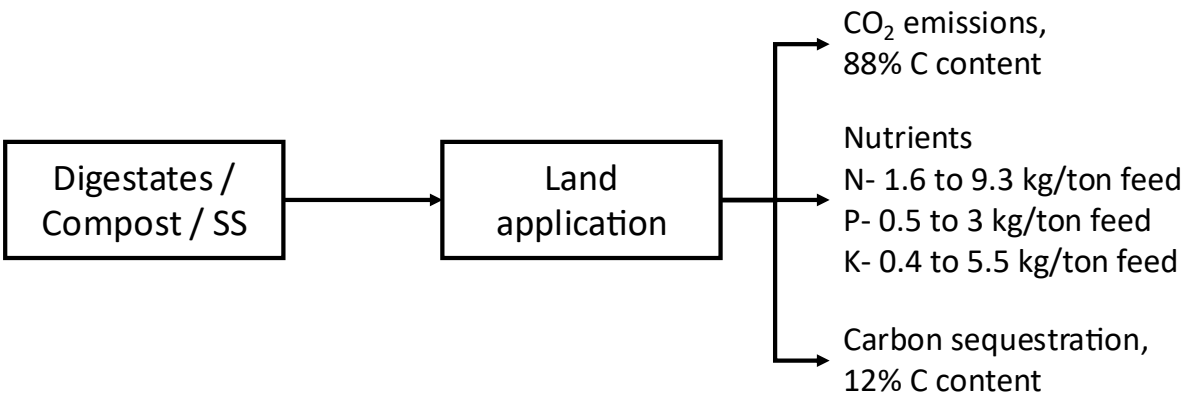


Figure 4: Carbon balance of digestate, compost and sewage sludge

3.1.3 Foregone electricity credits

The electricity lost from the diversion of the feedstocks from conventional processes such as AD and incineration is also considered. Currently, some energy generation is being done from food waste, digestates and SS processing through incineration and AD. The electricity generation potential of digestates is given in Table 21, computed based on the method by Đurdevic [36] and NNFCC [37]. AD and incineration produced electricity into the grid which helps reduce the emissions from national electricity generation. Electricity emission rates based on BEIS [38] data were used to compute the foregone electricity credits.

Table 21: Electricity potential for the waste feedstocks

Waste / Treatment	**Electricity potential**	**Units**	**Reference**
Incineration			
Digestate	1.33	MWh/tonne feed, dry	[39]
Food waste	1.42	MWh/tonne feed, dry	[39]
AD			
Food waste	0.30	MWh/tonne feed, wet	[37]

3.1.4 Avoided treatment emissions

The avoided emissions from the conventional waste treatment process are calculated and accounted for in the LCA. These processes include landfilling, composting and landspreading. The emission rates from the landfilling of biogenic waste are estimated at 400 tons CO2eq per ton MSW by Nordahl [40], while the emission rates from composting were based on Ecoinvent data. The wastes which are treated by either composting, landspreading or landfilling are food waste. The land application of digestates and SS are assumed to emit zero methane as the methane is stripped off during AD processes (maximum methane recovery).

3.2 Inventory data

The summary of the inventory data, from the waste generation/collection to fuel combustion, used in the LCA is outlined in Table 22. The data were collected across the various stages of fuel production ranging from feedstock collection and transportation to fuel transportation and distribution.

Table 22: Summary of the key inventory data used in the LCA evaluations

Description	Process values	Units	References for process and emissions factors
Raw materials collection and processing			
Dewatering	30	kWh/ton feed dewatered	[15], [17], [38]
Feed transportation			
Truck (14-20 t), payload 12 t	0.06	g CO_2/kgcargo.km	[14]
HTL unit			
Electricity (HTL plant)	1.6	kWh/GGE biocrude	[26], [38]
Natural gas	26.65	MJ/GGE biocrude	[12], [41]
Biocrude ($NaCO_3$) catalyst	0.0004	kg/kg feed	[12], [42]
Cooling water makeup	0.0469	L/kg biocrude	[43], [44]
Quicklime (CaO)	0.106	kg/kg biocrude	[43], [45], [46]
Solids to landfill (85% $CaCO_3$)	0.219	kg/kg biocrude	[43]
Biocrude upgrading			
Hydrogen	0.044	kg/kg biocrude	[12], [47]
Zeolite catalyst	0.0006	kg/kg biocrude	[12], [19], [48], Ecoinvent
Electricity (upgrading plant)	0.37	kWh/GGE biofuel	[12], [38]
Cooling water makeup	0.0153	L/kg biocrude	[43], [44]
Product distribution			
Truck (14-20 t), payload 12 t	0.06	g CO2eq/kg cargo.km	[14]

4 Production prices

4.1 Plant scale

The effect of plant scale on the fuel production price from food waste, landfilled BMW and SS are shown in

Figure 5.

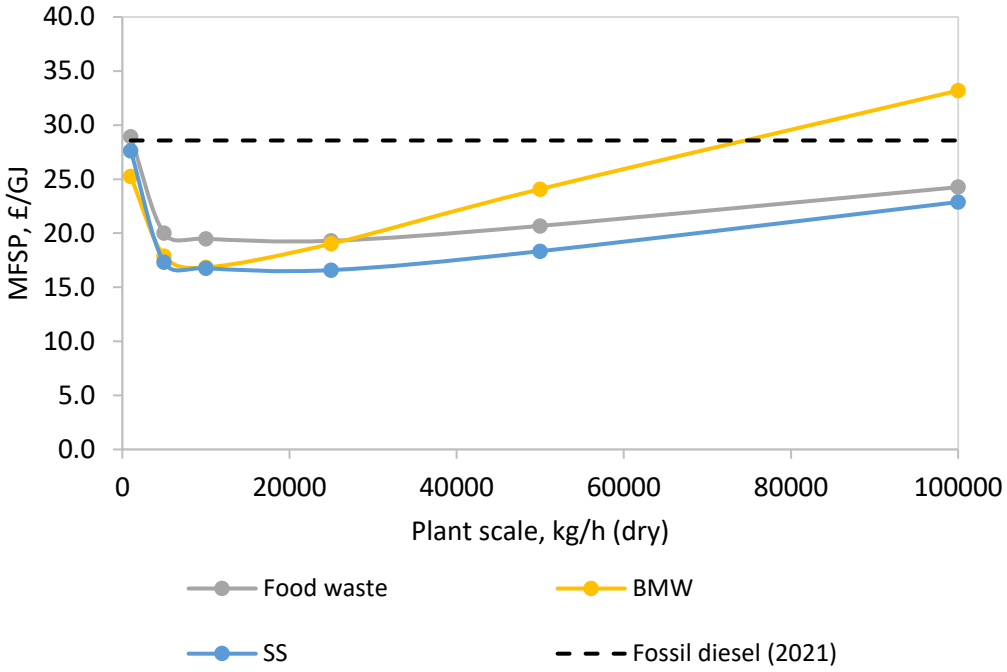
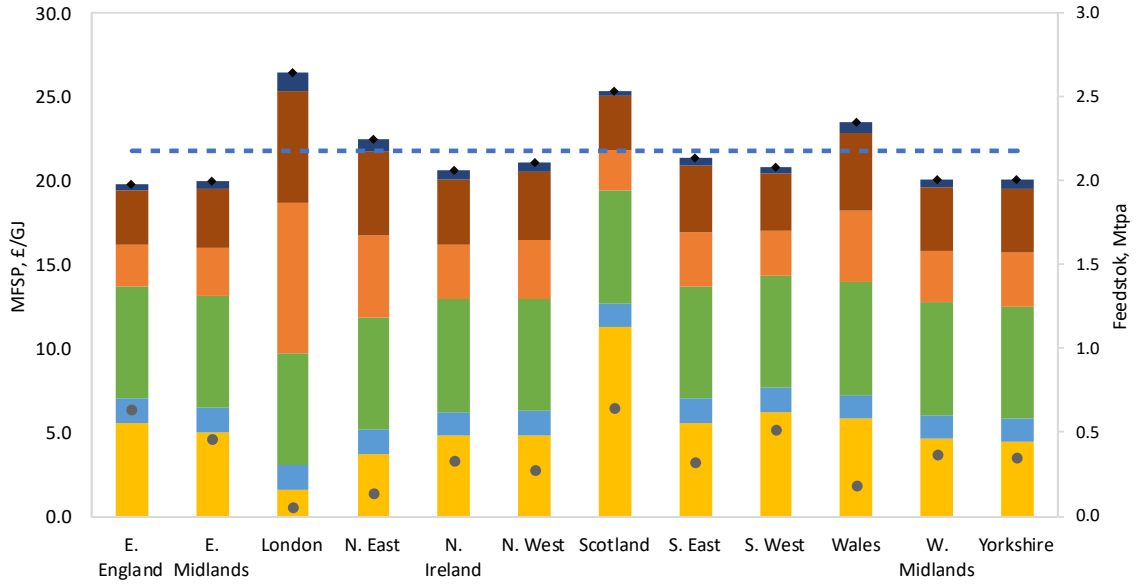


Figure 5: Effects of plant scale on the processing of food waste, BMW, and SS

4.2 Prices of feedstocks per region

Here, the results averages of Figure 6 in Section 3.1 of the main work are represented by feedstock and region as calculated in the economic analysis, as shown in Figure 6. The average of these results is used to plot Figure 6, Section 3.1 of the main work.

(a)



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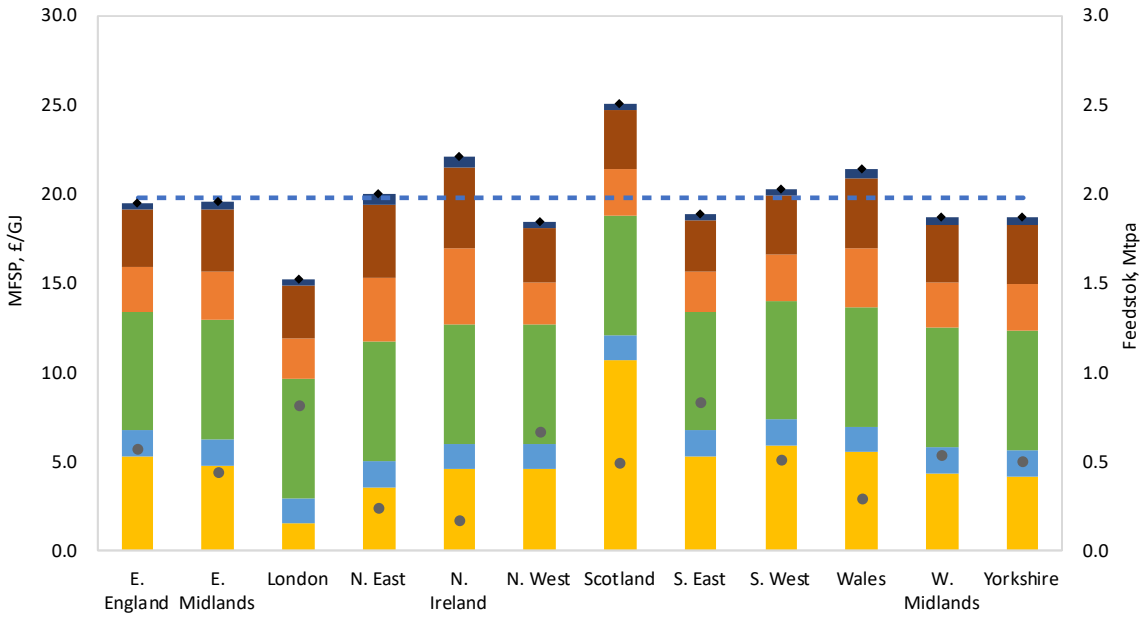
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MFSP, £/GJ
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Feedstok, Mtpa
E. England
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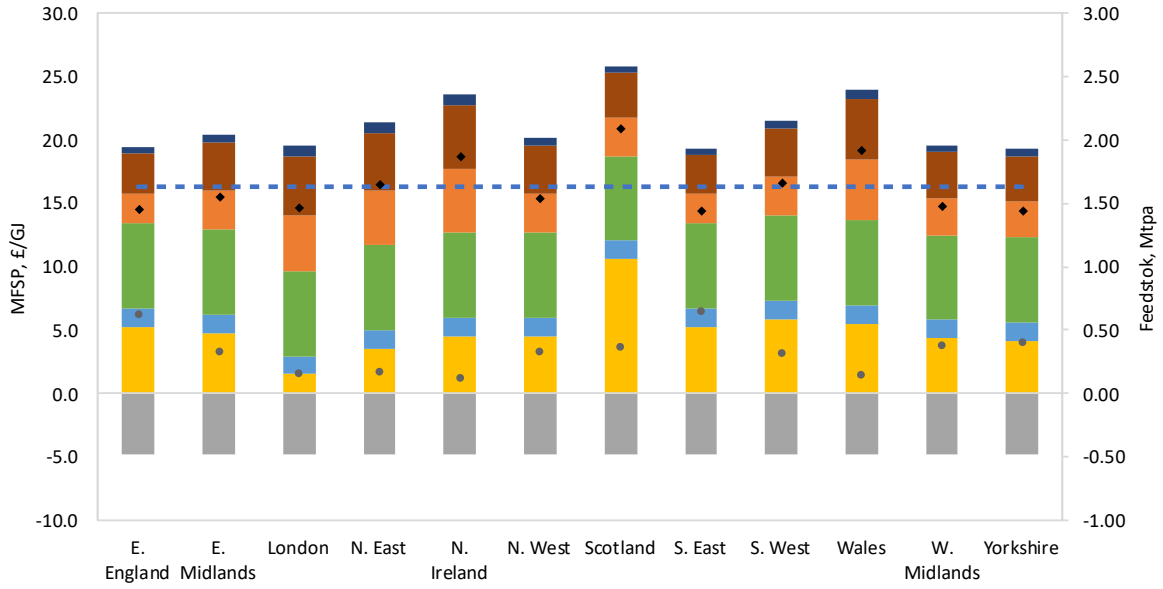
W. Midlands
Yorkshire

(c)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MFSP, £/GJ
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2.50
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Feedstok, Mtpa
E. England
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W. Midlands
Yorkshire

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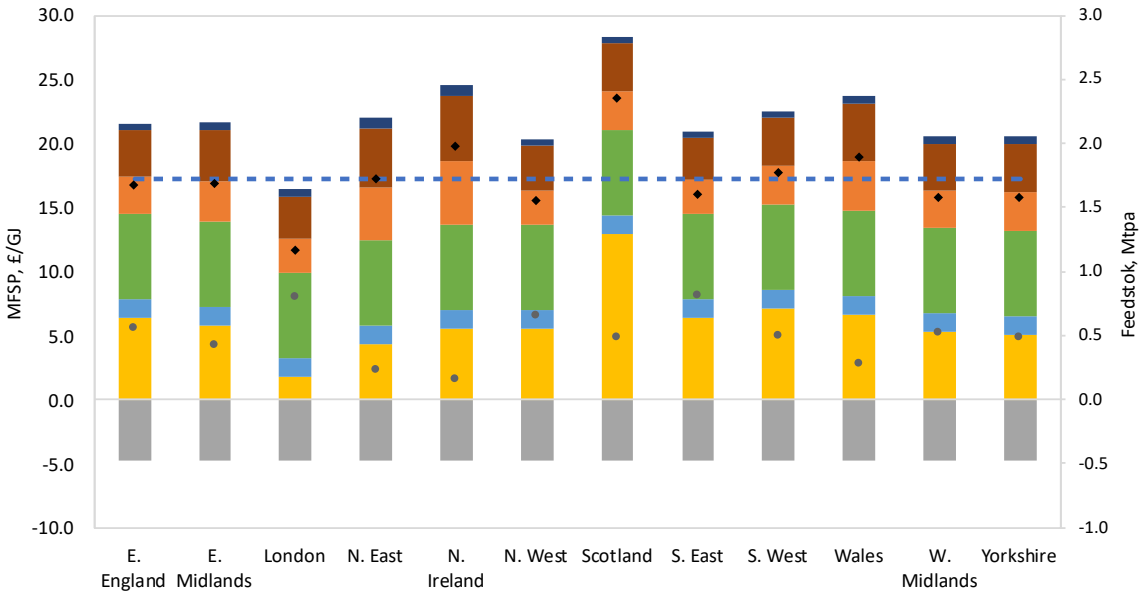

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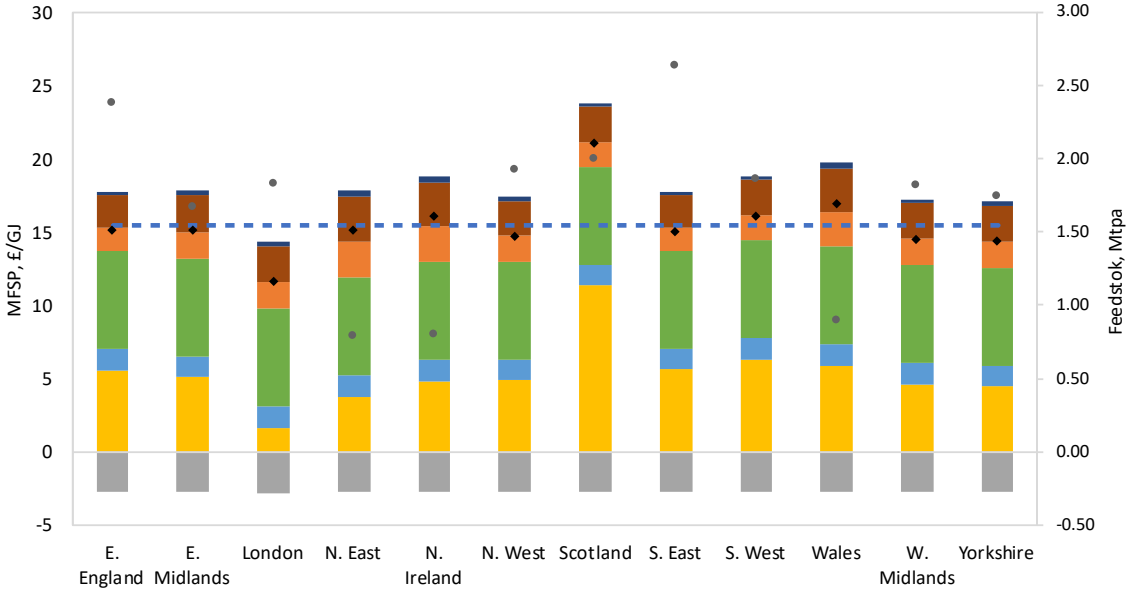
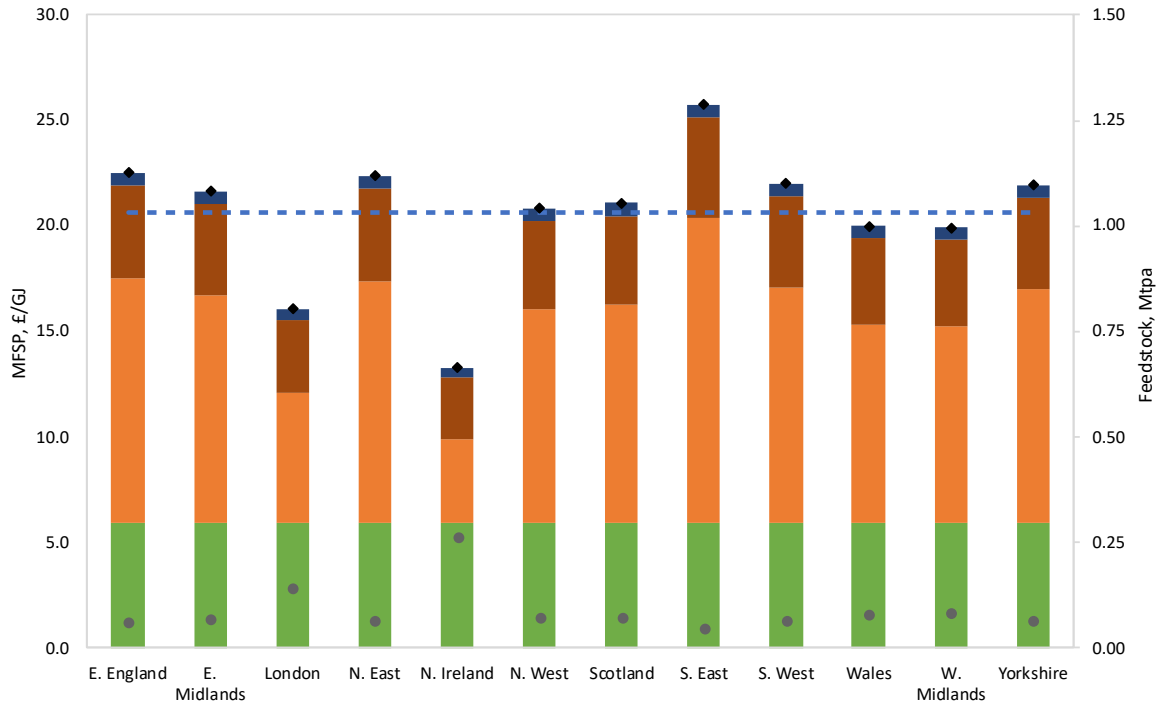




Figure 6: MFSP distribution of the HTL processing for (a) digestates (b) food waste (c) BMW (d) SS and (e) co-processing the digestates, food waste, BMW and SS, based on the Centralised, Grey H2 scenario

(a)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Feedstock, Mtpa
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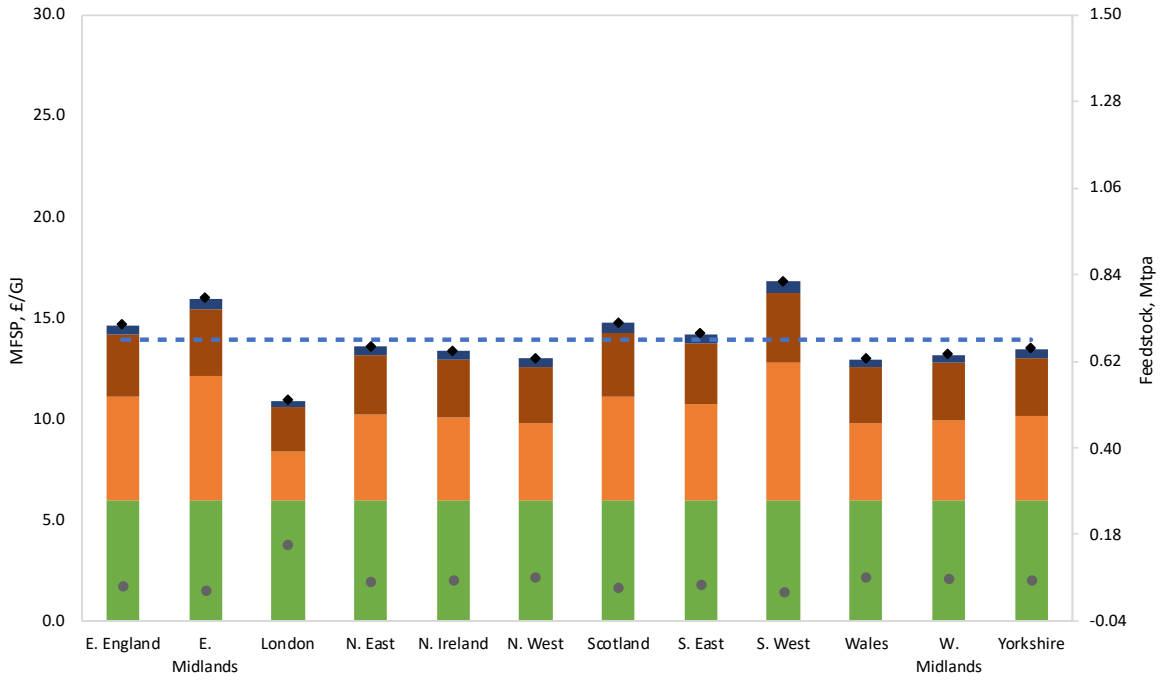
Wales
W. Midlands
Yorkshire

(b)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Feedstock, Mtpa
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N. Ireland
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Scotland
S. East
S. West
Wales
W. Midlands
Yorkshire

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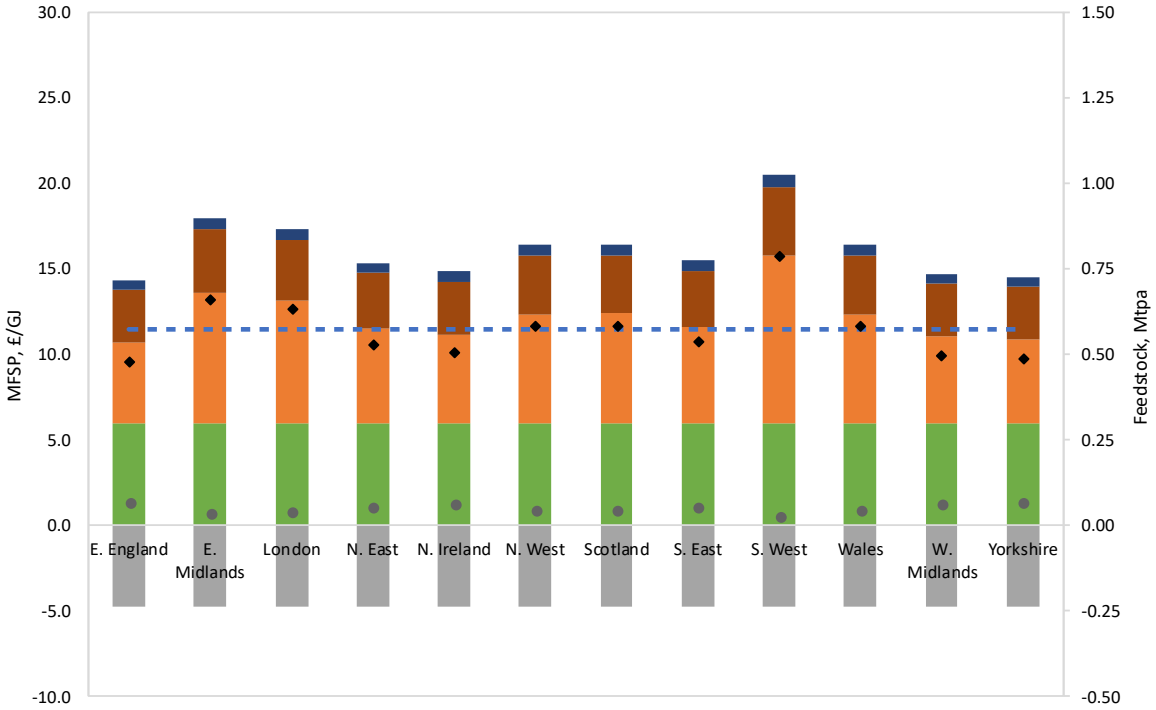
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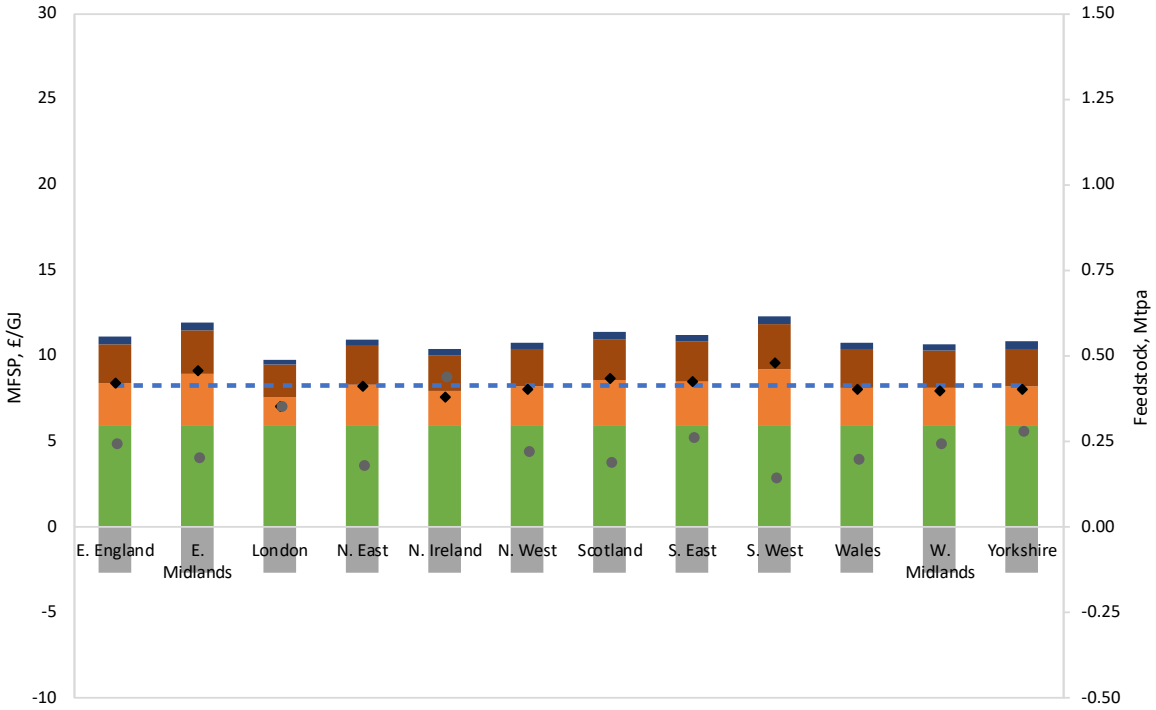
-0.25
-0.50
MFSP, £/GJ
Feedstock, Mtpa
E. England
E. Midlands
London
N. East
N. Ireland
N. West
Scotland
S. East
S. West
Wales
W. Midlands
Yorkshire

(d)


30
25
20
15
10
5
0
-5
-10
1.50
1.25
1.00
0.75
0.50
0.25
0.00
-0.25
-0.50
MFSP, £/GJ
Feedstock, Mtpa
E. England
E. Midlands
London
N. East
N. Ireland
N. West
Scotland
S. East
S. West
Wales
W. Midlands
Yorkshire

(e)

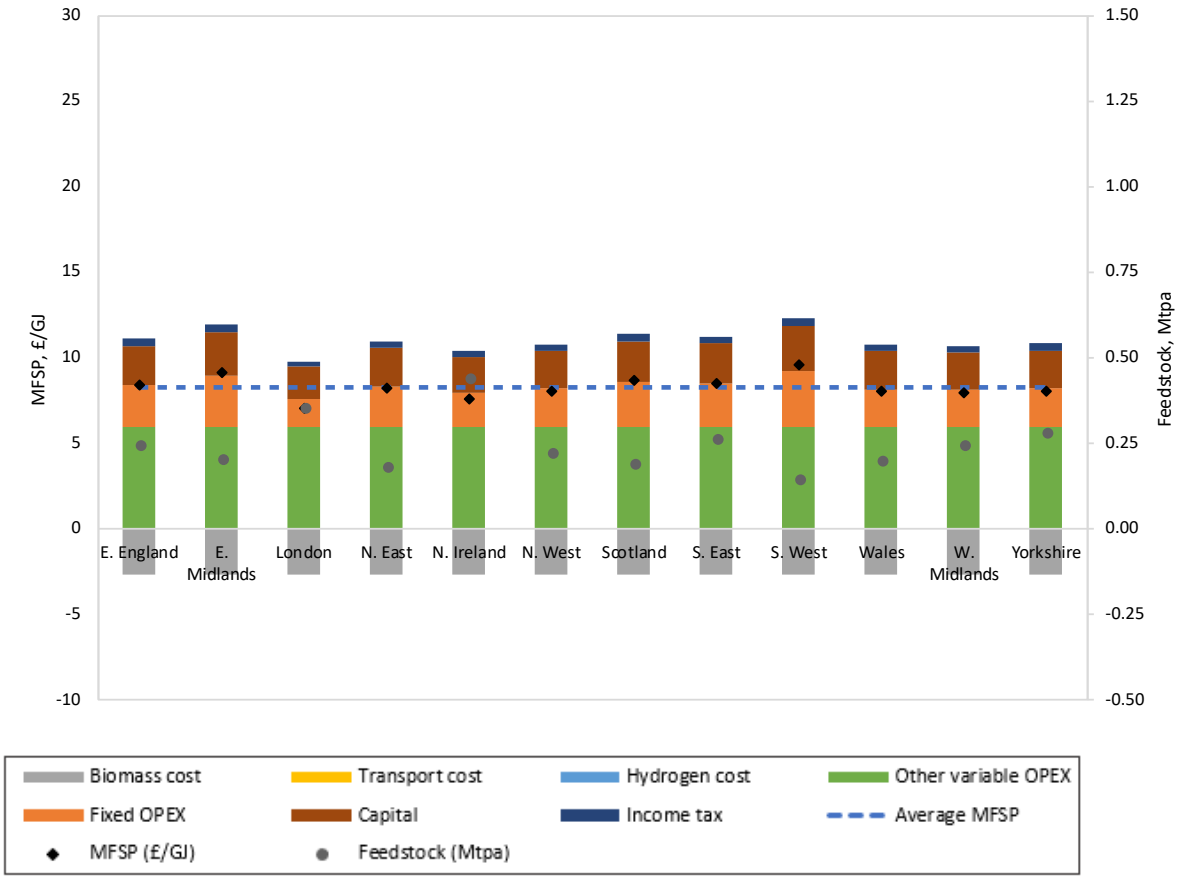
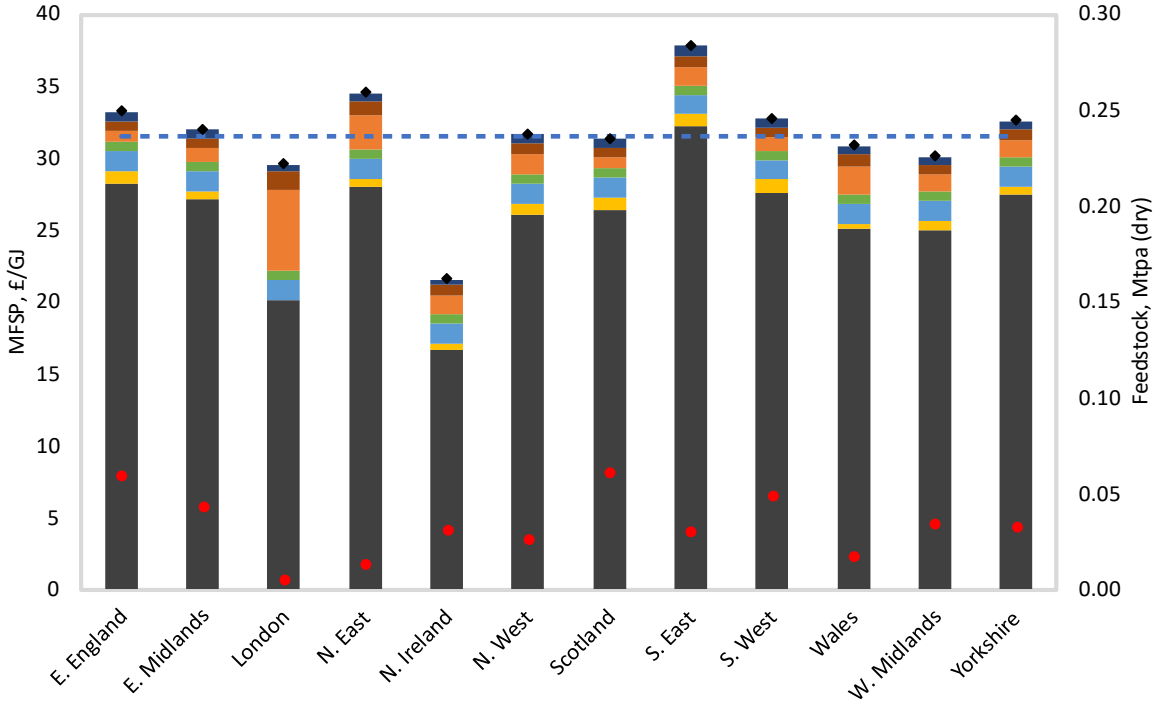


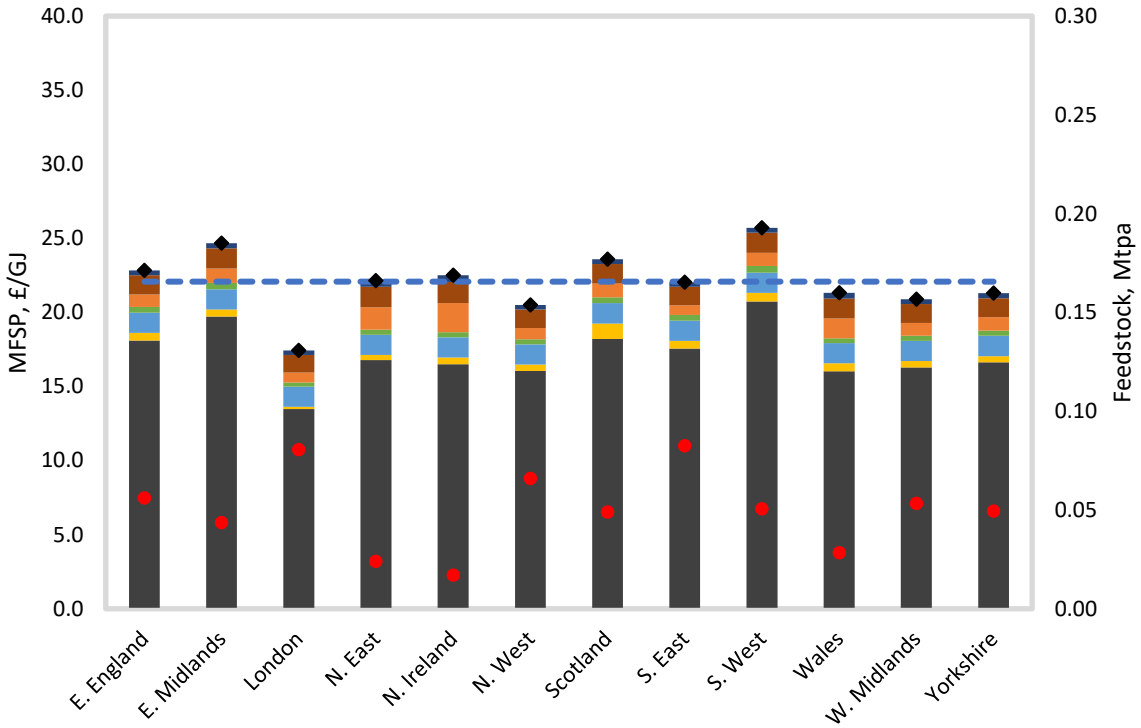
Figure 7: MFSP distribution of biocrude for the HTL of (a) digestates (b) food waste (c) BMW (d) SS and (e) co-processing the digestates, food waste, BMW and SS, at local sites (feedstocks to biocrude) used in the decentralised scenarios

(a)

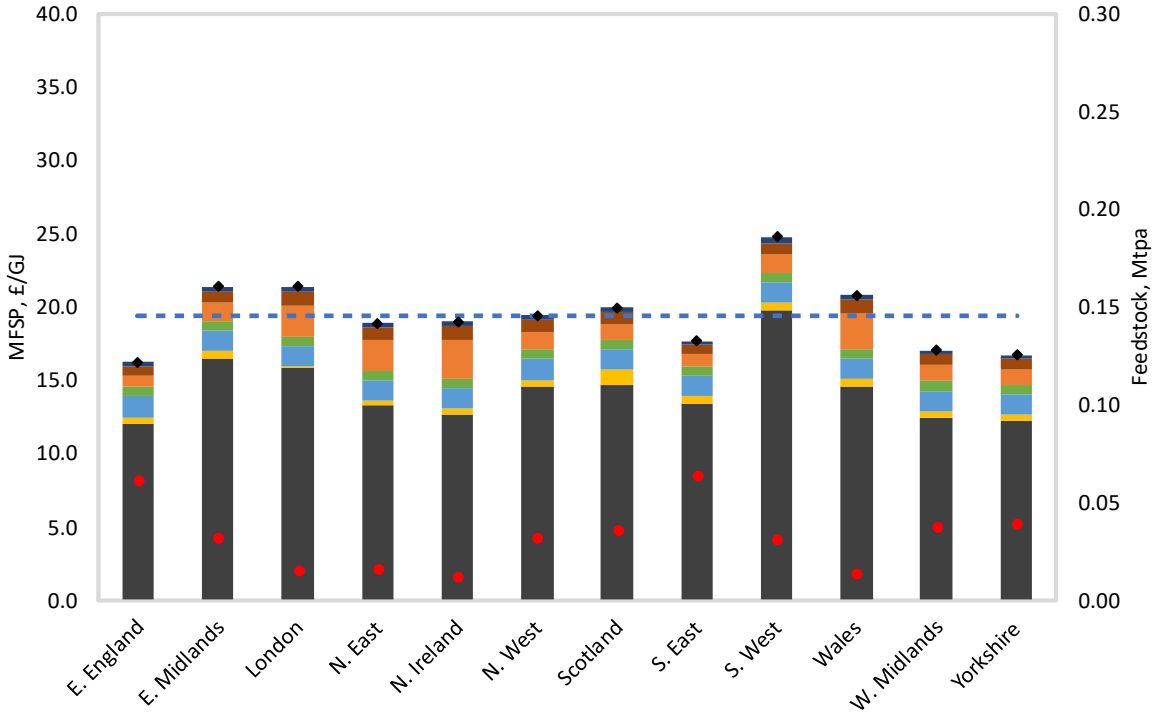


w

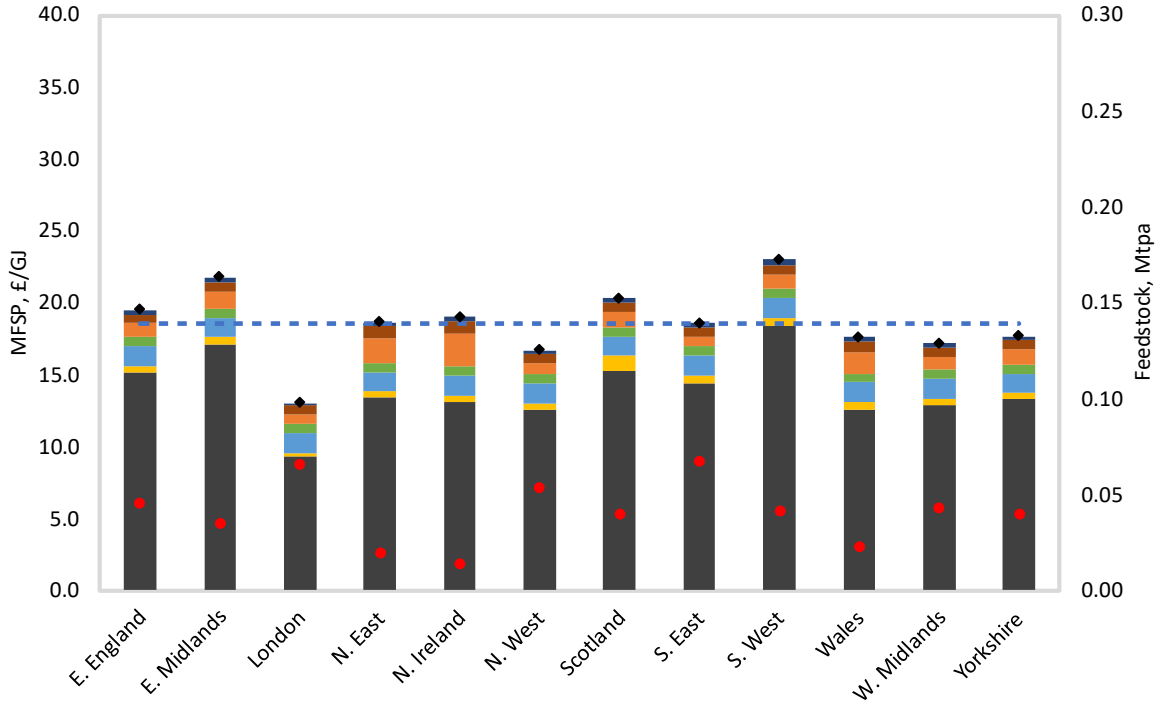
(b)


40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
MFSP, £/GJ
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Feedstock, Mtpa
E. England
E. Midlands
London
N. East
N. Ireland
N. West
Scotland
S. East
S. West
Wales
W. Midlands
Yorkshire

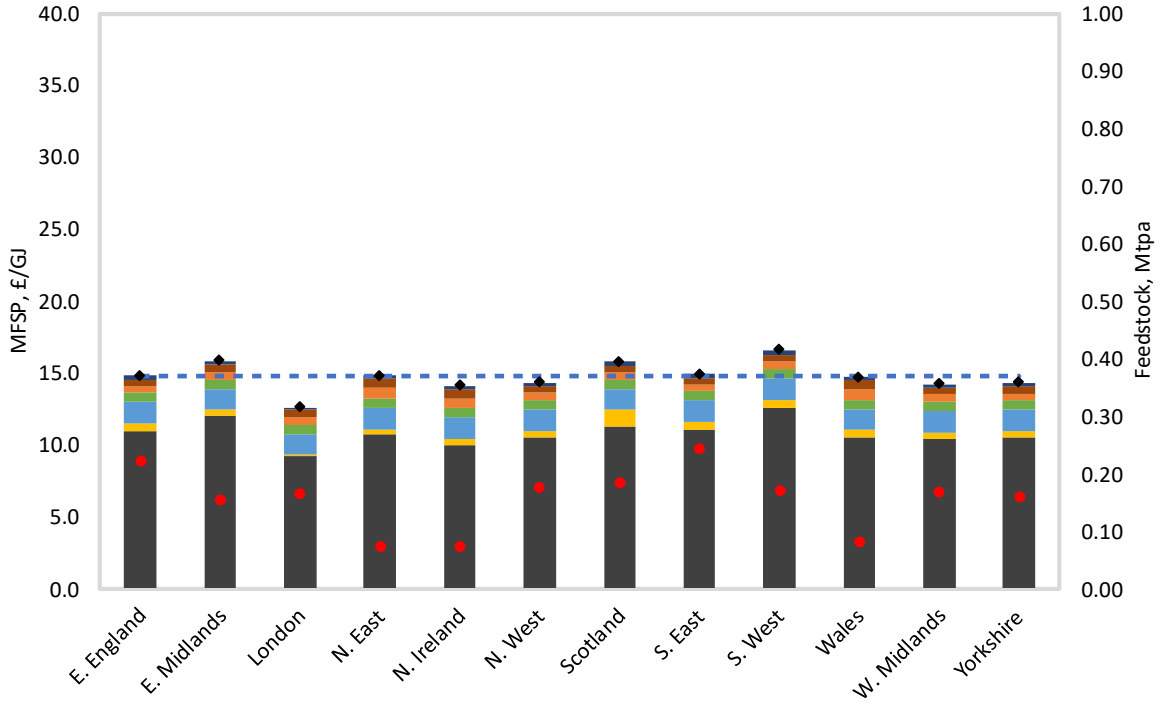
(c)


40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
MFSP, £/GJ
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Feedstock, Mtpa
E. England
E. Midlands
London
N. East
N. Ireland
N. West
Scotland
S. East
S. West
Wales
W. Midlands
Yorkshire

(d)



(e)



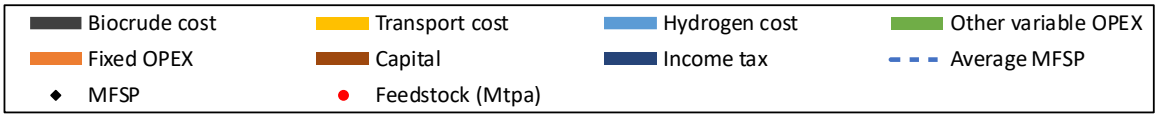


Figure 8: MFSP distribution of the HTL processing for (a) digestates (b) food waste (c) BMW (d) SS and (e) co-processing the digestates, food waste, BMW and SS, based on the Decentralised, Grey H2 scenario.

4.3 Summary of results

The summary of the key results of the cost and GHG emissions estimations for centralised and decentralised processing of the various feedstocks from across the different regions of the UK, using grey, blue and green hydrogen, are presented in Table 23 and Table 24.

1 Table 23: Summary of TEA results for the various feedstocks

Feedstock	Average fuel price across the UK (£/GJ)						Liquid fuel prod. volumes	
	Centralised, Grey H2	Decentralised, Grey H2	Centralised, Blue H2	Decentralised, Blue H2	Centralised, Green H2	Decentralised, Green H2	ML per yr	TJ per yr
Digestate	21.79	31.50	22.41	32.01	27.11	36.71	398	13,955
	0.69*	1.00*	0.71*	1.02*	0.86*	1.17*		
Food waste	19.81	22.08	20.43	22.70	25.15	27.40	594	20,847
	0.63*	0.70*	0.65*	0.72*	0.80*	0.87*		
Landfilled BMW	16.32	19.46	16.94	20.08	21.62	24.78	388	13,623
	0.52*	0.62*	0.54*	0.64*	0.69*	0.79*		
Sewage sludge	17.20	18.60	17.82	19.22	22.50	23.92	484	16,971
	0.55*	0.59*	0.57*	0.61*	0.72*	0.76*		
Co-processing	15.44	14.76	16.05	15.40	20.80	20.30	1,865	65,396
	0.49*	0.47*	0.51*	0.49*	0.66*	0.65*		
* Equivalent prices in £ per GLE								

2

3 Table 24: Summary of LCA results for the various feedstocks, based on the competing case

Feedstock	GHG emissions rate in 2021 (kg CO_2eq per GJ)						Total GHG emissions (Mt CO2eq/yr)		
	Centralised, Grey H2	Decentralised, Grey H2	Centralised, Blue H2	Decentralised, Blue H2	Centralised, Green H2	Decentralised, Green H2	Grey H2 cases	Blue H2 cases	Green H2 cases
Digestate	59.7	58.9	50.2	49.4	47.0	46.2	0.8	0.7	0.6
	35.7*	34.9*	26.3*	25.4*	23.0*	22.2*			
Food waste	35.0	34.2	25.5	24.8	22.3	21.5	0.7	0.5	0.5
	33.7*	32.9*	24.3*	23.5*	21.0*	20.3*			
Landfilled BMW	-68.5	-69.3	-78.0	-78.8	-81.2	-82.0	-0.9	-1.0	-1.1
	33.7*	32.9*	24.3*	23.5*	21.0*	20.3*			
Sewage sludge	59.1	58.1	49.6	48.6	46.4	45.4	1.0	0.8	0.8
	36.1*	35.2*	26.7*	25.7*	23.5*	22.5*			

Feedstock	GHG emissions rate in 2021 (kg CO_2eq per GJ)						Total GHG emissions (Mt CO2eq/yr)		
	Centralised, Grey H2	**Decentralised, Grey H2**	**Centralised, Blue H2**	**Decentralised, Blue H2**	**Centralised, Green H2**	**Decentralised, Green H2**	**Grey H2 cases**	**Blue H2 cases**	**Green H2 cases**
Co-processing	24.9	24.1	15.5	14.6	12.3	11.4	1.6	1.0	0.8
	34.8*	33.9*	25.3*	24.5*	22.1*	21.2*			
* Attributional emissions: Direct life cycle emissions when consequential factors are unaccounted for. Emissions based on an attributional approach are independent of current competing uses as only the direct fuel production and usage processes are considered.									

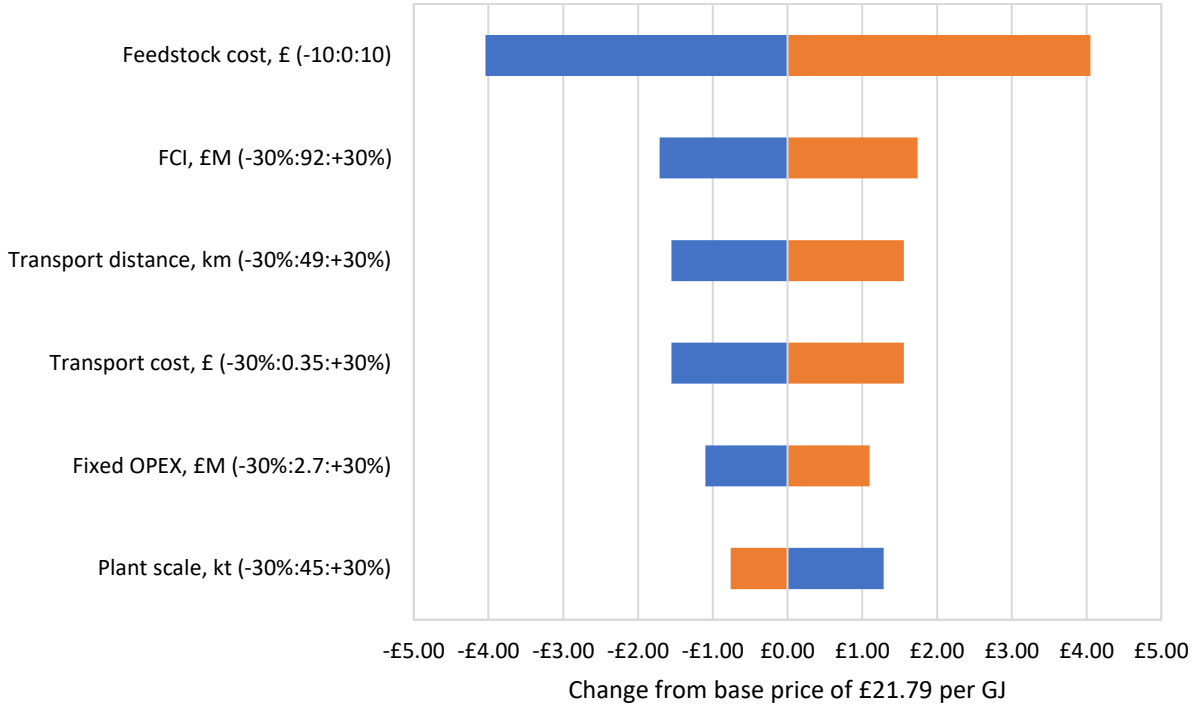
4

4.4 Sensitivity analysis of fuel price

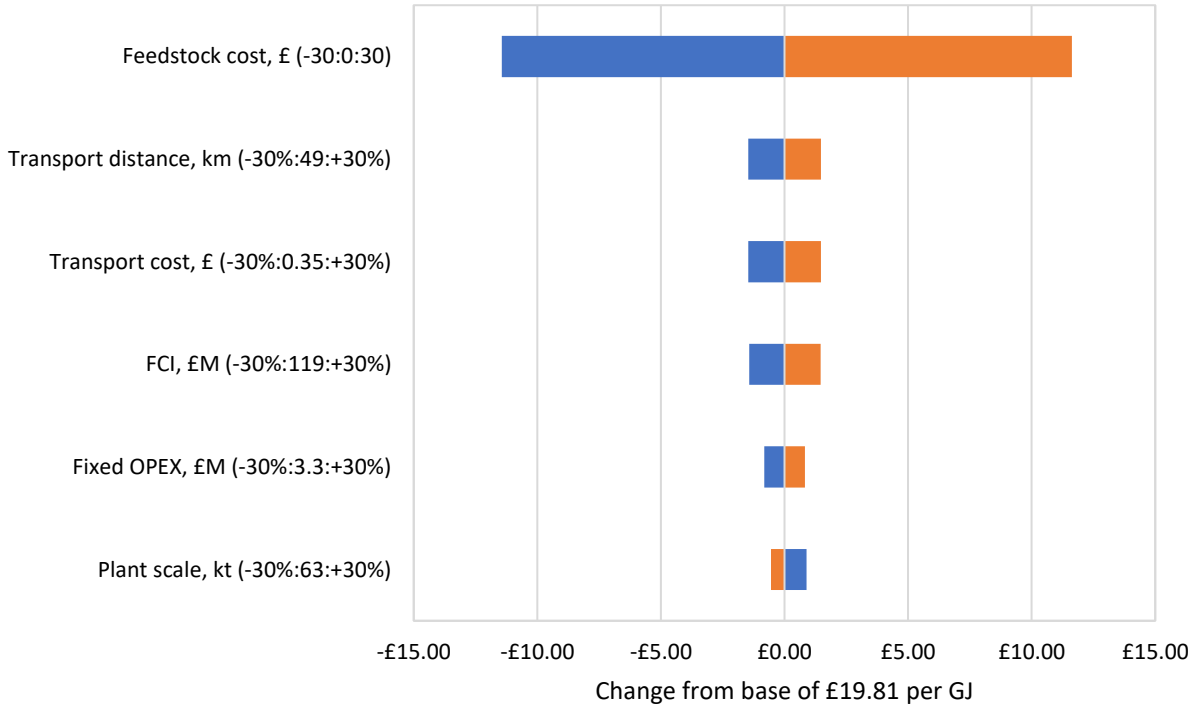
This section discusses the sensitivity analysis of the economics of digestates, food waste, BMW and SS studied. Some parameters were considered to have an important impact on the MFSP. These parameters which include feedstock price, transportation cost, hydrogen cost, fixed OPEX and capital cost were used to perform a sensitivity analysis of the fuel production cost, to determine how changes in these factors impact the plant economics.

As seen in Figure 9, the feedstock price had the highest impact on the production price of drop-in fuels from the various feedstocks. For digestates feedstocks, a variation in digestates price between £10 and £10 was analysed, based on the price range published by WRAP [16]. For food waste, the feedstock cost range of -£30 to £30 was adopted based on the cost ranges by WRAP [49] and letsrecycle.com. The feedstock costs range of landfilled BMW and SS were based on costs published by WRAP [49] and Katsou [13]. The impact of the changes in the cost of the feedstocks based on published variations can cause a change of more than 50% in the fuel production price, as seen with food waste. FCI is seen to cause the second biggest change after feedstock cost, due to the impact of capital cost and scale of plant operations. Also, transportation distances and cost strongly impact the cost of fuels, as the wet biomass feedstocks are very distributed in various locations and have high moisture content. Other factors such as fixed OPEX and plant scale also had significant impacts on the fuel production price.

(a)

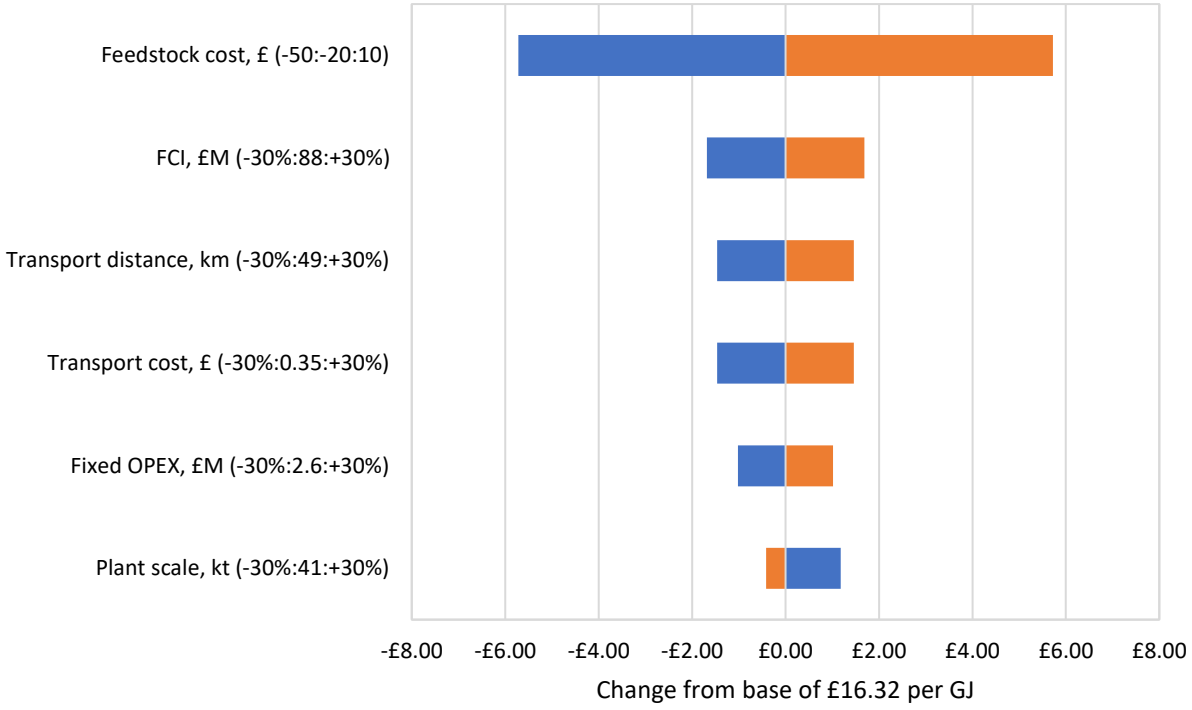

Feedstock cost, £ (-10:0:10)
FCI, £M (-30%:92:+30%)
Transport distance, km (-30%:49:+30%)
Transport cost, £ (-30%:0.35:+30%)
Fixed OPEX, £M (-30%:2.7:+30%)
Plant scale, kt (-30%:45:+30%)
-£5.00 -£4.00 -£3.00 -£2.00 -£1.00 £0.00 £1.00 £2.00 £3.00 £4.00 £5.00
Change from base price of £21.79 per GJ

(b)


Feedstock cost, £ (-30:0:30)
Transport distance, km (-30%:49:+30%)
Transport cost, £ (-30%:0.35:+30%)
FCI, £M (-30%:119:+30%)
Fixed OPEX, £M (-30%:3.3:+30%)
Plant scale, kt (-30%:63:+30%)
-£15.00 -£10.00 -£5.00 £0.00 £5.00 £10.00 £15.00
Change from base of £19.81 per GJ

dd

(c)



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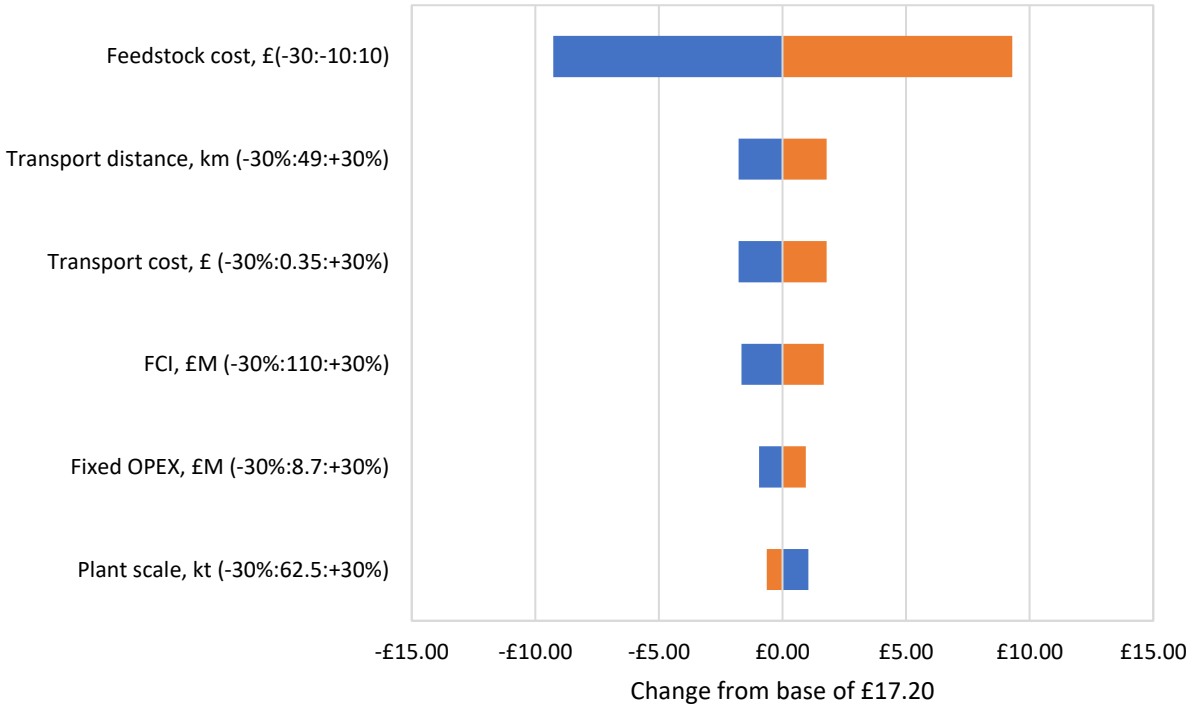


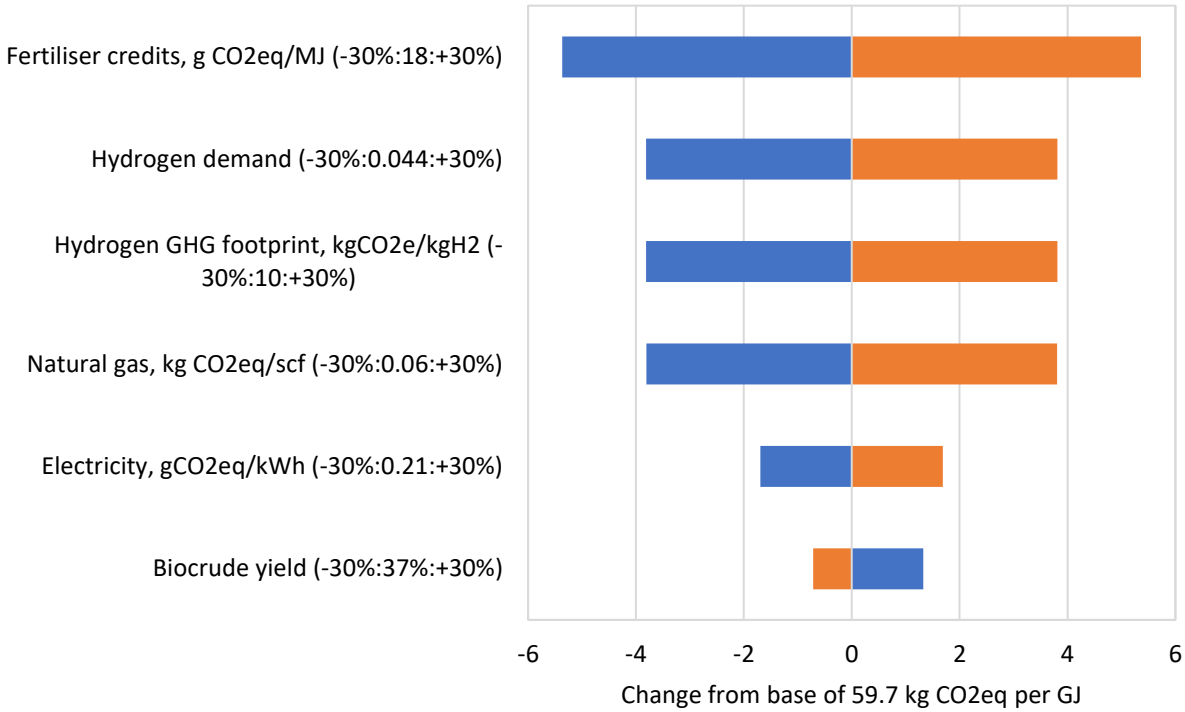
Figure 9: Sensitivity analysis results of (a) digestates (b) food waste (c) BMW and (d) SS, based on the Centralised, Grey H2 case

4.5 Sensitivity analysis of LCA emissions

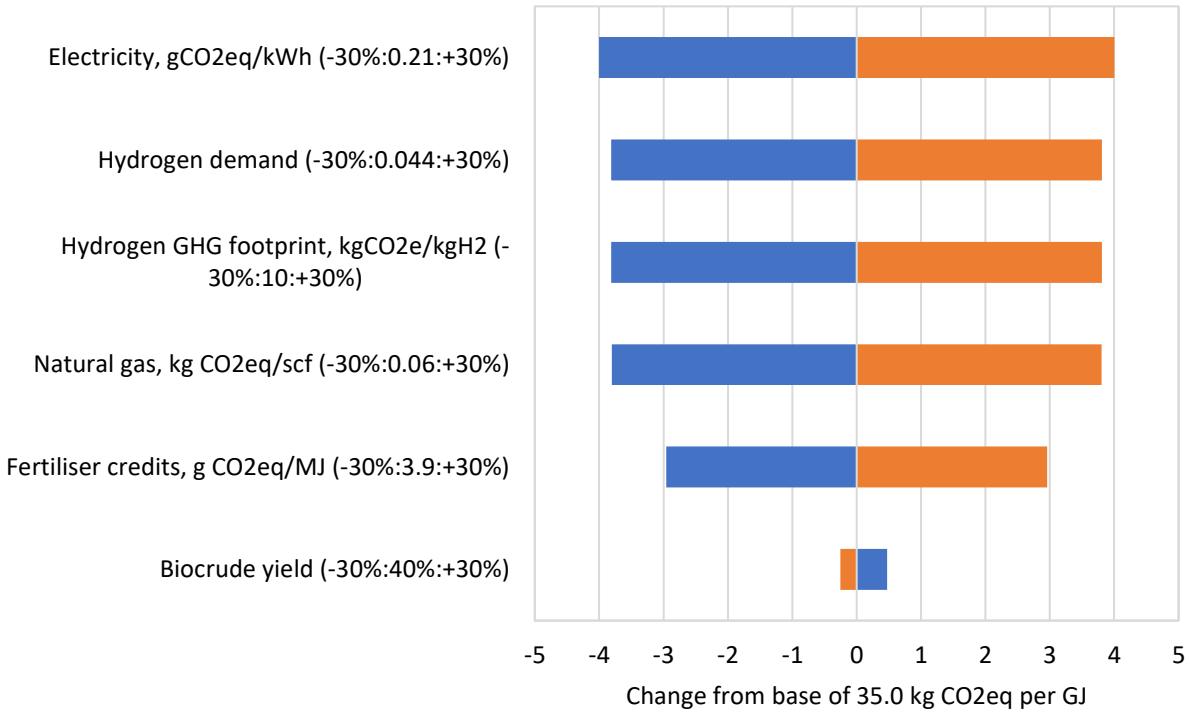
The sensitivity analysis of the life cycle GHG emissions of the various feedstocks- digestates, food waste, BMW and SS- are shown in Figure 10, based on the Centralised, Grey H2 scenario. The key

parameters directly impacting GHG emissions are hydrogen demand and emissions, natural gas emissions, and electricity emissions factors, amongst others. Indirect factors such as foregone fertiliser emissions benefits, foregone electricity benefits and avoided emissions benefits also had significant impacts on emissions, especially in digestates and landfilled BMW due to the nature of the current waste treatment methods.

a)



b)



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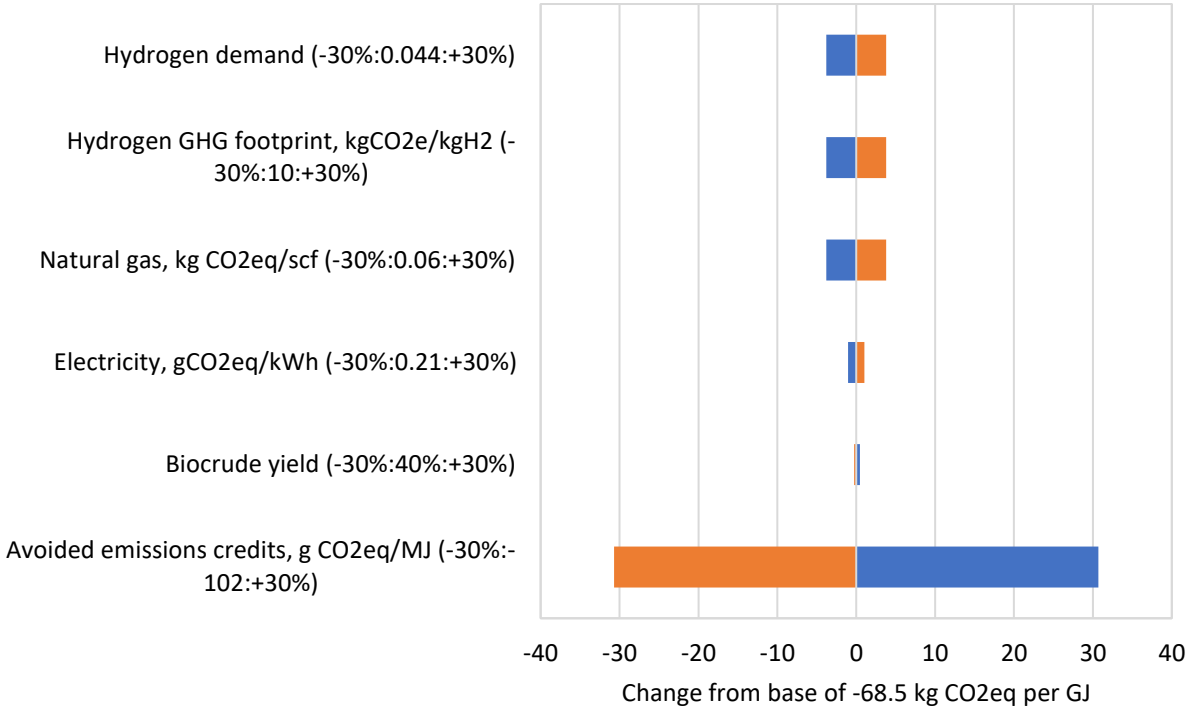

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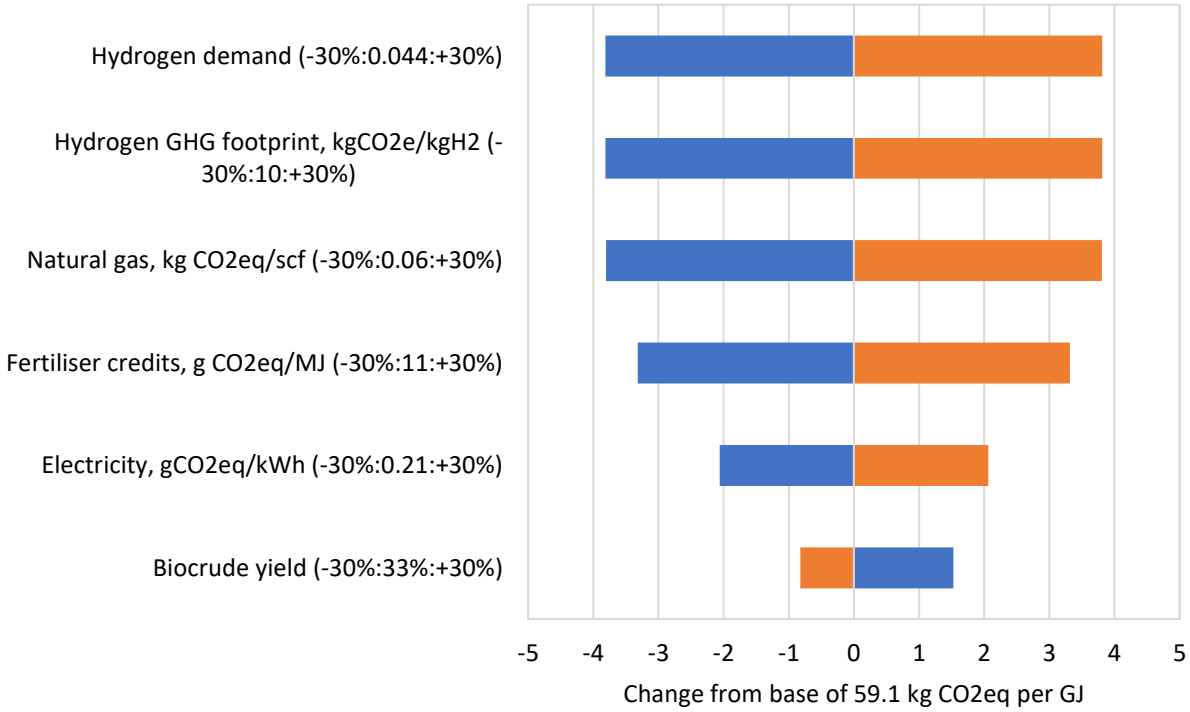

Figure 10: GHG emission sensitivity analysis results for (a) Digestates (b) Food waste (c) BMW and (d) SS, based on the Centralised, Grey H2 case

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Appendix A3: Supplementary information for Chapter 6: Technical, economic and lifecycle greenhouse gas emissions analyses of solid sorbent direct air capture technologies

Technical, economic and lifecycle greenhouse gas emissions analyses of solid sorbent direct air capture technologies

Supplementary Information

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Table S1: The kinetic parameters of Zeolite 4A-DEA [1]

Time	**Adsorption rate**
[min]	**[mol CO_2/kg sorbent]**
0.0	0.00
0.2	4.11
1.0	5.52
5.0	6.93
10.0	7.54
20.0	8.15
40.0	8.76
80.0	9.37

Table S2: The kinetic parameters of Zeolite 13X-Pz [2]

Time	**Adsorption rate**
[min]	**[mol CO_2/kg sorbent]**
0.0	0.00
0.2	0.50
1.0	1.56
5.0	2.71
10.0	2.99
20.0	3.15
40.0	3.23
80.0	3.28

Table S3: The kinetic parameters of MIL-101(Cr)-PEI [3]

Time	**Adsorption rate**
[min]	**[mol CO_2/kg sorbent]**
0.0	0.00
0.2	2.12
0.5	2.78
1.2	3.45
2.2	3.90
5.0	4.15
10.0	4.20
20.8	4.24

Time	Adsorption rate
[min]	[mol CO_2/kg sorbent]
80.0	4.24

Table S4: The kinetic parameters of mmen-Mg2(dobpdc) [4]

Time	Adsorption rate
[min]	[mol CO_2/kg sorbent]
0.0	0.00
0.2	0.04
1.0	0.08
5.0	0.27
10.0	0.50
20.0	0.97
40.0	1.91
50.3	2.40
63.1	2.85
70.9	2.94
80.0	2.94

Table S5: Process modelling parameters based on [4], [5]

Parameter	Value	Unit
Adsorbent channel inner radius d_1	0.000525	[m]
Adsorbent channel outer radius d_2	0.000585	[m]
Channel diameter d_3	0.00127	[m]
Contactor width side 1 w_1	1.1	[m]
Contactor width side 2 w_2	1.1	[m]
Adsorption capacity q	See Table S*1*–Table S*4* and Table S*14*	[mol CO_2/kg sorbent]
Operating (days) t_d	350	[days]
Channel Length (m) l	0.3	[m]
Cycle time t_c	Adsorption + Desorption time	[minutes]
Adsorption cycle time t_a	See Table S*1*–Table S*4* and Table S*14*	[minutes]
Desorption cycle time t_d	See Table S*1*–Table S*4* and Table S*14*	[minutes]
Sorbent lifetime t_s	Table S*14*	[years]
Plant lifetime t_l	30	[years]
Monolith lifetime t_{mo}	10	[years]
Monolith cost	50	[$/kg]
Desorption swing capacity θ	0.8	[mol/mol]
Air velocity v	3	[m/s]
Air viscosity μ	1.84E-05	[kg/m.s]

Ratio of specific heat CO_2	1.28	[-]
Adsorbent density	See Table S*14*	[kg/m^3]
Wall density	2050	[kg/m^3]
CO_2 desorption	55	[KJ/mol]
H_2O desorption	0	[KJ/mol]
H_2O:CO_2 uptake	2.2	[mol/mol]
Temperature at end of adsorption	348	[K]
Temperature for desorption	373	[K]
Steam latent heat	2257.60	[KJ/kg]
Channels per contactor	400	[cpsi]
Channels per contactor equivalent [per contactor dimensions]	750000	
Monolith heat capacity	840.00	[J/kg.K]
CO_2 capture efficiency	75%	

Formula used for monolith and contactor design [4], [5].

$$Volume\ of\ channel = 750000 \cdot \pi \left(\frac{d_3}{2}\right)^2 \cdot l \quad (S1)$$

$$Volume\ of\ adsorbent = 750000 \cdot \pi \left({d_2}^2 - {d_1}^2\right) \cdot l \quad (S2)$$

$$Volume\ of\ monolith = 750000 \cdot \pi \left\{\left(\frac{d_3}{2}\right)^2 - {d_1}^2\right\} \cdot l \quad (S3)$$

$$Volume\ of\ contactor = w_1 \cdot w_2 \cdot l \quad (S4)$$

$$CO_2\ uptake\ per\ contactor = \frac{\pi \cdot l \cdot \left({d_2}^2 - {d_1}^2\right) \cdot \rho \cdot (w_1/d_3) \cdot (w_2/d_3) \cdot q \cdot t_d \cdot 24 \cdot 60}{t_c} \quad (S5)$$

$$Number\ of\ contactor\ (n) = \frac{\alpha}{\theta \cdot CO_2\ uptake\ per\ contactor} \quad (S6)$$

Where α is the DAC CO_2 capture capacity in moles CO_2 per year.

$$CO_2\ uptake\ total = \ n \times CO_2\ uptake\ per\ contactor \quad (S7)$$

$$Fan\ duty = = \frac{\Delta P \cdot V}{\eta_{fan}} \quad (S8)$$

Where, V is the fan volumetric flowrate, ΔP is the pressure drop required to be overcome by fan power and η_{fan} is the fan efficiency.

$$\Delta P = \frac{8 l \mu v}{{d_1}^2} \quad (S9)$$

Table S6: Plant construction cost location factors [6]

Location	**Location Factor**
UK	1.02
US	1.02

Table S7: Zeolite 4A-DEA plant equipment cost based on methods by Seider et al. [7] and Bahmanzadegan and Ghaemi [1]

Major ISBL Equipment item	Quantity	Item Cost	Total Cost	Installation Factor	Installed Cost	Purchase cost CEPCI (2013)	2020 Installed Cost	Location Factor	Total Installed Cost
Dryer 1: Feed dryer	1	$49,210	$49,210	2.5	$123,025	567	$167,993	1.02	$171,353
Dryer 1: Product dryer	1	$54,669	$54,669	2.5	$136,674	567	$186,630	1.02	$190,362
Mixer	2	$283,156	$566,312	2.5	$1,415,780	567	$1,933,269	1.02	$1,971,934
Filter	1	$149,122	$149,122	2.5	$372,806	567	$509,072	1.02	$519,254
Total									**$2,852,903**

Table S8: Zeolite 13X-Pz plant equipment cost based on methods by Seider et al. [7] and Fashi et al. [2]

Major ISBL Equipment item	Quantity	Item Cost	Total Cost	Installation Factor	Installed Cost	Purchase cost CEPCI (2013)	2020 Installed Cost	Location Factor	Total Installed Cost
Dryer 1: Feed dryer	1	$42,966	$42,966	2.5	$107,414	567	$146,676	1.02	$149,609
Dryer 1: Product dryer	1	$46,692	$46,692	2.5	$116,729	567	$159,396	1.02	$162,584
Mixer	2	$341,955	$683,909	2.5	$1,709,773	567	$2,334,721	1.02	$2,381,415
Filter	1	$149,122	$149,122	2.5	$372,806	567	$509,072	1.02	$519,254
Total									**$3,212,862**

Table S9: MIL-101(Cr)-PEI and mmen-Mg2(dobpdc) plant equipment cost based on Table S7 and Table S8

Parameter	**Value**	**Unit**
Plant capacity	12000	tonne sorbent
Capital	373	$ per tonne sorbent
Working Capital	8.5%	Fraction of capital
Fixed operating	41.8%	Fraction of capital
Electricity demand	0.22 [MIL-101(Cr)-PEI]/0.30 [mmen-Mg2(dobpdc)]	kWh/kg

Table S10: Zeolite 4A-DEA mass and energy balance from [1]

Parameter	**Demand**	**Unit**	**Cost factor [$/kg]**	**Emission factor [kgCO_2e/kg parameter]**	**Ref.**
Zeolite	0.901	kg	0.14	2.0000	[8], [9]
DEA	0.100	kg	1.1	Ecoinvent	[10]
MeOH make-up	0.506	kg	0.35	2.0100	[11], [12], 30-year reagent life
MeOH initial	0.000	kg	0.35	2.0100	
Water	1.500	kg	See Table S*23*	Ecoinvent	
Energy	0.131	kWh	See Table S*21*	See Table S*21*	
Plant construction	1.000	plant	See Table S*7*	0.0002	[13]

Table S11: Zeolite 13X-Pz mass and energy balance from [2]

Sorbent	**Demand**	**Unit**	**Cost factor [$/kg]**	**Emission factor [kgCO_2e/kg parameter]**	**Ref.**
Zeolite	0.713	kg	0.14	Ecoinvent	[2], [8], [9]
Anhydrous Pz	0.285	kg	35	Ecoinvent	[14]
MeOH make-up	0.750	kg	0.35	2.0100	[11], [12], 30-year reagent life
MeOH initial	0.000	kg	0.35	2.0100	
Water	1.500	kg	See *Table S23*	Ecoinvent	
Energy	0.165	kWh	See *Table S21*	See *Table S21*	
Plant construction	1.000	plant	See Table S*8*	0.0002	[13]

FU: 1 kg MIL-101(Cr)-PEI sorbent

Sub-FU: 1 kg MIL-101(Cr)

Sub-FU: 1 kg $Cr(NO_3)_3 \cdot 9H_2O$

Sub-FU: 1 kg chromium (III) oxide (Cr_2O_3)

Table S12: MIL-101(Cr)-PEI mass and energy balance from [3], [4]

Group	**Sorbent**	**Demand**	**Unit**	**Cost factor [$/kg]**	**Emission factor [kgCO_2e /kg parameter]**	**Comment/Ref.**
Sub-FU: 1 kg Cr2O3	Sodium dichromate	1.7236	kg		Ecoinvent	[15]
	Sulphur	0.2110	kg		Ecoinvent	[15]
	Cr_2O_3	**1.0000**	**kg**		**6.8903**	**Calculated**
Sub-FU: 1 kg $Cr(NO_3)_3 \cdot 9H_2O$	Cr2O3	0.1899	kg		6.8903	[15]
	Nitric acid	0.4723	kg		Ecoinvent	[15]
	Water	0.3715	kg		Ecoinvent	[15]
	$Cr(NO_3)_3 \cdot 9H_2O$	**1.0000**	**kg**		**2.3052**	**Calculated**
Sub-FU:1 kg MIL-101(Cr)	$Cr(NO_3)_3 \cdot 9H_2O$	0.8000	kg	5.00	2.3052	[16], [17], [18]
	Terephthalic acid make-up	0.0332	kg	1.15	Ecoinvent	[19], [20], 10-year reagent life
	Terephthalic acid initial	0.0332	kg	1.15	Ecoinvent	[19], [20], 10-year reagent life
	MIL-101(Cr)	**1.0000**	**kg**	**4.08**	**1.9743**	**Calculated**
FU: 1 kg MIL-101(Cr)-PEI sorbent	MIL-101(Cr)	0.555	kg	4.08	1.9743	
	PEI	0.445	kg	19.50	11.0500	[18], [21], [22]
	MeOH make-up	0.220	kg	0.35	2.0100	[11], [12], 30-year reagent life
	MeOH initial	0.073	kg	0.35	2.0100	[11], [12], 30-year reagent life
	Deionised water	0.010	kg	0.0008	Ecoinvent	[10]
	Energy	0.222	kWh	See *Table S21*	See *Table S21*	
	Plant construction	1.000	plant	See Table S*9*	0.0002	[13]

FU: 1 kg mmen-Mg2(dobpdc) sorbent

Sub-FU: 1 kg Mg2(dobpdc)

Sub-FU: 1 kg 4,4′-Dihydroxy-(1,1′-biphenyl)-3,3′-dicarboxylic Acid (H4dobpdc)

Sub-FU: 1 kg 4,4′-dihydroxybiphenyl

Sub-FU: 1 kg vanadium tetrachloride

Table S13: Mmen-Mg2(dobpdc) mass and energy balance from [4], [23]

Group	**Sorbent**	**Demand**	**Unit**	**Cost factor [$/kg]**	**Emission factor [kgCO_2e /kg parameter]**	**Comment/reference**
Sub-FU:1 kg vanadium tetrachloride	Vanadium pentoxide	0.4718	kg		19.5000	[24], [25], [26]
	Chlorine	0.7357	kg		Ecoinvent	
	Carbon (graphite)	0.3115	kg		Ecoinvent	
	Vanadium tetrachloride [+ CO by product]	**1.0000**	**kg**		**11.2001**	**Calculated**
Sub-FU:1 kg 4,4′-dihydroxybiphenyl	Vanadium tetrachloride make-up	0.2070	kg		11.2001	30-year reagent life
	Vanadium tetrachloride initial	0.0690	kg		11.2001	30-year reagent life
	Phenol	1.0108	kg		Ecoinvent	
	4,4′-dihydroxybiphenyl	**1.0000**	**kg**		**6.3565**	**Calculated**
H4dobpdc	4,4′-dihydroxybiphenyl make-up	0.1706	kg	12.00	6.3565	[16], [18], [27], 10-year reagent life
	4,4′-dihydroxybiphenyl initial	0.1706	kg	12.00	6.3565	[16], [18], [27], 10-year reagent life
	KHCO3 make-up	0.2941	kg	0.95	Ecoinvent	[10], 10-year reagent life
	KHCO3 initial	0.2941	kg	0.95	Ecoinvent	[10], 10-year reagent life
	Ice	5.8824	kg	0.0012	Ecoinvent	
	1,2,4-trichlorobenzene make-up	0.6441	kg	7.00	Ecoinvent	[27], [28], [29], 10-year reagent life
	1,2,4-trichlorobenzene initial	0.6441	kg	7.00	Ecoinvent	[27], [28], [29], 10-year reagent life
	H4dobpdc	**1.0000**	**kg**	**13.68**	**7.8911**	**Calculated**

Mg2(dobpdc)	H4dobpdc	0.4174	kg	13.68	7.8911	
	MgBr2·6H2O	1.0435	kg	20.00	Ecoinvent	[16], [27], [30]
	1:1 N,N-diethylformamide:Ethanol make-up	0.7378	kg	1.29	Ecoinvent	[10], [18], 10-year reagent life
	1:1 N,N-diethylformamide:Ethanol initial	0.7378	kg	1.29	Ecoinvent	[10], [18], 10-year reagent life
	Mg2(dobpdc)	**1.0000**	**kg**	**28.48**	**12.1407**	
FU: 1 kg mmen-Mg2(dobpdc) sorbent	Mg2(dobpdc)	0.8851	kg	28.48	12.1407	
	N,N'-dimethylethylenediamine(mmen)	0.243	kg	25	Ecoinvent	[4], [18], [27]
	Energy	0.296	kWh	See *Table S21*	See *Table S21*	
	Plant construction	1.000	plant	See Table S*9*	0.0002	[13]

Table S14: Sorbent properties and the corresponding DAC mass and energy demand from modelling results.

Sorbent	**Type**	**Model**	**Adsorption rates [mol/kg]**	**Life [y]**	**Sorbent density [kg/m^3]**	**Sorbent heat capacity [J/kg.K]**	**Electricity demand [GJ/t CO_2]**	**Heat demand [GJ/t CO_2]**	**Water demand [m^3/t CO_2]**
Zeolite 4A-DEA	Zeolite	Experimental	6.9	0.5	466	1604	1.847	2.325	0.153
Zeolite 13X-Pz	Zeolite	Experimental	2.7	0.5	600	1239	1.847	2.325	0.153
MIL-101(Cr)-PEI	MOFs	Experimental	3.9	1.0	500	893	1.874	3.100	0.205
mmen-Mg2(dobpdc)	MOFs	Experimental	2.4	1.0	500	893	1.859	2.674	0.185
Zeolite 4A-DEA	Zeolite	Nth plant model	9.4	0.5	466	1604	1.884	3.384	0.218
Zeolite 13X-Pz	Zeolite	Nth plant model	3.3	0.5	600	1239	1.840	2.118	0.159
MIL-101(Cr)-PEI	MOFs	Nth plant model	4.2	1.0	500	893	1.865	2.829	0.192
mmen-Mg2(dobpdc)	MOFs	Nth plant model	2.9	1.0	500	893	1.856	2.583	0.180
Generic sorbent model	Generic	Nth plant model	10.0	1.0	500	1000	1.872	3.045	0.202

Table S15: Zeolite 4A-DEA sorbent cost

Year	Country	Electricity	Prices [$$_{2024}$/tonne]
2025	UK	Grid	1,224
2025	US	Grid	1,166
2030	UK	Grid	1,223
2030	US	Grid	1,166
2040	UK	Grid	1,223
2040	US	Grid	1,166
2050	UK	Grid	1,223
2050	US	Grid	1,166

Table S16: Zeolite 13X-Pz sorbent cost

Year	Country	Electricity	Prices [$$_{2024}$/tonne]
2025	UK	Grid	14,201
2025	US	Grid	14,107
2030	UK	Grid	14,200
2030	US	Grid	14,107
2040	UK	Grid	14,200
2040	US	Grid	14,107
2050	UK	Grid	14,200
2050	US	Grid	14,107

Table S17: MIL-101(Cr)-PEI sorbent cost

Year	Country	Electricity	Prices [$$_{2024}$/tonne]
2025	UK	Grid	14,438
2025	US	Grid	14,453
2030	UK	Grid	14,436
2030	US	Grid	14,453
2040	UK	Grid	14,436
2040	US	Grid	14,454
2050	UK	Grid	14,436
2050	US	Grid	14,453

Table S18: Mmen-Mg2(dobpdc) sorbent cost

Year	Country	Electricity	Prices [$$_{2024}$/tonne]
2025	UK	Grid	40,459
2025	US	Grid	40,436
2030	UK	Grid	40,457
2030	US	Grid	40,436
2040	UK	Grid	40,457
2040	US	Grid	40,436
2050	UK	Grid	40,457
2050	US	Grid	40,436

Table S19: Calculated GHG emissions of sorbents in 2025

Country	Electricity	Sorbent	GHG emissions [$kgCO_2e/kg$ sorbent]
UK	Grid	MIL-101(Cr)-PEI	**6.3753**
US	Grid	MIL-101(Cr)-PEI	**6.6758**
UK	Grid	mmen-Mg2(dobpdc)	**10.4477**
US	Grid	mmen-Mg2(dobpdc)	**12.3466**
UK	Grid	Zeolite 4A - DEA	**3.1487**
US	Grid	Zeolite 4A - DEA	**3.1671**
UK	Grid	Zeolite 13X - Pz	**4.3640**
US	Grid	Zeolite 13X - Pz	**4.7583**
UK	Grid	Generic sorbent model	**4.0000**
US	Grid	Generic sorbent model	**4.0000**
UK	Grid	Generic for 2050	**4.0000**
US	Grid	Generic for 2050	**4.0000**

Table S20: Grid electricity emissions factors for 2025 to 2050 based on IEA

Country	Country	IEA Scenario	30-year average emission factor [$kgCO_2e/kWh$]	Weighted average emission factor used [$kgCO_2e/kWh$]
UK	2025	Stated Policies	0.16640	0.1664
UK	2025	Sustainable	0.09862	
UK	2030	Stated Policies	0.15486	0.1322
UK	2030	Sustainable	0.07936	
UK	2040	Stated Policies	0.14063	0.0986
UK	2040	Sustainable	0.05666	
UK	2050	Stated Policies	0.13655	0.0748
UK	2050	Sustainable	0.04827	
US	2025	Stated Policies	0.30769	0.3077
US	2025	Sustainable	0.15003	
US	2030	Stated Policies	0.27867	0.2287
US	2030	Sustainable	0.11226	
US	2040	Stated Policies	0.24023	0.1587
US	2040	Sustainable	0.07711	
US	2050	Stated Policies	0.22564	0.1167
US	2050	Sustainable	0.07005	

Table S21: Energy parameters used in the analysis

Year	Country	Technology	Cost [$/kWh]	Capacity factor	Load hours	Emission factor [$kgCO_2e/kWh$]	Comment
2025	UK	Wind	0.05473	61%	5344	0.0044	[31]
2025	UK	Solar	0.05099	11%	964	0.0276	[31]
2025	UK	Grid	0.14863	96%	8400	0.1664	30-year avg. from 2025 of [32], Table S*20*

2025	UK	NG	0.03744	96%	8400	0.2027	30-year avg. from 2025 of [32]
2025	US	Wind	0.03060	46%	4015	0.0127	[33]
2025	US	Solar	0.04501	24%	2098	0.0180	[33]
2025	US	Grid	0.06765	96%	8400	0.3077	30-year avg. from 2025, [34], Table S*20*
2025	US	NG	0.01583	96%	8400	0.2027	30-year avg. from 2025, [34]
2030	UK	Wind	0.04851	65%	5694	0.0044	[31]
2030	UK	Solar	0.04602	11%	964	0.0276	[31]
2030	UK	Grid	0.14204	96%	8400	0.1322	30-year avg. from 2030 of [32], Table S*20*
2030	UK	NG	0.03570	96%	8400	0.2027	30-year avg. from 2030 of [32]
2030	US	Wind	0.02677	48%	4165	0.0127	[33]
2030	US	Solar	0.03543	27%	2348	0.0180	[33]
2030	US	Grid	0.06767	96%	8400	0.2287	30-year avg. from 2030, [34], Table S*20*
2030	US	NG	0.01616	96%	8400	0.2027	30-year avg. from 2030, [34]
2040	UK	Wind	0.05099	69%	6044	0.0044	[31]
2040	UK	Solar	0.03731	11%	964	0.0276	[31]
2040	UK	Grid	0.141169	96%	8400	0.0986	30-year avg. from 2040 of [32], Table S*20*
2040	UK	NG	0.03582	96%	8400	0.2027	30-year avg. from 2040 of [32]
2040	US	Wind	0.02404	48%	4198	0.0127	[33]
2040	US	Solar	0.02402	34%	2961	0.0180	[33]
2040	US	Grid	0.06895	96%	8400	0.1587	30-year avg. from 2040, [34], Table S*20*
2040	US	NG	0.01674	96%	8400	0.2027	30-year avg. from 2040, [34]
2050	UK	Wind	0.05099	69%	6044	0.0044	[31]
2050	UK	Solar	0.03731	11%	964	0.0276	[31]
2050	UK	Grid	0.141801	96%	8400	0.0748	30-year avg. from 2050 of [32], Table S*20*
2050	UK	NG	0.03593	96%	8400	0.2027	30-year avg. from 2050 of [32]
2050	US	Wind	0.02135	48%	4232	0.0127	[33]
2050	US	Solar	0.01950	36%	3127	0.0180	[33]
2050	US	Grid	0.06724	96%	8400	0.1167	30-year avg. from 2050, [34], Table S*20*
2050	US	NG	0.01628	96%	8400	0.2027	30-year avg. from 2050, [34]

Table S22: Heating efficiency

NG to heat	90%
Electricity to heat	85%

Table S23: Other variable cost

Input Parameter	**Value**	**Unit**	**Ref.**
Cooling water	0.06	[$/m^3]	[10]
Process water	0.35	[$/m^3]	[10]
Sorbent transportation cost	9.66063E-05	[$/kg/km]	[35], [36]
Monolith	50	[$/kg]	[5]

Table S24: Air composition

	Volume fraction	Density [kg/m^3]	Mass [kg]	Mass fraction
N_2	78%	1.25	0.976125	75.56%
O_2	21%	1.4291	0.299396	23.18%
Argon	1%	1.69	0.015548	1.20%
CO_2	0%	1.87	0.000748	0.06%

Table S25: DAC plant equipment cost based on methods by Seider et al. [7]

Major ISBL Equipment item	**Quantity**	**Item Cost**	**Total Cost**	**Installation Factor**	**Installed Cost**	**Purchase cost CEPCI (2013)**	**2025 Installed Cost**	**Location Factor**	**Total Installed Cost**
Fans	165	$216,878	$35,784,852	2.5	$89,462,129	567	$122,161,913	1.02	$124,605,152
Vacuum pump	49	$66,834	$3,274,874	4	$13,099,494	567	$17,887,561	1.02	$18,245,312
Condenser	1	$111,509	$111,509	3.5	$390,281	567	$532,935	1.02	$543,594
Condenser flash drum	1	$376,926	$376,926	4	$1,507,706	567	$2,058,796	1.02	$2,099,971
DAC steam heat exchanger 1	1	$111,715	$111,715	3.5	$391,001	567	$533,918	1.02	$544,596
DAC steam heat exchanger 2	1	$62,492	$62,492	3.5	$218,722	567	$298,668	1.02	$304,642
DAC steam heat exchanger external	1	$56,400	$56,400	3.5	$197,401	567	$269,554	1.02	$274,945
Compressor 1	1	$7,847,160	$7,847,160	2.5	$19,617,901	567	$26,788,546	1.02	$27,324,317
Condenser flash drum 2	1	$219,933	$219,933	4	$879,733	567	$1,201,289	1.02	$1,225,315
Compressor 2	1	$7,305,199	$7,305,199	2.5	$18,262,996	567	$24,938,403	1.02	$25,437,171
Total									**$200,605,014**

Table S26: DAC plant capital and other material cost with scale (capacity factor-independent)

Plant scales [t/h]	Capital cost [$/(t/h)]		Other material cost (95% monolith and 5% sorbent) [$/(t/h) yearly]	
	2025	2050	2025	2050
11.90	5,043,356	4,260,325	18,979	16,164
59.52	2,858,712	2,414,868	18,971	16,157
119.05	2,485,089	2,099,254	18,917	16,157
178.57	2,330,849	1,968,962	18,968	16,155

Table S27: DAC plant capital cost by plant commissioning year, based on a 1 Mtpa plant

Year	Capital cost [$/(t/h)]	Monolith cost [$/(t/h) yearly]
2025	2,485,089	17,775
2030	2,254,305	16,125
2040	2,157,478	15,432
2050	2,099,254	15,016

Table S28: DAC plant emissions factors

Element	Emission factor	Units	Ref.
Sorbent	See Table S*19*	$kgCO_2e$/kg sorbent	
Sorbent transportation	0.05	gCO_2e/kg cargo/km	GaBi [37]
DAC plant construction	0.0035	$kgCO_2e$/kg CO_2 captured	[13], [38]
Injection pipeline	0.000003	$kgCO_2e$/(km.kg CO_2 captured)	[39]
Cooling water	Ecoinvent	$kgCO_2e$/kg water	
Steam	Table S*21* and Table S*22*	$kgCO_2e$/kWh source	
Electricity	Table S*21* and Table S*22*	$kgCO_2e$/kWh electricity	

Table S29: Optimal experimental and commercial plant results in 2025 with UK Wind.

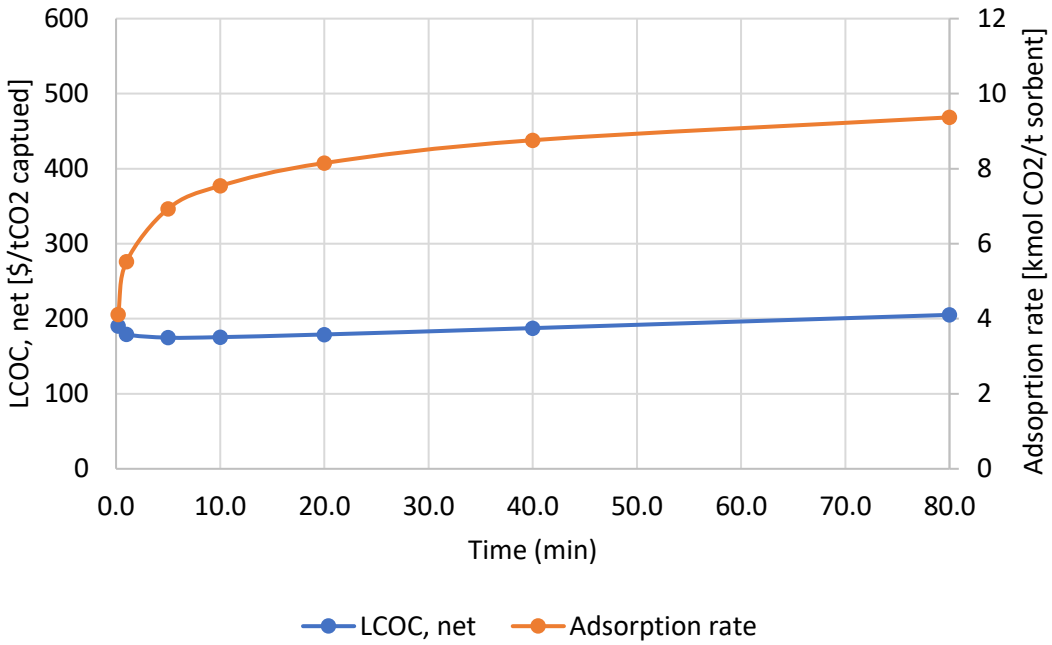
Sorbent	Plant model	Sorbent cost (2024)	Adsorption rate	Adsorption time	Desorption time	Sorbent density	Sorbent heat capacity	Sorbent demand	$LCOC_{gross}$ (2025)	$LCOC_{net}$ (2025)	DAC GHG emissions (2025)
		[$\$_{2024}$/t sorbent]	[mol/kg]	[min]	[min]	[kg/m^3]	[J/kg/K]	[kg sorbent/tCO_2 captured]	[$\$_{2024}$/t$CO_2$ captured]	[$\$_{2024}$/t$CO_2$ captured]	[tCO2/tCO_2 captured]
Zeolite 4A-DEA	Experimental	1,200	6.9	5.0	15	466	1604	0.7	173	175	0.0113
Zeolite 13X-Pz	Experimental	14,200	2.7	5.0	15	600	1239	1.7	232	236	0.0179
MIL-101(Cr)-PEI	Experimental	14,400	3.9	2.2	20.5	500	893	0.7	202	205	0.0140
mmen-Mg2(dobpdc)	Experimental	40,400	2.4	50.3	15	500	893	3.2	456	477	0.0443
Zeolite 4A-DEA	Nth plant model	1,200	9.4	5	10	466	1604	0.4	163	164	0.0100
Zeolite 13X-Pz	Nth plant model	14,200	3.3	5	10	600	1239	1.1	205	208	0.0146
MIL-101(Cr)-PEI	Nth plant model	14,400	4.2	2	10	500	893	0.3	183	185	0.0117
mmen-Mg2(dobpdc)	Nth plant model	40,400	2.9	10	10	500	893	0.8	244	249	0.0187
Generic nth plant model	Nth plant model	1,200	10.0	5	10	500	1000	0.2	159	160	0.0093

Table S30: Summary of cost and GHG emissions of DAC commercial plant.

Year	Country	Energy source	Boundary	Sorbent	Sorbent demand	LCOC, gross	LCOC, net	DAC GHG emissions
					[kg sorbent/tCO_2 captured]	[$/t$CO_2$ captured]	[$/t$CO_2$ captured]	tCO_2/tCO_2 captured
2025	UK	Wind	Plant	Generic sorbent model	0.2	159	160	0.0093
2025	UK	Solar	Plant	Generic sorbent model	1.0	588	612	0.0394
2025	UK	Wind & Grid	Plant	Generic sorbent model	0.1	164	178	0.0775
2025	UK	Grid	Plant	Generic sorbent model	0.1	233	290	0.1971
2025	UK	Grid & NG	Plant	Generic sorbent model	0.1	159	203	0.2134
2025	US	Wind	Plant	Generic sorbent model	0.2	164	167	0.0191
2025	US	Solar	Plant	Generic sorbent model	0.5	299	307	0.0262

Year	Country	Energy source	Boundary	Sorbent	Sorbent demand	LCOC, gross	LCOC, net	DAC GHG emissions
					[kg sorbent/tCO_2 captured]	[$/$tCO_2$ captured]	[$/$tCO_2$ captured]	tCO_2/tCO_2 captured
2025	US	Wind & Grid	Plant	Generic sorbent model	0.2	145	160	0.0952
2025	US	Grid	Plant	Generic sorbent model	0.1	140	219	0.3612
2025	US	Grid & NG	Plant	Generic sorbent model	0.1	106	148	0.2855
2025	UK	Wind	Reservoir	Generic sorbent model	0.2	168	170	0.0106
2025	UK	Solar	Reservoir	Generic sorbent model	1.0	597	623	0.0410
2025	UK	Wind & Grid	Reservoir	Generic sorbent model	0.1	174	189	0.0795
2025	UK	Grid	Reservoir	Generic sorbent model	0.1	244	305	0.2003
2025	UK	Grid & NG	Reservoir	Generic sorbent model	0.1	170	217	0.2166
2025	US	Wind	Reservoir	Generic sorbent model	0.2	173	177	0.0205
2025	US	Solar	Reservoir	Generic sorbent model	0.5	308	317	0.0276
2025	US	Wind & Grid	Reservoir	Generic sorbent model	0.2	154	171	0.0974
2025	US	Grid	Reservoir	Generic sorbent model	0.1	150	236	0.3660
2025	US	Grid & NG	Reservoir	Generic sorbent model	0.1	115	163	0.2903
2030	UK	Wind	Plant	Generic sorbent model	0.2	137	138	0.0093
2030	UK	Solar	Plant	Generic sorbent model	1.0	531	553	0.0394
2030	UK	Wind & Grid	Plant	Generic sorbent model	0.1	146	155	0.0569
2030	UK	Grid	Plant	Generic sorbent model	0.1	220	261	0.1574
2030	UK	Grid & NG	Plant	Generic sorbent model	0.1	149	186	0.1959
2030	US	Wind	Plant	Generic sorbent model	0.2	143	146	0.0191
2030	US	Solar	Plant	Generic sorbent model	0.4	240	246	0.0260
2030	US	Wind & Grid	Plant	Generic sorbent model	0.2	123	136	0.0955
2030	US	Grid	Plant	Generic sorbent model	0.1	134	184	0.2695
2030	US	Grid & NG	Plant	Generic sorbent model	0.1	100	133	0.2452
2040	UK	Wind	Plant	Generic sorbent model	0.2	132	133	0.0092
2040	UK	Solar	Plant	Generic sorbent model	1.0	500	520	0.0394
2040	UK	Wind & Grid	Plant	Generic sorbent model	0.1	141	147	0.0397
2040	UK	Grid	Plant	Generic sorbent model	0.1	216	245	0.1184

Year	Country	Energy source	Boundary	Sorbent	Sorbent demand	LCOC, gross	LCOC, net	DAC GHG emissions
					[kg sorbent/tCO_2 captured]	[$/$tCO_2$ captured]	[$/$tCO_2$ captured]	tCO_2/tCO_2 captured
2040	UK	Grid & NG	Plant	Generic sorbent model	0.1	146	178	0.1788
2040	US	Wind	Plant	Generic sorbent model	0.2	134	137	0.0191
2040	US	Solar	Plant	Generic sorbent model	0.3	179	183	0.0256
2040	US	Wind & Grid	Plant	Generic sorbent model	0.1	110	121	0.0953
2040	US	Grid	Plant	Generic sorbent model	0.1	133	164	0.1881
2040	US	Grid & NG	Plant	Generic sorbent model	0.1	99	125	0.2094
2050	UK	Wind	Plant	Generic sorbent model	0.2	130	131	0.0092
2050	UK	Solar	Plant	Generic sorbent model	1.0	487	507	0.0394
2050	UK	Wind & Grid	Plant	Generic sorbent model	0.1	140	144	0.0320
2050	UK	Grid	Plant	Generic sorbent model	0.1	216	237	0.0907
2050	UK	Grid & NG	Plant	Generic sorbent model	0.1	145	174	0.1666
2050	US	Wind	Plant	Generic sorbent model	0.2	127	130	0.0191
2050	US	Solar	Plant	Generic sorbent model	0.3	161	166	0.0256
2050	US	Wind & Grid	Plant	Generic sorbent model	0.1	103	112	0.0786
2050	US	Grid	Plant	Generic sorbent model	0.1	130	151	0.1394
2050	US	Grid & NG	Plant	Generic sorbent model	0.1	96	118	0.1881
2050	UK	Wind	Reservoir	Generic sorbent model	0.2	139	141	0.0105
2050	UK	Solar	Reservoir	Generic sorbent model	1.0	496	517	0.0410
2050	UK	Wind & Grid	Reservoir	Generic sorbent model	0.1	149	154	0.0335
2050	UK	Grid	Reservoir	Generic sorbent model	0.1	226	249	0.0928
2050	UK	Grid & NG	Reservoir	Generic sorbent model	0.1	156	187	0.1688
2050	US	Wind	Reservoir	Generic sorbent model	0.2	136	139	0.0205
2050	US	Solar	Reservoir	Generic sorbent model	0.3	170	175	0.0270
2050	US	Wind & Grid	Reservoir	Generic sorbent model	0.1	112	122	0.0806
2050	US	Grid	Reservoir	Generic sorbent model	0.1	139	162	0.1421
2050	US	Grid & NG	Reservoir	Generic sorbent model	0.1	105	130	0.1907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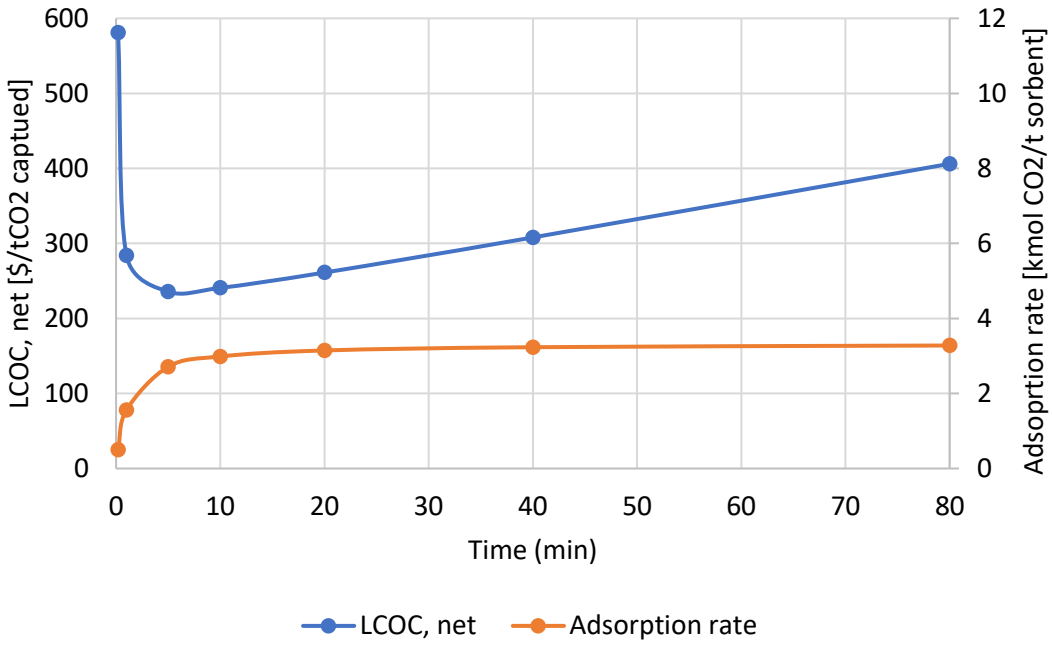
Time (min)
LCOC, net
Adsorption rate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Time (min)
LCOC, net
Adsorption rate

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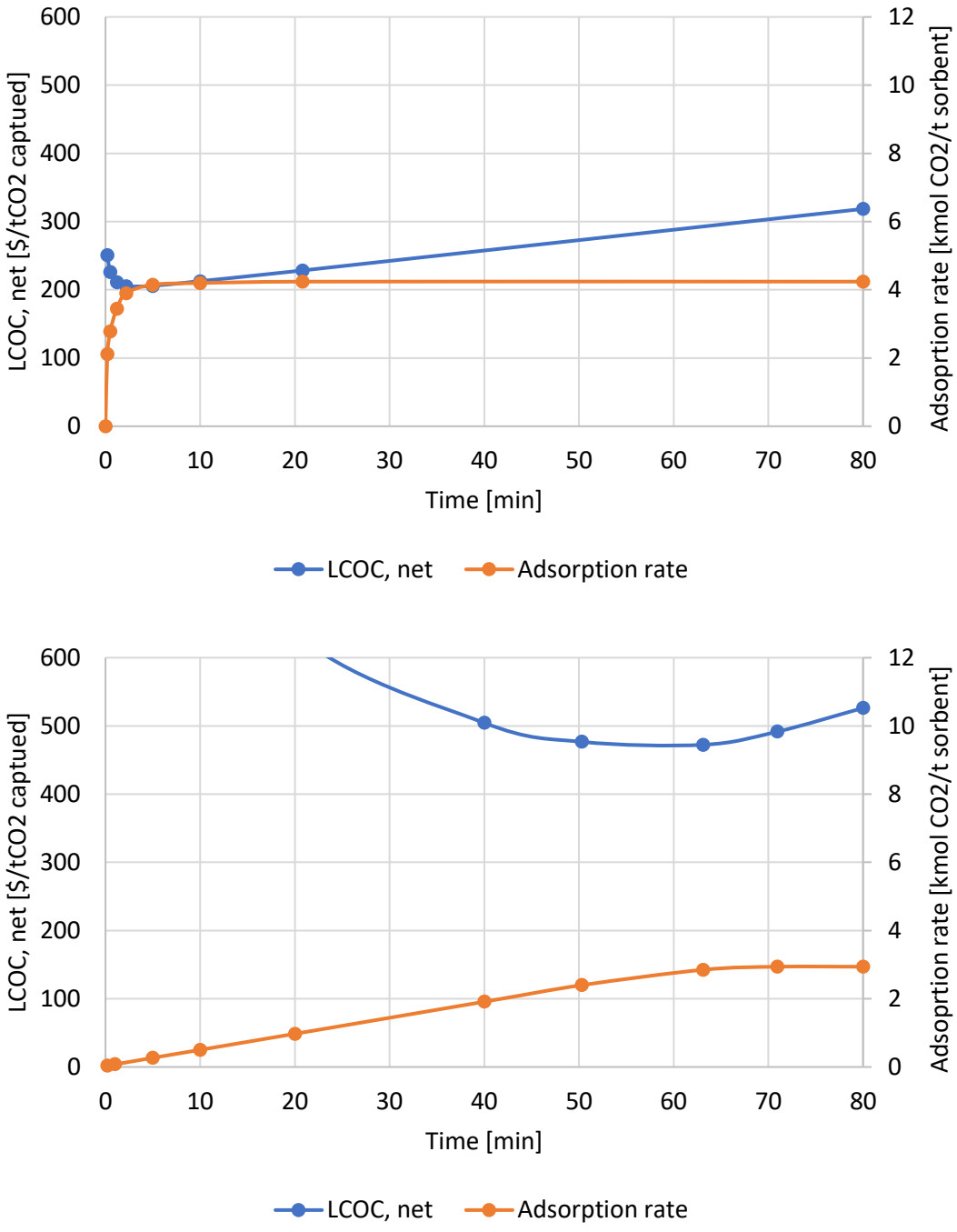
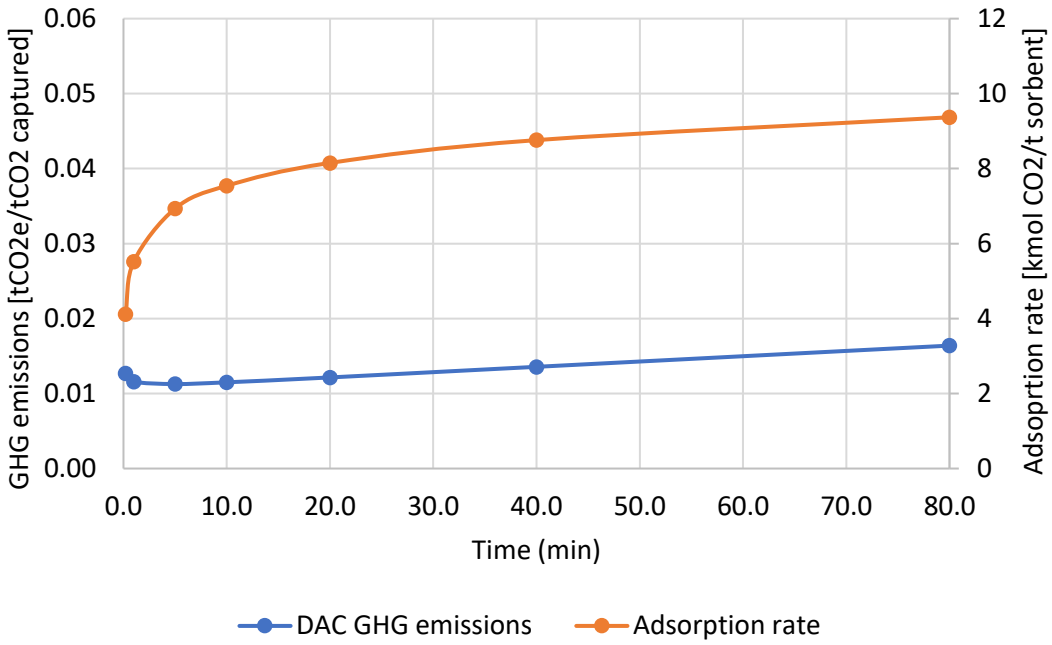
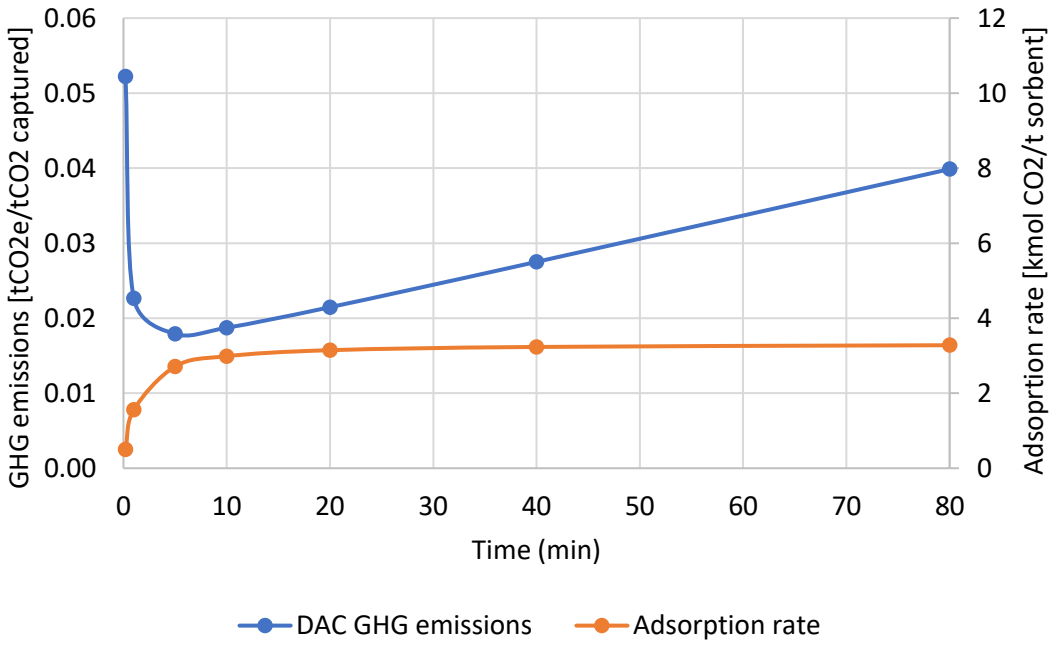


Figure S1a–*d*: Variation in DAC cost with adsorption rate and time, based on the 2025 commissioning year using UK Wind for (a) Zeolite 4A-DEA with kinetic data from Bahmanzadegan and Ghaemi [1] (b) Zeolite 13X-Pz with kinetic data from Fashi et al. [2] (c) MIL-101(Cr)-PEI with kinetic data from Lin et al. [3] and (d) mmen-Mg2(dobpdc) with kinetic data from Sinha et al. [4].


GHG emissions [tCO2e/tCO2 captured]
0.06
0.05
0.04
0.03
0.02
0.01
0.00
Adsoprtion rate [kmol CO2/t sorbent]
12
10
8
6
4
2
0
0.0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
Time (min)
DAC GHG emissions
Adsorption rate


GHG emissions [tCO2e/tCO2 captured]
0.06
0.05
0.04
0.03
0.02
0.01
0.00
Adsoprtion rate [kmol CO2/t sorbent]
12
10
8
6
4
2
0
0
10
20
30
40
50
60
70
80
Time (min)
DAC GHG emissions
Adsorption rate

t

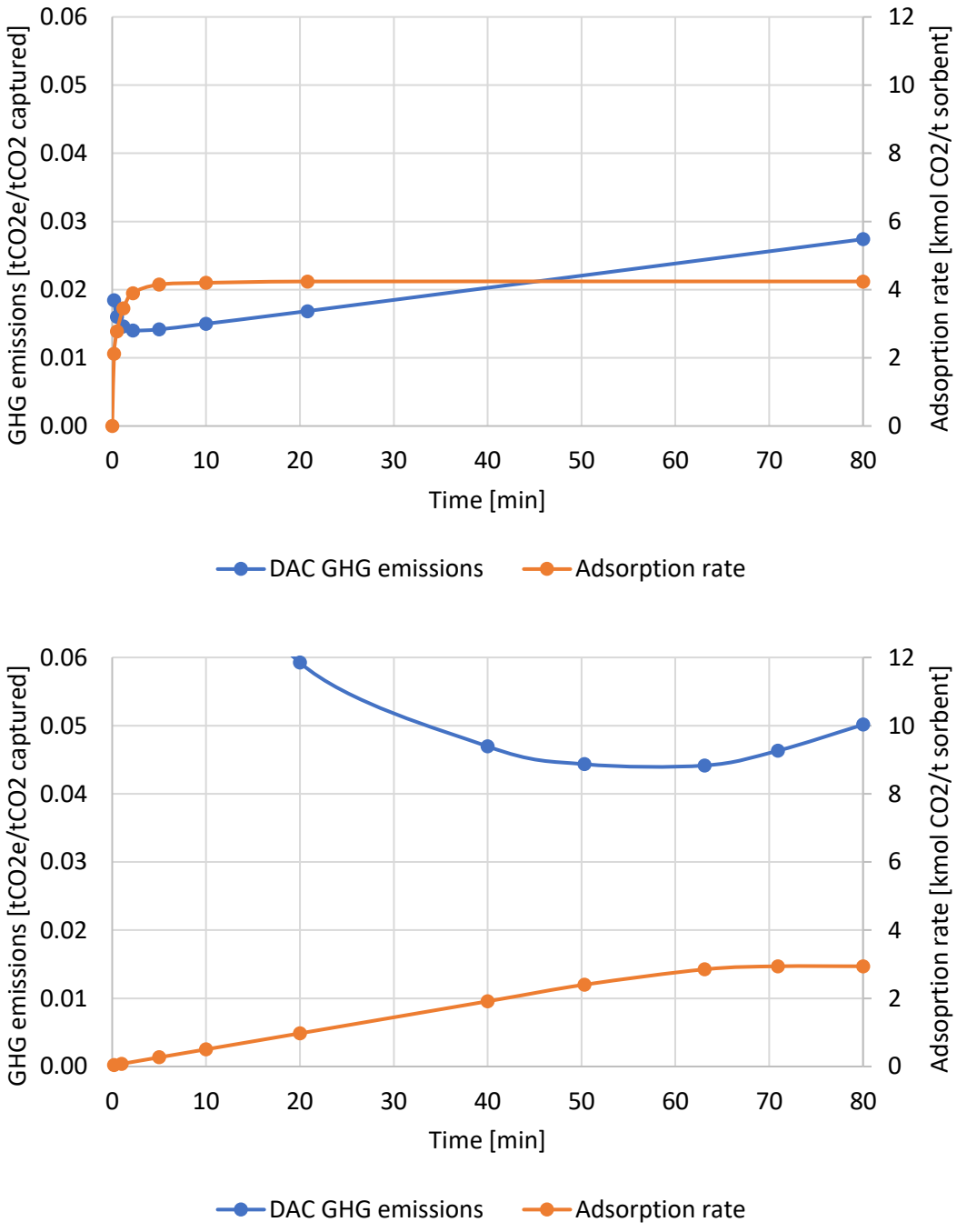


Figure S2a–*d*: Variation in DAC GHG emissions with adsorption rate and time, based on the 2025 commissioning year using UK Wind for (a) Zeolite 4A-DEA with kinetic data from Bahmanzadegan and Ghaemi [1] (b) Zeolite 13X-Pz with kinetic data from Fashi et al. [2] (c) MIL-101(Cr)-PEI with kinetic data from Lin et al. [3] and (d) mmen-Mg2(dobpdc) with kinetic data from Sinha et al. [4].

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Appendix A4: Supplementary information for Chapter 7: Life cycle greenhouse gas implications of low-carbon gaseous fuel supply chains from technological, geospatial, and temporal perspectives

Supplementary Information (SI) 1

Life cycle greenhouse gas implications of low-carbon gaseous fuel supply chains from technological, geospatial, and temporal perspectives

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1 Methodology

Table S1: Chemical properties [1], [2], [3], [4].

Chemical	Parameter	Value	Unit
Hydrogen	LHV	119.95	MJ/kg
Hydrogen	HHV	141.88	MJ/kg
Hydrogen	Density as Liquid, STP	0.072	kg/L
Hydrogen	Density as CH2, 80 bar	0.006313607	kg/L
Hydrogen	Density as CH2, 500 bar and 15 °C	0.033808916	kg/L
Hydrogen	Density as CH2, 700 bar and 15 °C	0.043350326	kg/L
SNG	LHV	50.00	MJ/kg
SNG	HHV	55.00	MJ/kg
LSNG	Density	0.45	kg/L
SNG	Density, 80 bar and 15 °C	0.066713	kg/L
SNG	Density, STP	0.000768	kg/L
SNG	Density, 200 bar and 15 °C	0.179626	kg/L
MeOH	Density	0.794	kg/L
NH_3	Density	0.700	kg/L
MCH	Density	0.770	kg/L

Table S2: Process yield of H_2-related process.

Chemical	Yield basis				Unrecoverable system loss		Comment/data based on ref.
SNG	0.010	kg H_2	0.0200	SNG	25.18%	kg H_2	SNG formation produces almost 50% of H_2O as a by-product, [3], [5]
NH_3	0.010	kg H_2	0.0535	kg NH_3	0.5%	kg H_2	Losses from casing leaks, [3], [6], [7]
MCH	0.062	kg H_2	1.0000	kg MCH	0.2%	kg H_2	Losses from casing leaks, [3], [6], [7]
MeOH	0.010	kg H_2	0.0502	kg MeOH	32.3%	kg H_2	MeOH formation produces high amount H_2O as a by-product [3]

Table S3: CO_2 capture and N_2 liquefaction material, energy balance, and emission factors data.

Operation	**Electricity [kWh/kg fuel product]**	**Net heat [MJ/kg fuel product]**	**Embodied emissions [kgCO_2e/kg fuel product]**	**Reference**
DAC w/MeOH, H_2 basis	3.66	34.37	0.025020	[3], [8], [9], [10] and Ecoinvent
DAC w/SNG, SNG basis	1.51	8.61	0.010350	
N_2 liquefaction [for NH_3]	1.467836	0.00	0.001263	

Table S4: Rail transportation parameters based on tank cars by Federal Railroad Administration [11].

Rail	**Units**	**CH2**	**LH2**	**as MCH**	**as MeOH**	**as NH_3**	**Data based on ref.**
Train life (years)	40	40	40	40	40	40	
Tank capacity	t (cargo)	1.1	4	34	36	32	[3], [11], [12], [13]
Product stored pressure	bar	500	<5	1	1	1	[12], [14]
Boil-off	Per h for CH2 and per kg H_2 for LH2	0.0075%	0.43%	N/A	N/A	N/A	[6], [14]
Speed	km/h	69.20	69.20	69.20	69.20	69.20	[11]
Speed (unloaded)	km/h	80.00	80.00	80.00	80.00	80.00	
Delivery distance	km	400	400	400	400	400	
Travel time (loaded)	h	5.78	5.78	5.78	5.78	5.78	
Travel time (unloaded)	h	5.00	5.00	5.00	5.00	5.00	
Numbers of rail cars	h	30	30	30	30	30	[11]
Loading/unloading time per rail tank car	h	0.55	0.55	0.55	0.55	0.55	[15]
Loading/unloading time (total)	h	16.36	16.36	16.36	16.36	16.36	
Total time	h	22.14	22.14	22.14	22.14	22.14	
Total time with empty return	h	27.14	27.14	43.51	27.14	27.14	
Total time with toluene return	h	43.51	43.51	59.87	43.51	43.51	
Energy consumption	MJ/kg fuel product/km	0.00155	0.00081	0.00406	0.00131	0.00142	[11]
Energy consumption with empty return	MJ/kg fuel product/km	0.00296	0.00147		0.00185	0.00201	
Energy consumption with toluene return	MJ/kg fuel product/km	0.00338	0.00263	0.00812			
Embodied emissions (single trip basis)	kgCO_2e/kg fuel product	0.06751	0.03170	0.08170	0.02627	0.02852	Train (long-distance), Ecoinvent

Table S5: Ship transportation parameters.

Shipping	**Units**	**LH2**	**as MCH**	**as MeOH**	**as NH_3**	**LNG**	**Ref.**
Capacity	t (cargo)	11,000	110,000	90,402	53,000	57,624	[3], [16], [17]
Lifetime	years	35	35	35	35	35	
Ship speed	km/h	30	30	30	30	30	
Fuel use	MJ/km	1487	3300	5469	2500	10787	
Fuel use	MJ/km/kg cargo (fuel/carrier product) transported	0.000135	0.000484	0.000314	0.000266	0.0001872	
Boil-off rate	%/day	0.20%	0	0	0	0.10%	
Loading/unloading time	Days	2	2	2	2	2	
Embodied emissions (single trip basis)	$kgCO_2e$/ kg fuel product	0.00786	0.01515	0.00487	0.00529	0.00150	Tanker (liquefied natural gas), Ecoinvent

Table S6: Pipeline transportation parameters.

Pipeline	**Leakage rate [per 1000 km]**	**Electricity demand [kWh/kg fuel product/km]**	**Embodied emissions [$kgCO_2e$/kg fuel product/km]**	**Comment/Ref.**
Transport by Pipeline: as CH2 (Booster LP Distribution)	0.3%	0.000000	0.000000	[18], [19], [20], [21] and Ecoinvent
Transport by Pipeline: as CH2 (Booster HP Distribution)	0.5%	0.000699	0.000000	
Transport by Pipeline: as CH2 (plant to terminal)	0.5%	0.000699	0.000075	
Transport by Pipeline: as CH2 (Booster Long Dist. Transmission)	0.5%	0.000699	0.000075	
Transport by Pipeline: as LH2	~0%	0.000030	0.000046	[4] and Ecoinvent
Transport by Pipeline: as LH2 (plant to terminal)	~0%	0.000030	0.000046	
Transport by Pipeline: as MCH	0%	0.000005	0.000097	
Transport by Pipeline: as MCH w/toluene return	0%	0.000011	0.000194	
Transport by Pipeline: as MCH (plant to terminal)	0%	0.000005	0.000097	
Transport by Pipeline: as MCH w/toluene return (plant to terminal)	0%	0.000011	0.000194	
Transport by Pipeline: as MeOH, H_2 Product basis	0%	0.000016	0.000031	
Transport by Pipeline: as MeOH (plant to terminal), H2 Product basis	0%	0.000016	0.000031	
Transport by Pipeline: as NH_3, H_2 Product basis	0%	0.000020	0.000027	

Pipeline	Leakage rate [per 1000 km]	Electricity demand [kWh/kg fuel product/km]	Embodied emissions [$kgCO_2e$/kg fuel product/km]	Comment/Ref.
Transport by Pipeline: as NH_3 (plant to terminal), H_2 Product basis	0%	0.000020	0.000027	
Transport by Pipeline: as SNG (LP Distribution)	0.13%	0.000000	0.000000	[22] and grid pipeline
Transport by Pipeline: as SNG (HP Distribution)	0.13%	0.000201	0.000000	
Transport by Pipeline: as SNG (plant to terminal)	0.13%	0.000201	0.000007	[18], [22], [23]
Transport by Pipeline: as SNG (Long Dist. Transmission)	0.13%	0.000269	0.000007	
Transport by Pipeline: as LSNG (plant to terminal)	~0%	0.000009	0.000018	

Table S7: Countries and supply chain routes.

Market operation	Countries	Abbreviation	Port
Fuel production	Saudi Arabia	SA	Jeddah
Fuel production	Morrocco	MR	Casablanca
Fuel production	Nigeria	NG	Port Harcourt
Fuel production	Algeria	AL	Skikda
Fuel production	Chile	CL	San Antonio
Fuel production	Australia	AU	Fremantle
Fuel use	United Kingdom	UK	Southampton
Fuel use	Netherlands	NL	Rotterdam

Table S8: Transportation distance parameters.

Location	**Transportation mode**	**Distance [km]**	**Ref.**
Local [Import to distribution terminal]	Any	400	Own assumption
Local [Distribution terminal to station]	Any	150	[24]
SA to UK	Transport by Pipeline	6245	Jeddah to Southampton, Google
SA to UK	Transport by Ship	8,099	Jeddah to Southampton, Ports.com
SA to NL	Transport by Pipeline	5799	Jeddah to Rotterdam, Google
SA to NL	Transport by Ship	8,627	Jeddah to Rotterdam, Ports.com
MR to UK	Transport by Pipeline	2564	Casablanca to Southampton, Google
MR to UK	Transport by Ship	2589	Casablanca to Southampton, Ports.com
MR to NL	Transport by Pipeline	2755	Casablanca to Rotterdam, Google
MR to NL	Transport by Ship	3117	Casablanca to Rotterdam, Ports.com
NG to UK	Transport by Pipeline	7001	Port Harcourt to Southampton, Google
NG to UK	Transport by Ship	8649	Port Harcourt to Southampton, Ports.com
NG to NL	Transport by Pipeline	7192	Port Harcourt to Rotterdam, Google
NG to NL	Transport by Ship	9175	Port Harcourt to Rotterdam, Ports.com
AL to UK	Transport by Pipeline	3635	Google
AL to UK	Transport by Ship	3691	Port.com
AL to NL	Transport by Pipeline	3783	Google, Haumann et al. [25]
AL to NL	Transport by Ship	4219	Port.com
CL to UK	Transport by Pipeline	11780	www.fluentcargo.com, assumes air flight distance
CL to UK	Transport by Ship	17492	Ports.com
CL to NL	Transport by Pipeline	12184	www.fluentcargo.com, assumes air flight distance
CL to NL	Transport by Ship	18020	Ports.com
AU to UK	Transport by Pipeline	14712	www.fluentcargo.com, assumes air flight distance
AU to UK	Transport by Ship	20791	Ports.com
AU to NL	Transport by Pipeline	14443	www.fluentcargo.com, assumes air flight distance
AU to NL	Transport by Ship	21318	Jeddah to Southampton, Google

Table S9: Fuel to electricity parameters.

Turbine for electricity	Efficiency (Gas to Electricity)	Reference
Natural gas turbine	39.10%	[26]
Hydrogen gas turbine	39.82%	
Oil plants	35%	

Table S10: Electricity to motor power and heat parameters.

Electricity to motor power	Efficiency	Reference
Compressors	95%	[27]
Pumps	58%	
Electricity to heat	85%	

Table S11: 2030 to 2050 grid electricity emissions factors by IEA.

Grid electricity	Year	Scenario	Carbon footprint [kg CO_2e/kWh]	Comments
Grid-SA	2030	IEA Sustainable Dev.	0.448669972	
Grid-SA	2050	IEA Sustainable Dev.	0.116710585	
Grid-SA	2030	IEA Stated Policies	0.574577978	
Grid-SA	2050	IEA Stated Policies	0.420475259	
Grid-MR	2030	IEA Sustainable Dev.	0.404840367	
Grid-MR	2050	IEA Sustainable Dev.	0.120239076	
Grid-MR	2030	IEA Stated Policies	0.546549934	
Grid-MR	2050	IEA Stated Policies	0.382524211	
Grid-NG	2030	IEA Sustainable Dev.	0.278911816	Based on IEA estimates of West Africa countries (Cote d'Ivoire, Ghana and Guinea)
Grid-NG	2050	IEA Sustainable Dev.	0.086367623	
Grid-NG	2030	IEA Stated Policies	0.349599830	
Grid-NG	2050	IEA Stated Policies	0.268947265	
Grid-AL	2030	IEA Sustainable Dev.	0.295025159	Based on IEA [28], [29] and [29] energy mix for 2030 and estimates of African countries with similar 2025 numbers (Ghana and Cote d'Ivoire)
Grid-AL	2050	IEA Sustainable Dev.	0.085262241	
Grid-AL	2030	IEA Stated Policies	0.395895157	
Grid-AL	2050	IEA Stated Policies	0.289892067	
Grid-CL	2030	IEA Sustainable Dev.	0.112484157	
Grid-CL	2050	IEA Sustainable Dev.	0.057330125	
Grid-CL	2030	IEA Stated Policies	0.207605549	
Grid-CL	2050	IEA Stated Policies	0.148191653	
Grid-AU	2030	IEA Sustainable Dev.	0.428696645	
Grid-AU	2050	IEA Sustainable Dev.	0.063207333	
Grid-AU	2030	IEA Stated Policies	0.735077279	
Grid-AU	2050	IEA Stated Policies	0.366138846	
Grid-NL	2030	IEA Sustainable Dev.	0.136186901	Based on IEA estimates of neighbouring countries (Belgium, Germany and the UK)
Grid-NL	2050	IEA Sustainable Dev.	0.048270622	
Grid-NL	2030	IEA Stated Policies	0.186353285	
Grid-NL	2050	IEA Stated Policies	0.117268013	

Grid electricity	Year	Scenario	Carbon footprint [kg CO_2e/kWh]	Comments
Grid-UK	2030	IEA Sustainable Dev.	0.134630945	
Grid-UK	2050	IEA Sustainable Dev.	0.048268992	
Grid-UK	2030	IEA Stated Policies	0.194628877	
Grid-UK	2050	IEA Stated Policies	0.136554383	

Table S12: Electricity emissions factors with future grid estimates based on IEA Sustainable Development scenario.

Electricity	Year	Carbon footprint [kg CO_2e/kWh]
Green	2025	0.000
Green	2030	0.000
Green	2050	0.000
Grid-SA	2025	0.593
Grid-SA	2030	0.449
Grid-SA	2050	0.117
Grid-MR	2025	0.644
Grid-MR	2030	0.405
Grid-MR	2050	0.120
Grid-NG	2025	0.459
Grid-NG	2030	0.279
Grid-NG	2050	0.086
Grid-AL	2025	0.468
Grid-AL	2030	0.295
Grid-AL	2050	0.085
Grid-CL	2025	0.325
Grid-CL	2030	0.112
Grid-CL	2050	0.057
Grid-AU	2025	0.590
Grid-AU	2030	0.429
Grid-AU	2050	0.063
Grid-NL	2025	0.268
Grid-NL	2030	0.136
Grid-NL	2050	0.048
Grid-UK	2025	0.183
Grid-UK	2030	0.135
Grid-UK	2050	0.048
HFO	2025	0.792
HFO	2030	0.792
HFO	2050	0.792
Fossil diesel	2025	0.974
Fossil diesel	2030	0.974
Fossil diesel	2050	0.974
e-diesel	2025	0.061
e-diesel	2030	0.041

Electricity	Year	Carbon footprint [kg CO_2e/kWh]
e-diesel	2050	0.031
e-MeOH	2025	0.056
e-MeOH	2030	0.031
e-MeOH	2050	0.021
e-gasoline	2025	0.059
e-gasoline	2030	0.041
e-gasoline	2050	0.031
e-NH_3	2025	0.051
e-NH_3	2030	0.031
e-NH_3	2050	0.021
SNG	2025	0.138
SNG	2030	0.064
SNG	2050	0.037
NG	2025	0.516
NG	2030	0.516
NG	2050	0.516
e-H_2	2025	0.136
e-H_2	2030	0.063
e-H_2	2050	0.036

Table S13: Fuel emissions factors with future grid estimates based on IEA Sustainable Development scenario. E-fuel emission factors obtained from own preliminary analysis and Concawe [3].

Fuel/Heat	Year	Carbon footprint [kg CO_2e/MJ]
Green heat	2025	0.0000
Green heat	2030	0.0000
Green heat	2050	0.0000
Grid-SA to heat	2025	0.1938
Grid-SA to heat	2030	0.1466
Grid-SA to heat	2050	0.0381
Grid-MR heat	2025	0.2104
Grid-MR heat	2030	0.1323
Grid-MR heat	2050	0.0393
Grid-NG heat	2025	0.1498
Grid-NG heat	2030	0.0911
Grid-NG heat	2050	0.0282
Grid-AL heat	2025	0.1529
Grid-AL heat	2030	0.0964
Grid-AL heat	2050	0.0279
Grid-CL heat	2025	0.1062
Grid-CL heat	2030	0.0368
Grid-CL heat	2050	0.0187
Grid-AU heat	2025	0.1927
Grid-AU heat	2030	0.1401

Grid-AU heat	2050	0.0207
Grid-NL heat	2025	0.0877
Grid-NL heat	2030	0.0445
Grid-NL heat	2050	0.0158
Grid-UK heat	2025	0.0599
Grid-UK heat	2030	0.0440
Grid-UK heat	2050	0.0158
HFO	2025	0.0770
HFO	2030	0.0770
HFO	2050	0.0770
Fossil diesel	2025	0.0947
Fossil diesel	2030	0.0947
Fossil diesel	2050	0.0947
e-diesel	2025	0.0059
e-diesel	2030	0.0040
e-diesel	2050	0.0030
e-MeOH	2025	0.0054
e-MeOH	2030	0.0030
e-MeOH	2050	0.0020
e-gasoline	2025	0.0057
e-gasoline	2030	0.0040
e-gasoline	2050	0.0030
e-NH_3	2025	0.0050
e-NH_3	2030	0.0030
e-NH_3	2050	0.0020
SNG	2025	0.0150
SNG	2030	0.0070
SNG	2050	0.0040
NG	2025	0.0560
NG	2030	0.0560
NG	2050	0.0560
e-H_2	2025	0.0150
e-H_2	2030	0.0070
e-H_2	2050	0.0040

Table S14: Emissions of electrolytic H_2 from 50% wind and 50% solar PV calculated using Equations (6) and (7), Ecoinvent, [30], [31] and Smith et al. [32]. Grey and blue H_2 calculated from [33], [34], [35].

H_2 type	**Country**	**Electrolyser/CCS efficiency**	**Emission factor [kg CO_2e/kg H_2]**	**Embodied emission factor [kg CO_2e/kg H_2]**
Electrolytic H_2	SA	65.4%	0.0000	0.7167
Electrolytic H_2	SA	75.0%	0.0000	0.6249
Electrolytic H_2	MR	65.4%	0.0000	1.1368
Electrolytic H_2	MR	75.0%	0.0000	0.9913
Electrolytic H_2	NG	65.4%	0.0000	2.0093
Electrolytic H_2	NG	75.0%	0.0000	1.7521

Electrolytic H_2	AL	65.4%	0.0000	0.9442
Electrolytic H_2	AL	75.0%	0.0000	0.8233
Electrolytic H_2	CL	65.4%	0.0000	0.8811
Electrolytic H_2	CL	75.0%	0.0000	0.7683
Electrolytic H_2	AU	65.4%	0.0000	0.7168
Electrolytic H_2	AU	75.0%	0.0000	0.6250
Blue SMR H_2	Generic	Generic	2.5000 (in 2025 to 2030 based on Longden et al. [34] and IEA [35]) 2.0000* (in 2050 based on IEA [35])	0.2999
Grey SMR H_2	Generic	Generic	10.5500 (in 2025 to 2030 based on Longden et al. [34] and IEA [35]) 10.0000 (in 2050 based on IEA [35])	0.2999
* Note IEA blue H_2 BAT of 1.5 kg CO_2e/kg H_2 at plant gate was also analysed, and a note is indicated where this is done.				

Table S15: Electricity use by processes.

Operation type	**Electricity source, 2025**	**Fuel source, 2025**	**Electricity source, 2030**	**Fuel source, 2030**	**Electricity source, 2050**	**Fuel source, 2050**
Processes occurring at plant location: Green and synthetic fuels	Green	Green heat	Green	Green heat	Green	Green heat
Processes occurring at plant location: Blue and grey H_2	NG	NG	NG	NG	NG	NG
Processes occurring at terminals	Grid electricity	NG	Grid electricity	NG	Grid electricity	Grid electricity
Processes occurring at terminals (sensitivity analysis)	Synthetic fuel	Synthetic fuel	Synthetic fuel	Synthetic fuel	Synthetic fuel	Synthetic fuel
Transportation: Trucks, rail, local pipeline and ship	Grid electricity	Fossil diesel	Grid electricity	Synthetic fuel	Grid electricity	Synthetic fuel
Transportation: Trans-continental pipeline	Synthetic fuel	Synthetic fuel	Synthetic fuel	Synthetic fuel	Synthetic fuel	Synthetic fuel
Processes occurring at stations	Grid electricity	NG	Grid electricity	NG	Grid electricity	Grid electricity

Table S16: Electricity and embodied emission factors of fuel stations and gas boilers [based on 10-kW boiler]. A service station with 310,000 m^3 gas sold per year (in 365 days) was assumed for the embodied emission factors based on Ecoinvent data of NG refuelling station.

Process	**Boil off/losses [per kg H_2]**	**Electricity demand [kWh/kg fuel product]**	**Embodied emissions [kgCO_2e/kg fuel product]**	**Ref.**
H_2 Dispensing Station: as CH2 (from LP)	0.5%	3.522544	0.000036	[3], [16], [27], [36], [37], [38], and Ecoinvent
H_2 Dispensing Station: as CH2 (from initial 80-100 bar)	0.5%	2.692836	0.000036	
H_2 Dispensing Station: as CH2 (from initial 500 bar)	0.5%	0.618567	0.000036	
H_2 Dispensing Station: as LH2	1.85%	0.549400	0.000022	
H2 Dispensing Station: as CH2 w/NH_3 at station	1.5%	0.618567	0.000002	
CNG Dispensing Station: as SNG	0.02%	0.305556	0.000009	
Gas boilers: as H_2	0.02%	0.618567	0.070588	
Gas boilers: as SNG	0.02%	0.000000	0.029424	

Table S17: Electricity and embodied emission factors of terminals.

Process	**Boil off/losses [per kg H_2]**	**Electricity demand [kWh/kg fuel product]**	**Embodied emissions [kgCO_2e/kg fuel product]**	**Comments/Ref.**
H_2 Storage: CH2 Terminal (Import)	0.50%	0.200000	0.083750	Assumed 10 days storage in terminals, [3], [16], [38], and Ecoinvent
H_2 Storage: CH2 Terminal (Export)	0.50%	0.610000	0.083750	
H_2 Storage: CH2 Terminal (Distribution)	0.50%	0.200000	0.083750	
H_2 Storage: LH2 Terminal (Import)	0.70%	0.200000	0.007344	
H_2 Storage: LH2 Terminal (Import) w/re-LH2	0.70%	0.224500	0.007344	
H_2 Storage: LH2 Terminal (Export)	0.70%	0.610000	0.007344	
H_2 Storage: LH2 Terminal (Export) w/re-LH2	0.70%	0.634500	0.007344	
H_2 Storage: LH2 Terminal (Distribution)	0.70%	0.200000	0.007344	
H_2 Storage: LH2 Terminal (Distribution) w/re-LH2	0.70%	0.224500	0.007344	
MeOH Storage: Terminal (Import), H_2 Product basis	0.00%	0.024322	0.003454	
MeOH Storage: Terminal (Export), H_2 Product basis	0.00%	0.024322	0.003454	
MeOH Storage: Terminal (Distribution), H_2 Product basis	0.00%	0.024322	0.003454	
NH_3 Storage: Terminal (Import), H_2 Product basis	0.00%	0.003000	0.004254	

NH_3 Storage: Terminal (Export), H_2 Product basis	0.00%	0.001000	0.004254	
NH_3 Storage: Terminal (Distribution), H_2 Product basis	0.00%	0.003000	0.004254	
MCH Storage: Terminal (Import)	0.00%	0.013000	0.011076	
MCH Storage: Terminal (Export)	0.00%	0.013000	0.011076	
MCH Storage: Terminal (Distribution)	0.00%	0.013000	0.011076	
LSNG Storage: Terminal (Import)	0.03%	0.028322	0.001175	
LSNG Storage: Terminal (Export)	0.03%	0.028322	0.001175	

Table S18: Emission factors for fuel oxidation in combustion engines and fuel cell vehicles.

Parameter	**Model**	**Embodied emissions [$kgCO_2e$/kg fuel]**	**Oxidation GHG emissions factor [$kgCO_2e$/kg fuel]**	**Data based on ref.**
Road transport: H_2 oxidation	Truck	0.001104	0	[39], Ecoinvent (trailer, agricultural trailer production)
Road transport: SNG oxidation	Truck	0.001104	0.00521	[39], Ecoinvent (trailer, agricultural trailer production)
Rail transport: H_2 oxidation	Train	0.017776	0	[39], Ecoinvent (train production, passenger, long-distance)
Rail transport: SNG oxidation	Train	0.017776	0.00521	[39], Ecoinvent (train production, passenger, long-distance)
Water transport: H_2 oxidation	Ship	0.004610	0	[39], Ecoinvent (tanker production for liquefied natural gas)
Water transport: SNG	Ship	0.004610	0.00521	[39], Ecoinvent (tanker production for liquefied natural gas)
Air transport: H_2 oxidation	Aircraft	0.007238	0	[39], Ecoinvent medium-haul aircraft
Gas boiler: H_2	10 kW boiler	0.070588	0	[39], Ecoinvent 10 kW boiler

Gas boiler: SNG	10 kW boiler	0.029424	0.00521	[39], Ecoinvent 10 kW boiler

Table S19: Emissions for toluene production based on data obtained from Ecoinvent and IEA [16]

Parameter	**Value**
Lifetime of toluene in supply chains [y]	30
GHG emissions over a process lifetime of 30 years [kgCO_2e/kg toluene/year]	0.052
Toluene installed capacity [kt/y]	4200
H_2 equiv. carried [kt/y]	277.612
Toluene installed capacity [kg toluene/kg H_2]	15
Toluene installed capacity [kg toluene/y/kg H_2]	0.504301075
Toluene makeup [kt/y]	100
Toluene makeup [kt toluene/kt toluene]	2.4%
Toluene makeup [kg toluene/kg H_2 carried]	0.360215054

Table S20: 100-year GWP of GHGs

GWP	**Value**	**Unit**	**Reference**
H_2	11	CO_2e	[40]
CH_4	28	CO_2e	[41]
N_2O	265	CO_2e	
CO_2	1	CO_2e	

2 Results

2.1 Gaseous fuel Losses in transport applications

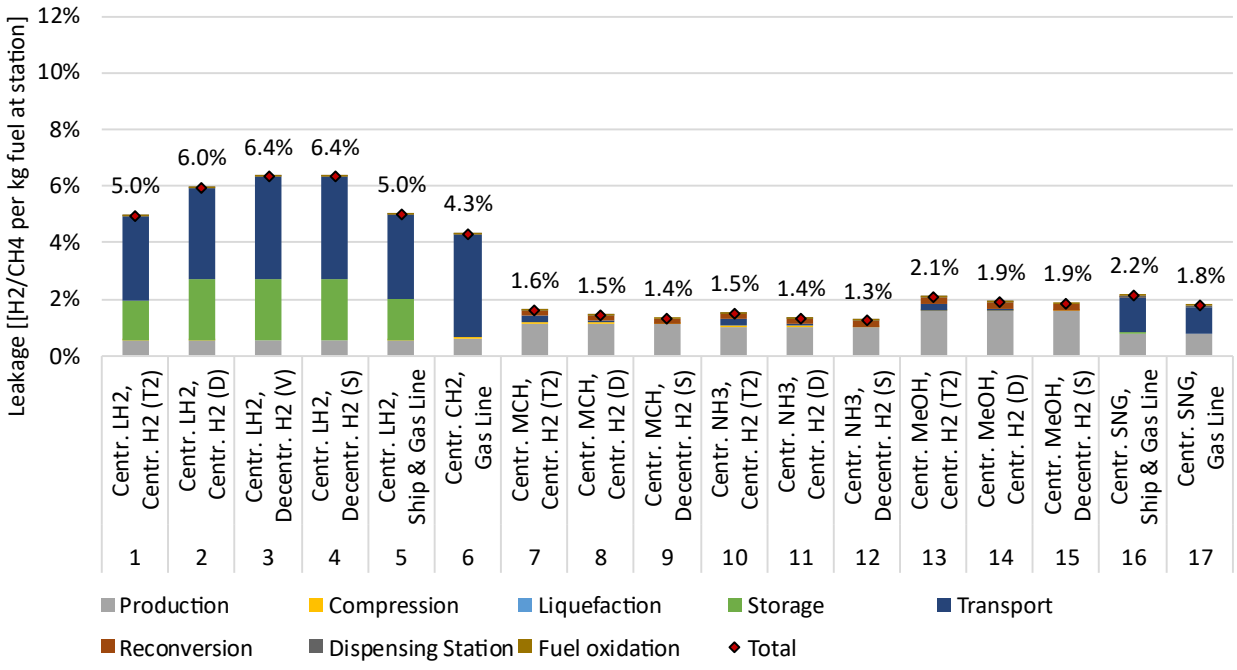

Figure S1: H_2-related losses to the environment in 2025, SA to UK.

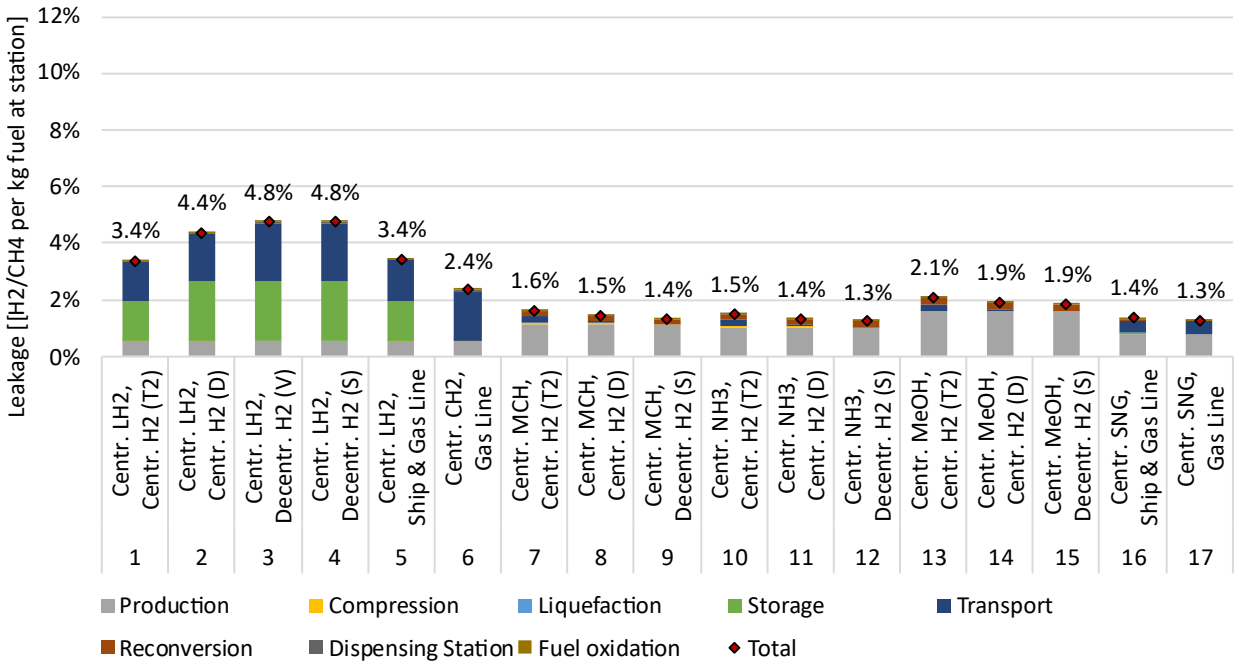

Figure S2: H_2-related losses to the environment in 2025, MR to UK.

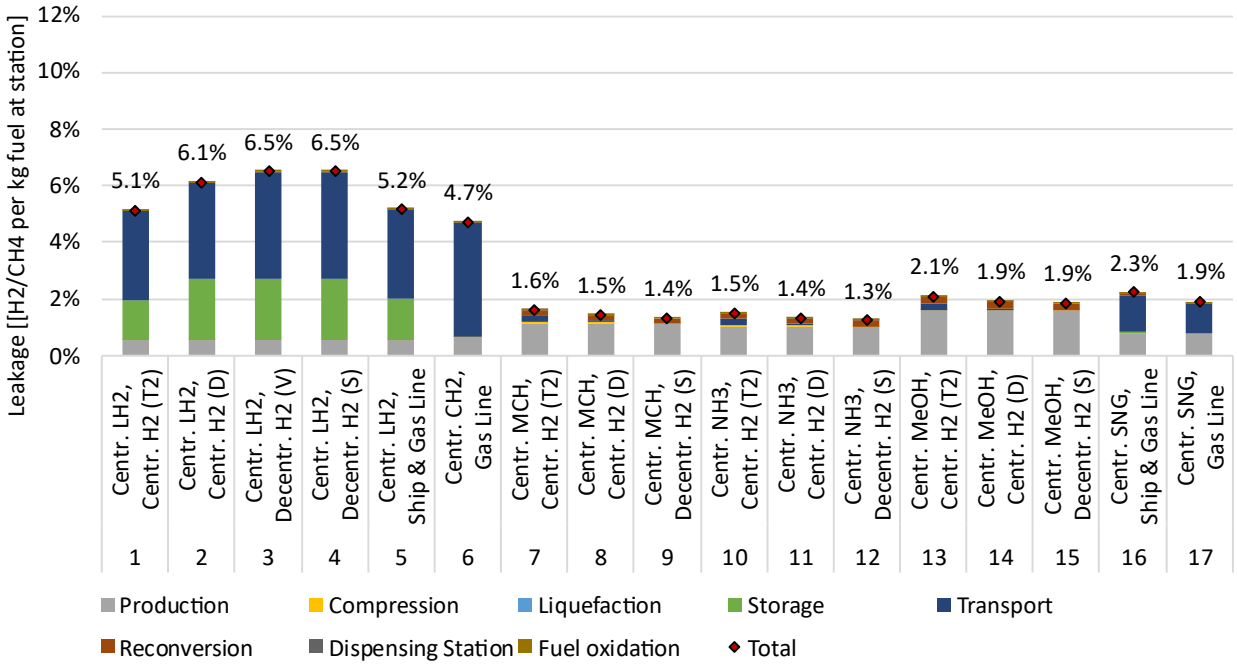

Figure S3: H_2-related losses to the environment in 2025, NG to UK.

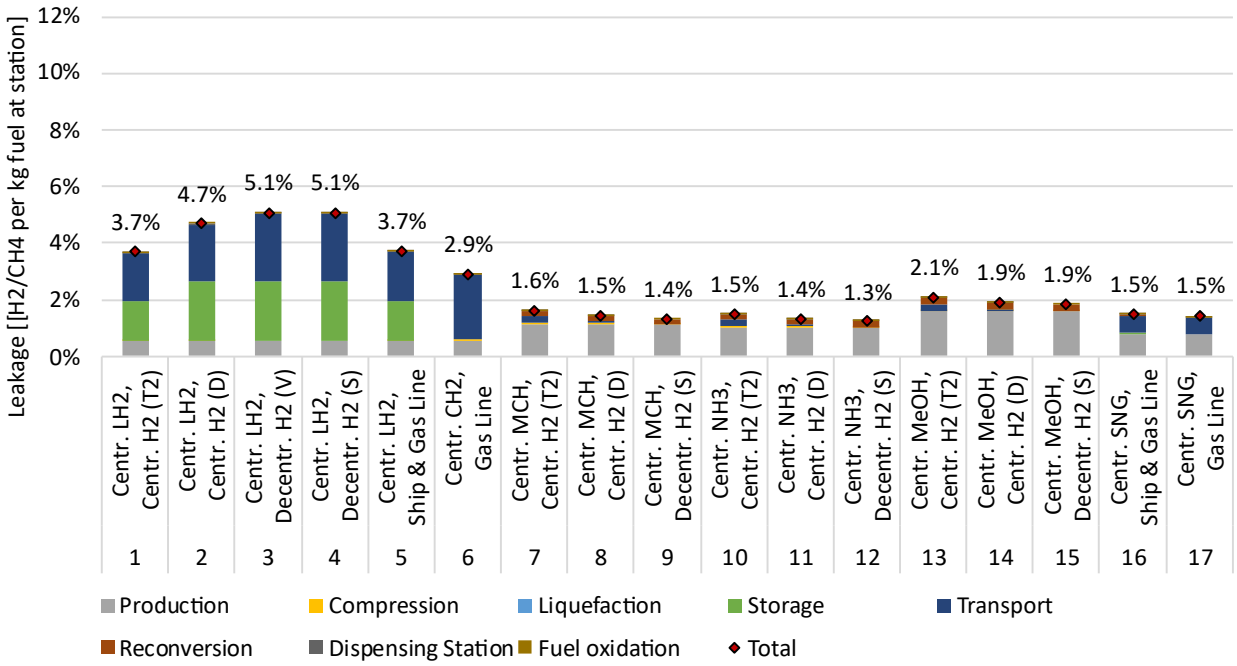

Figure S4: H_2-related losses to the environment in 2025, AL to UK.

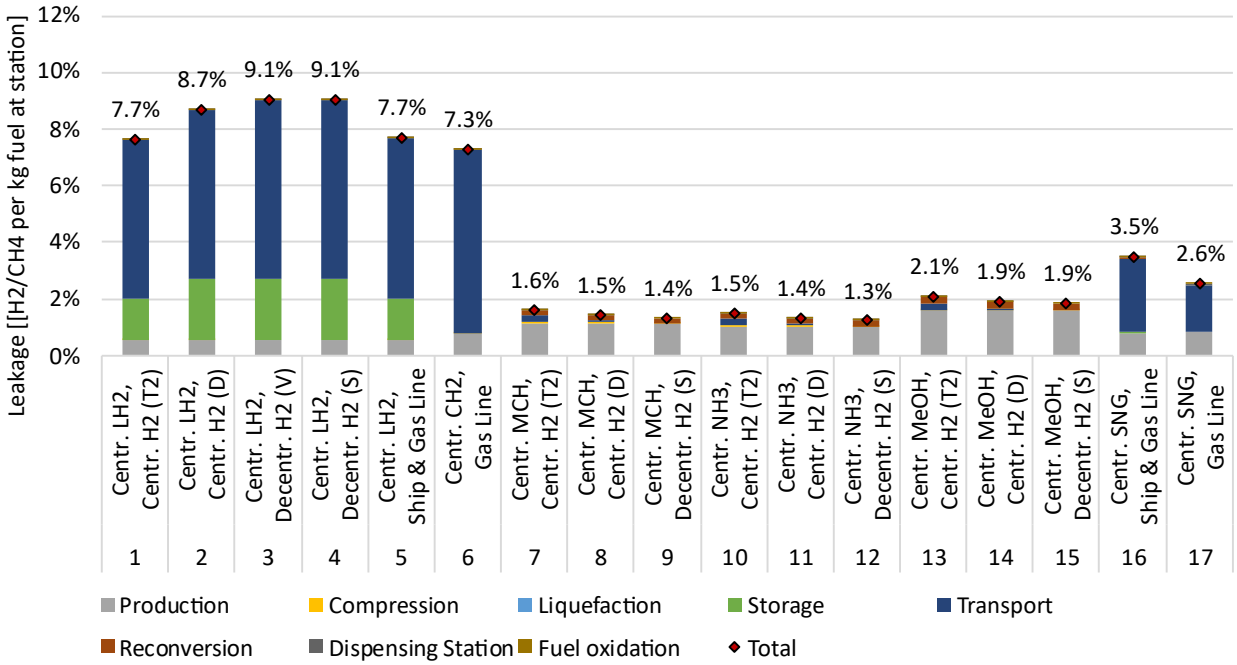

Figure S5: H_2-related losses to the environment in 2025, CL to UK.

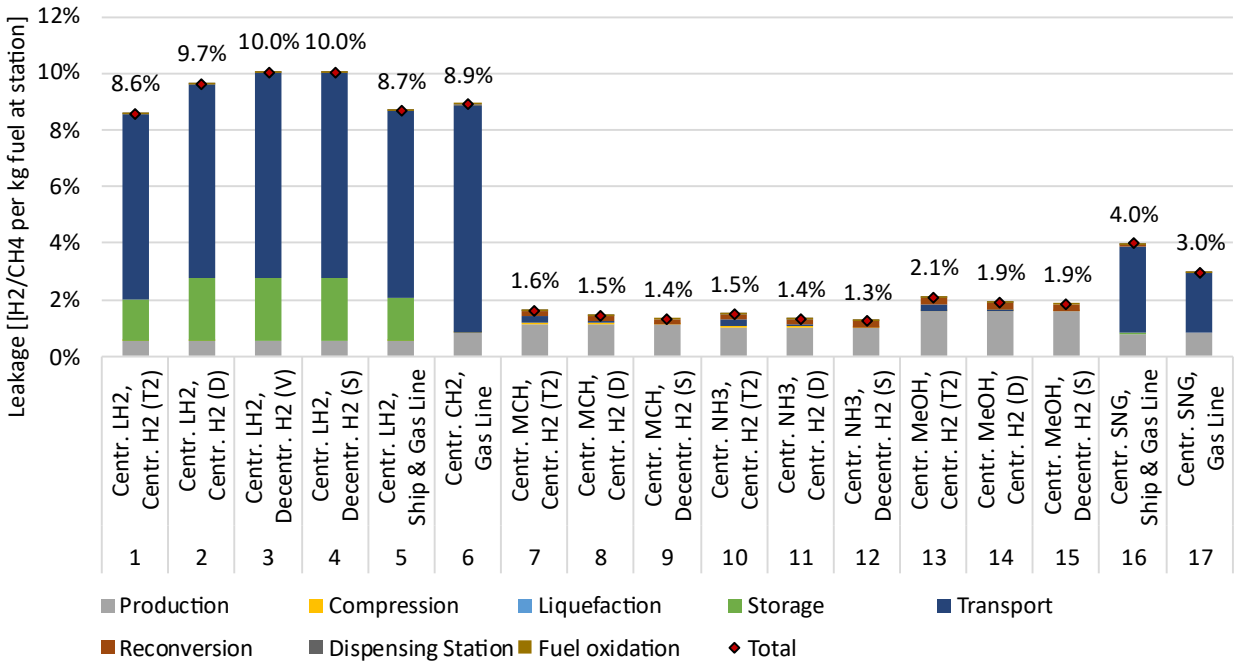

Figure S6: H_2-related losses to the environment in 2025, AU to UK.

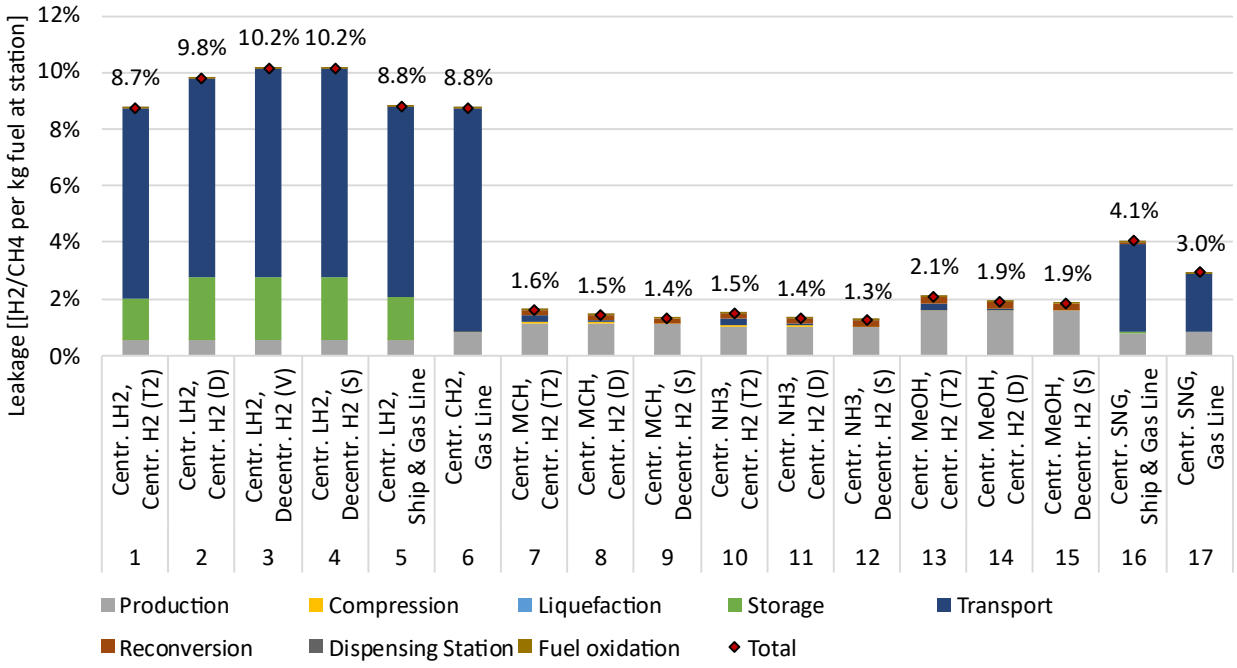

Figure S7: H_2-related losses to the environment in 2025, AU to NL.

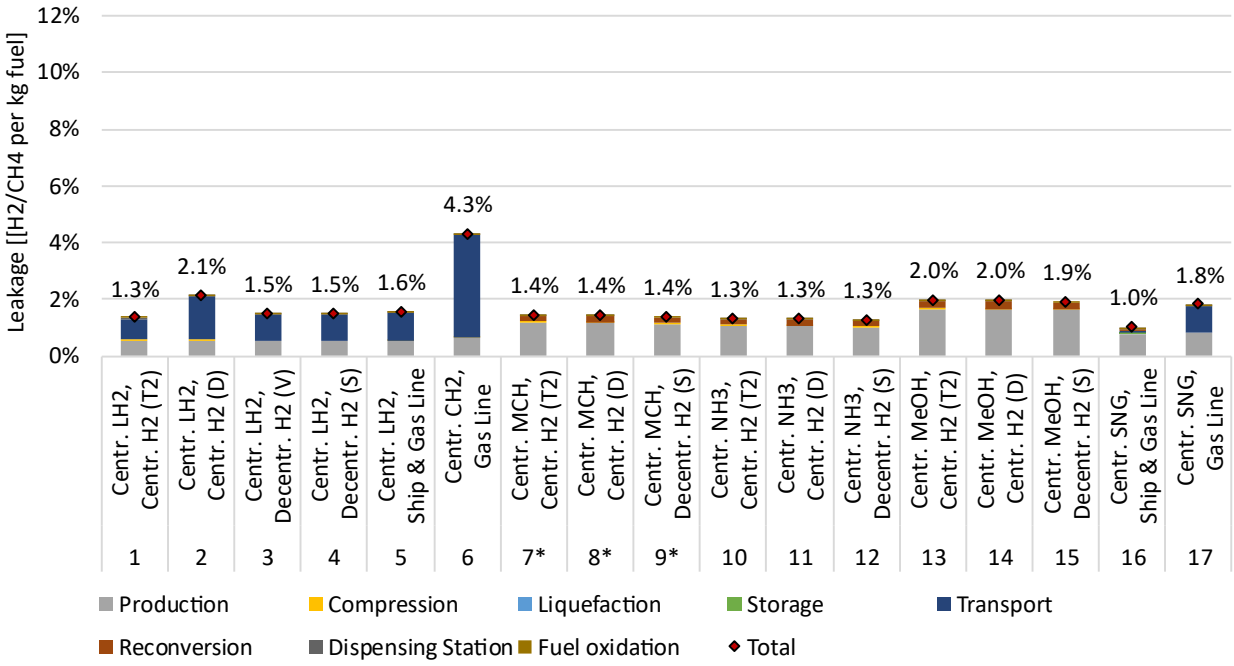

Figure S8: H_2-related losses to the environment in 2030 to 2050 with boil-off gas recovery, SA to UK.

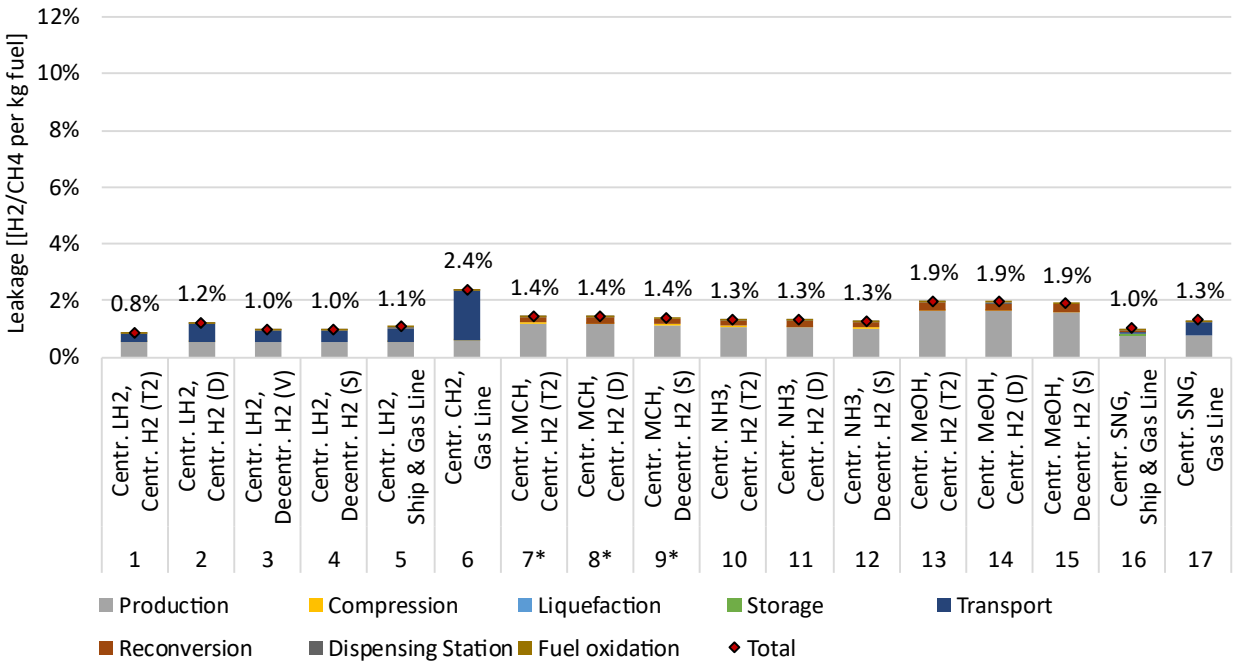

Figure S9: H_2-related losses to the environment in 2030 to 2050 with boil-off gas recovery, MR to UK.

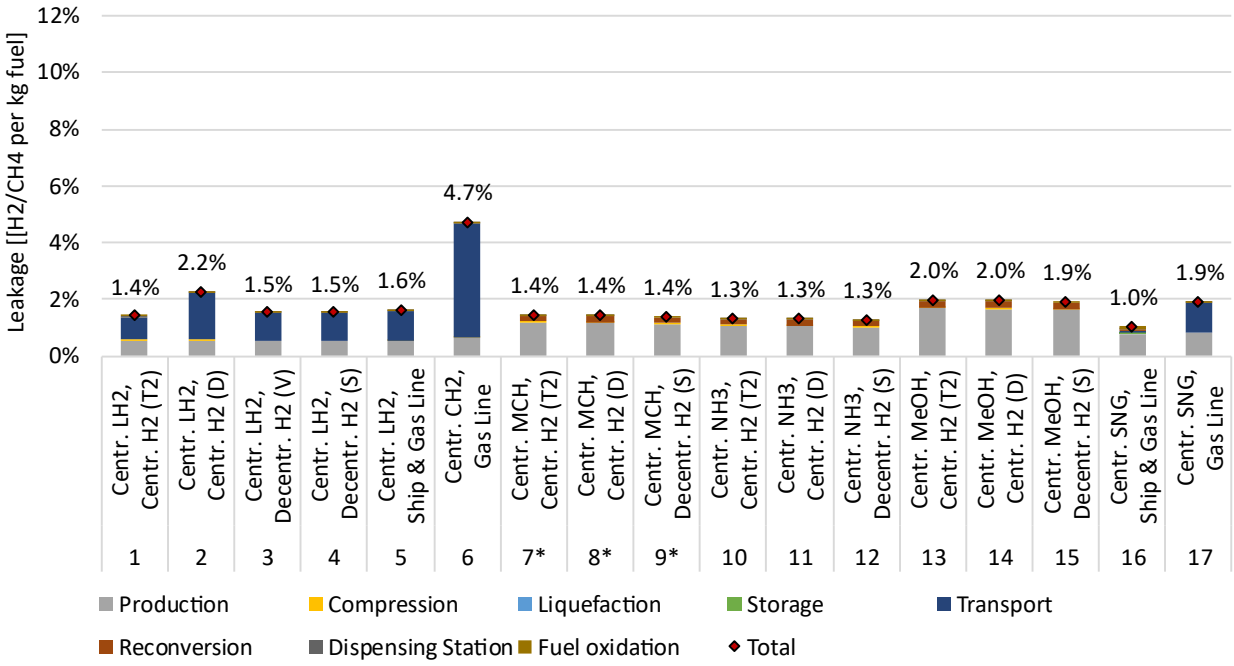

Figure S10: H_2-related losses to the environment in 2030 to 2050 with boil-off gas recovery, NG to UK.

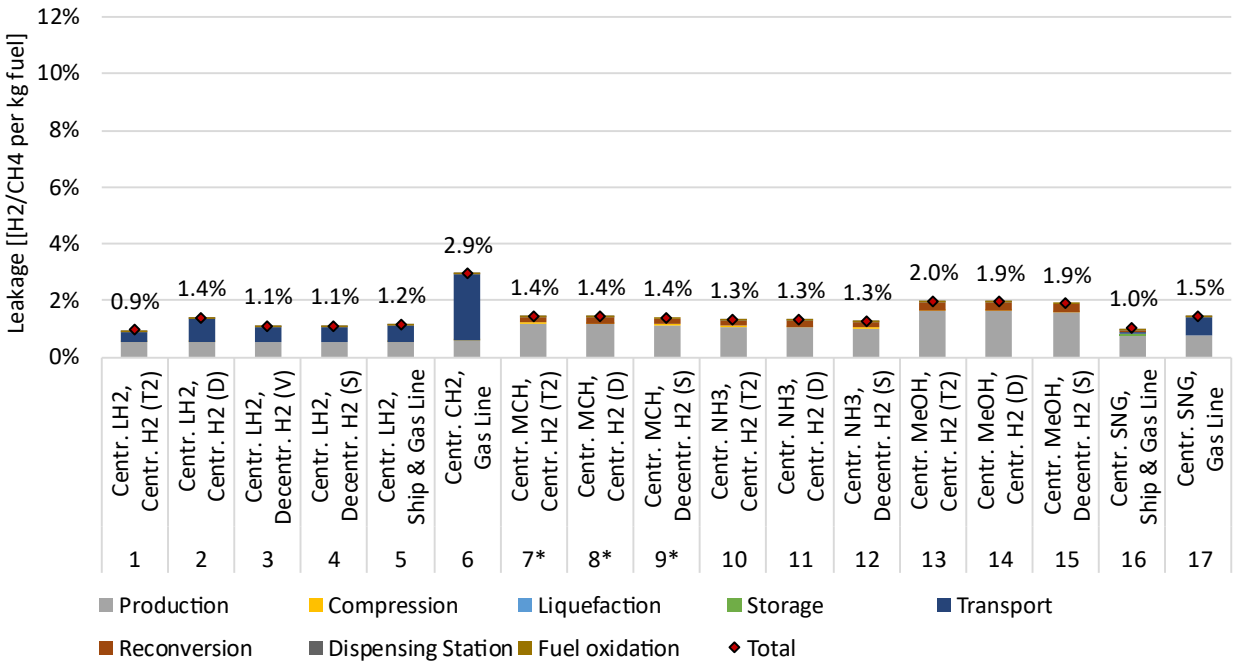

Figure S11: H_2-related losses to the environment in 2030 to 2050 with boil-off gas recovery, AL to UK.

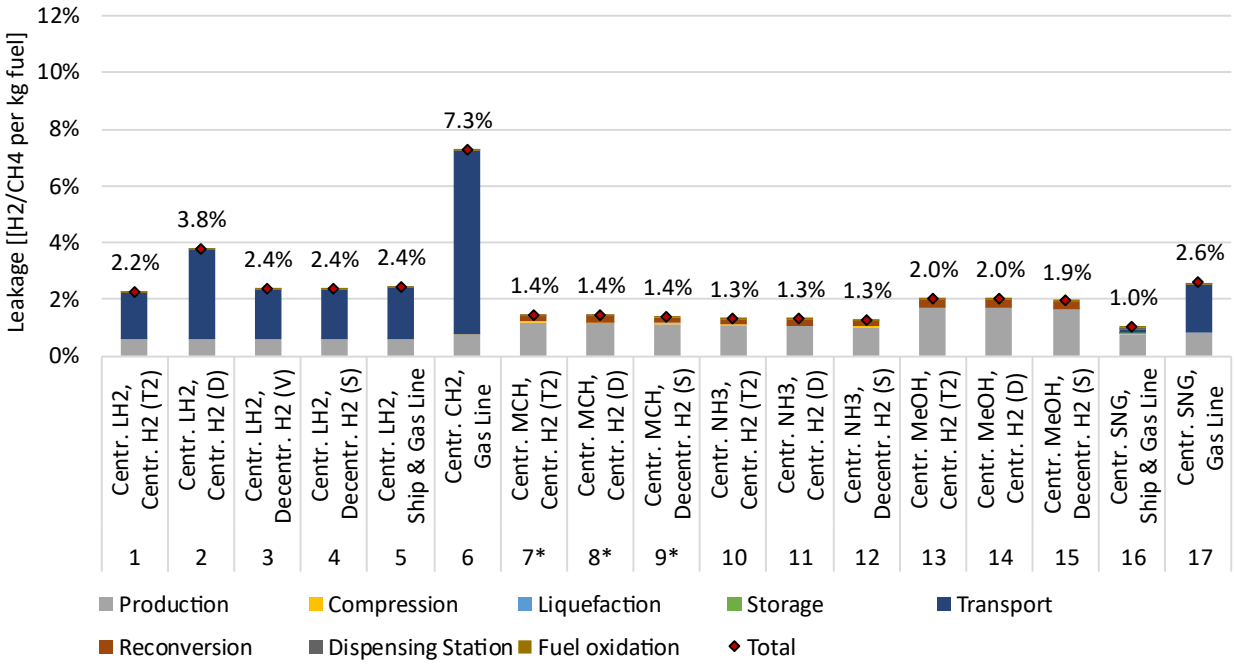

Figure S12: H_2-related losses to the environment in 2030 to 2050 with boil-off gas recovery, CL to UK.

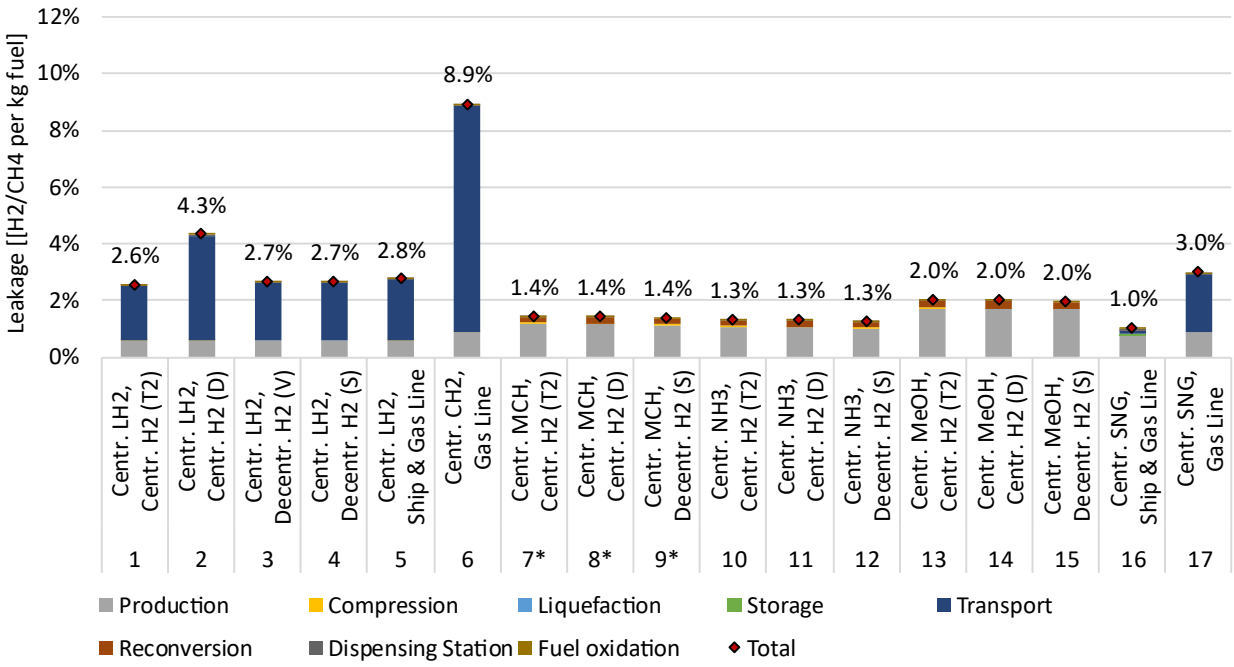

Figure S13: H_2-related losses to the environment in 2030 to 2050 with boil-off gas recovery, AU to UK.

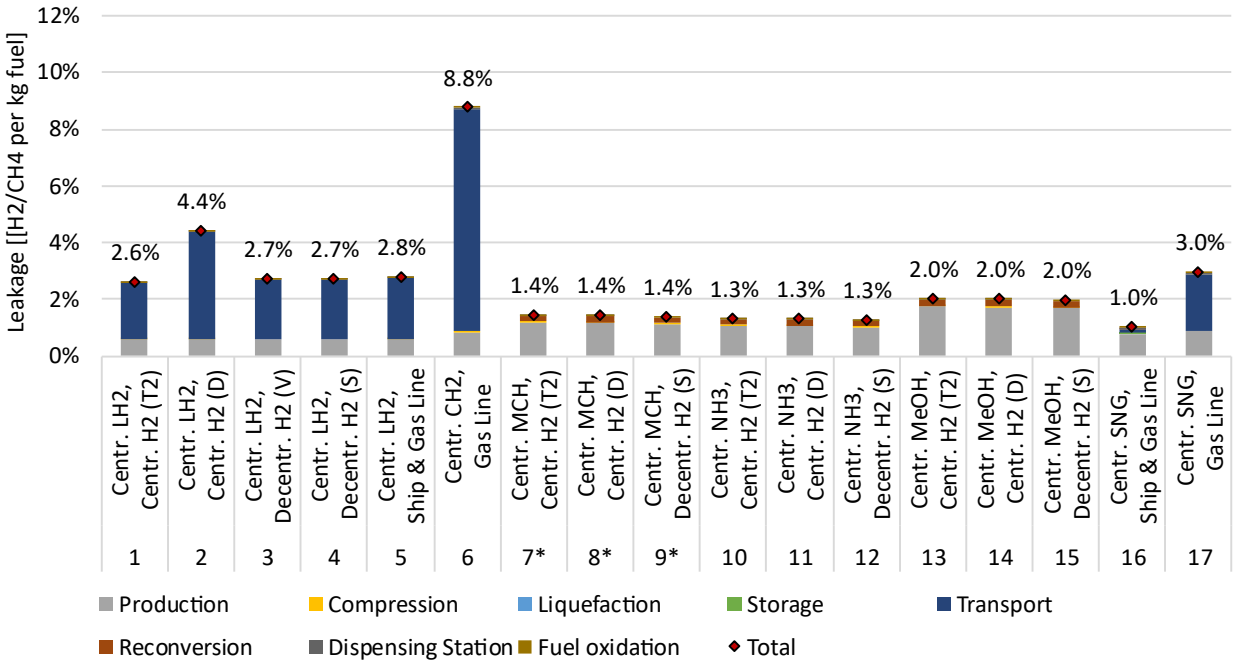

Figure S14: H_2-related losses to the environment in 2030 to 2050 with boil-off gas recovery, AU to NL.

2.2 Gaseous fuel energy balance in transport applications

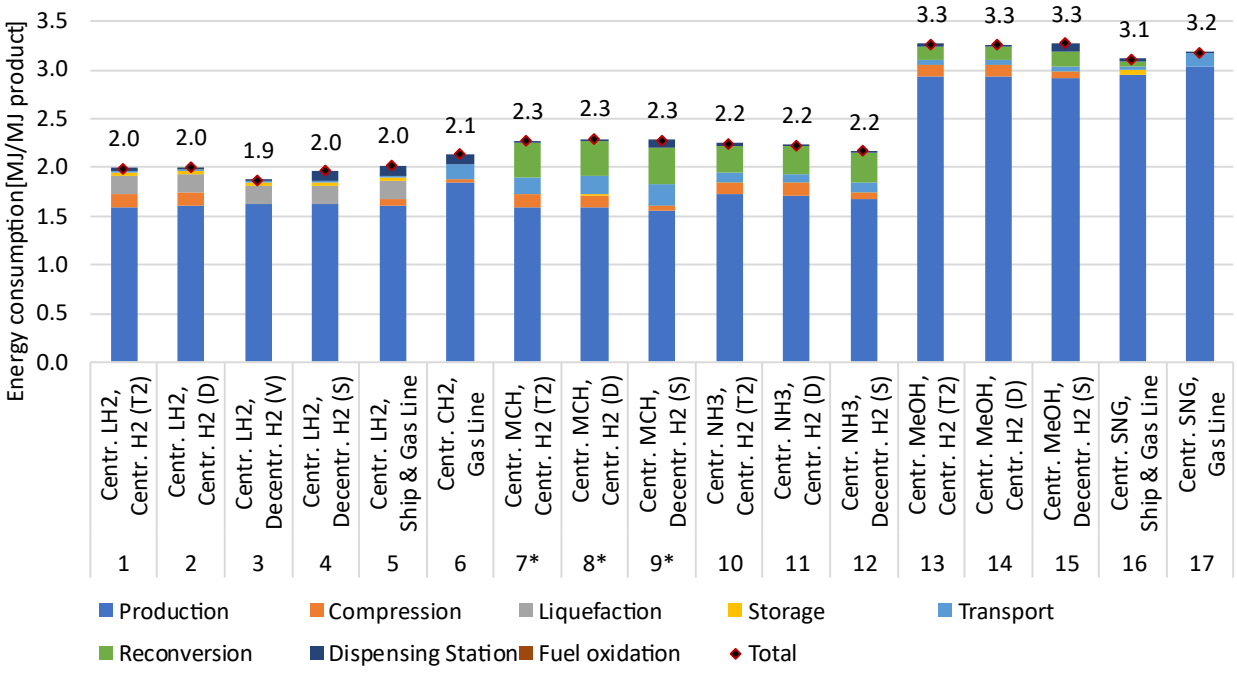

Figure S15: The energy consumption of various gaseous fuel supply chains for the SA to UK route in 2025. Note that the MCH supply chains in * do not include the energy consumption in producing toluene from the refinery, as toluene is a byproduct in the production of gasoline from crude oil and coke from coal.

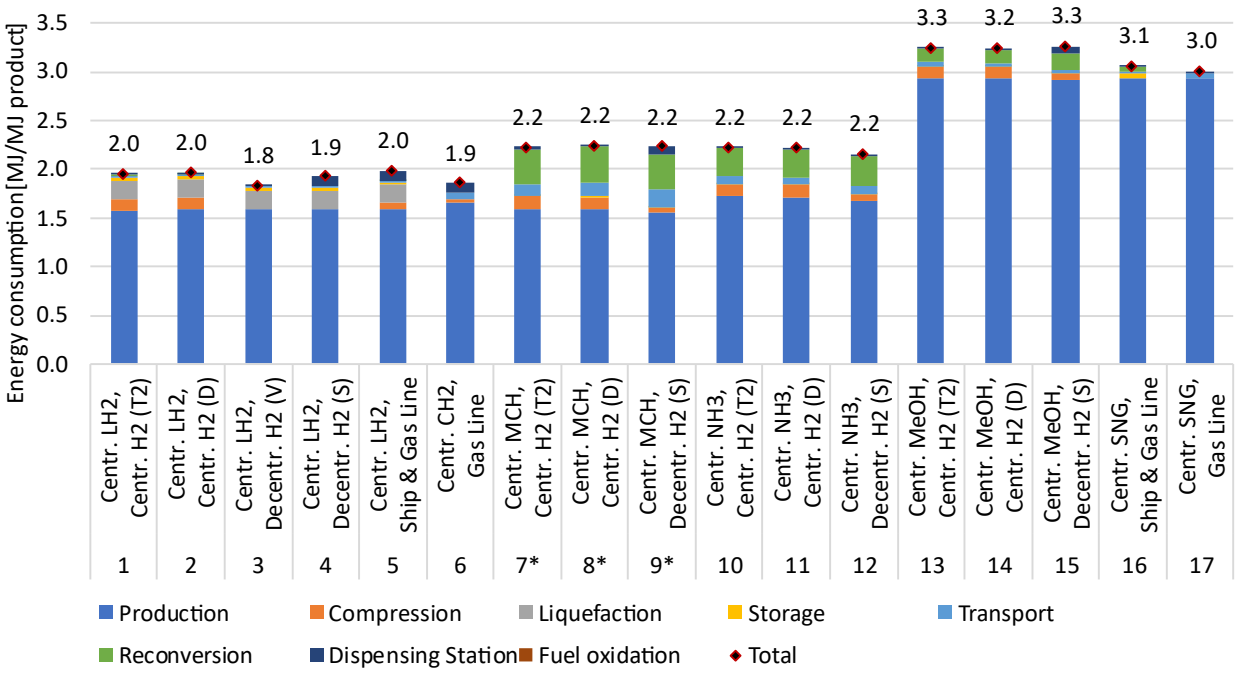

Figure S16: The energy consumption of various gaseous fuel supply chains for the MR to UK route in 2025.

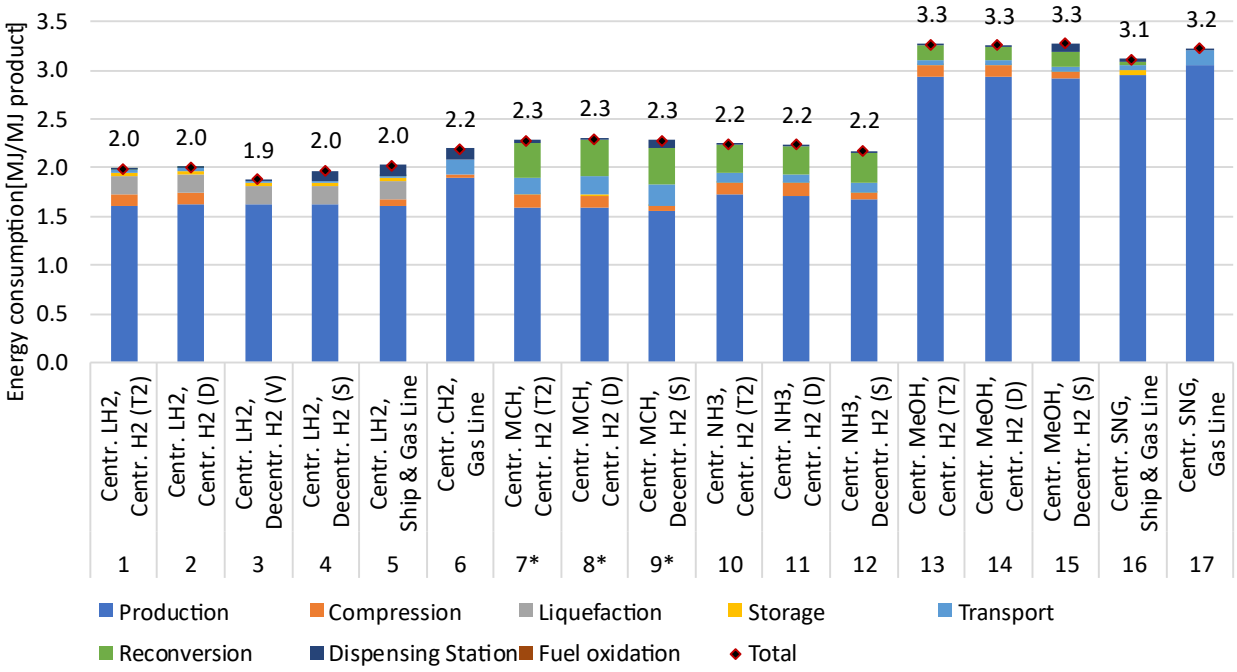

Figure S17: The energy consumption of various gaseous fuel supply chains for the NG to UK route in 2025.

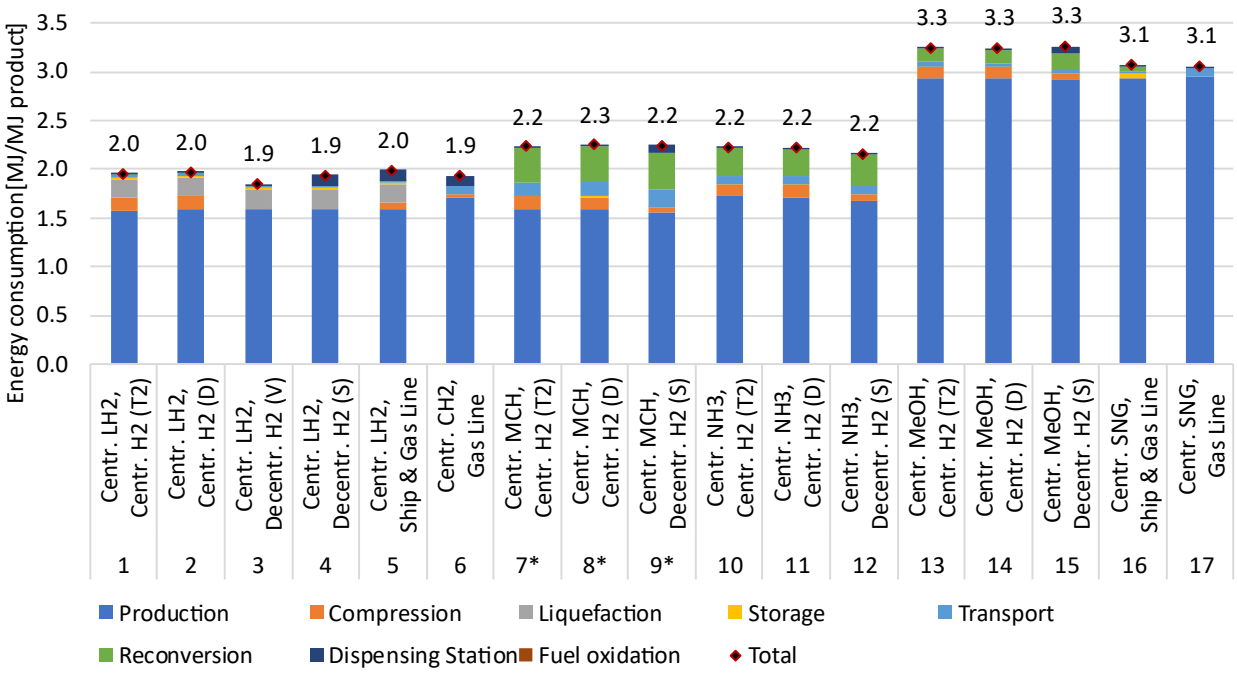

Figure S18: The energy consumption of various gaseous fuel supply chains for the AL to UK route in 2025.

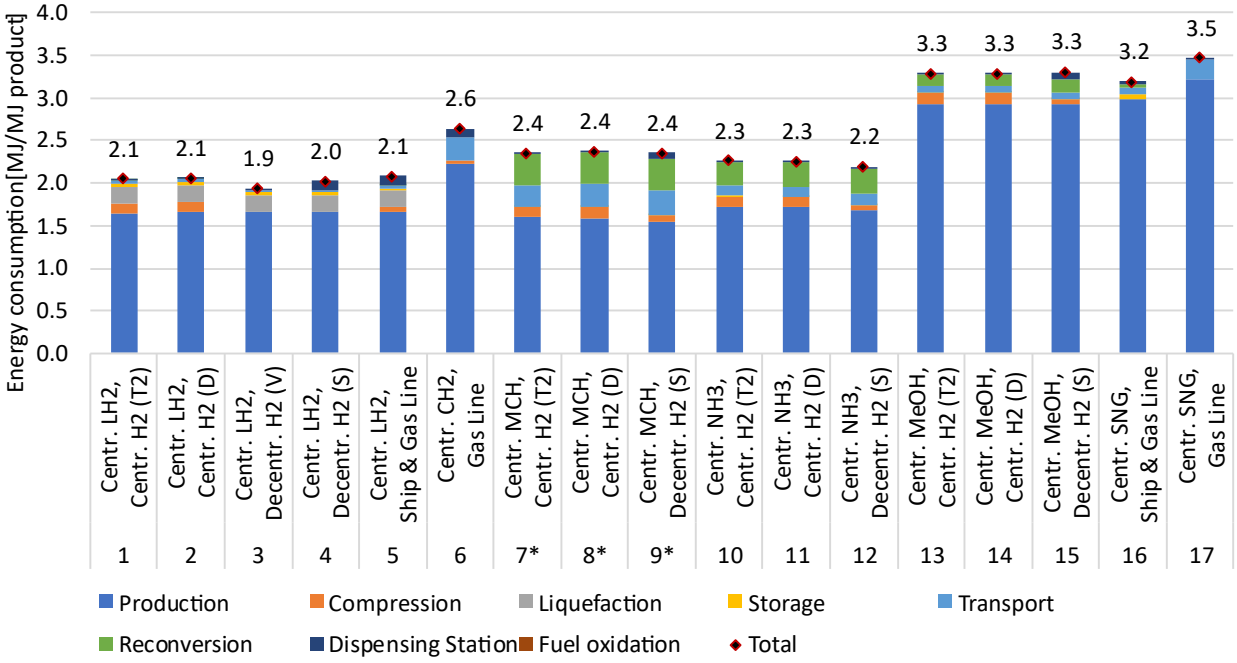

Figure S19: The energy consumption of various gaseous fuel supply chains for the CL to UK route in 2025.

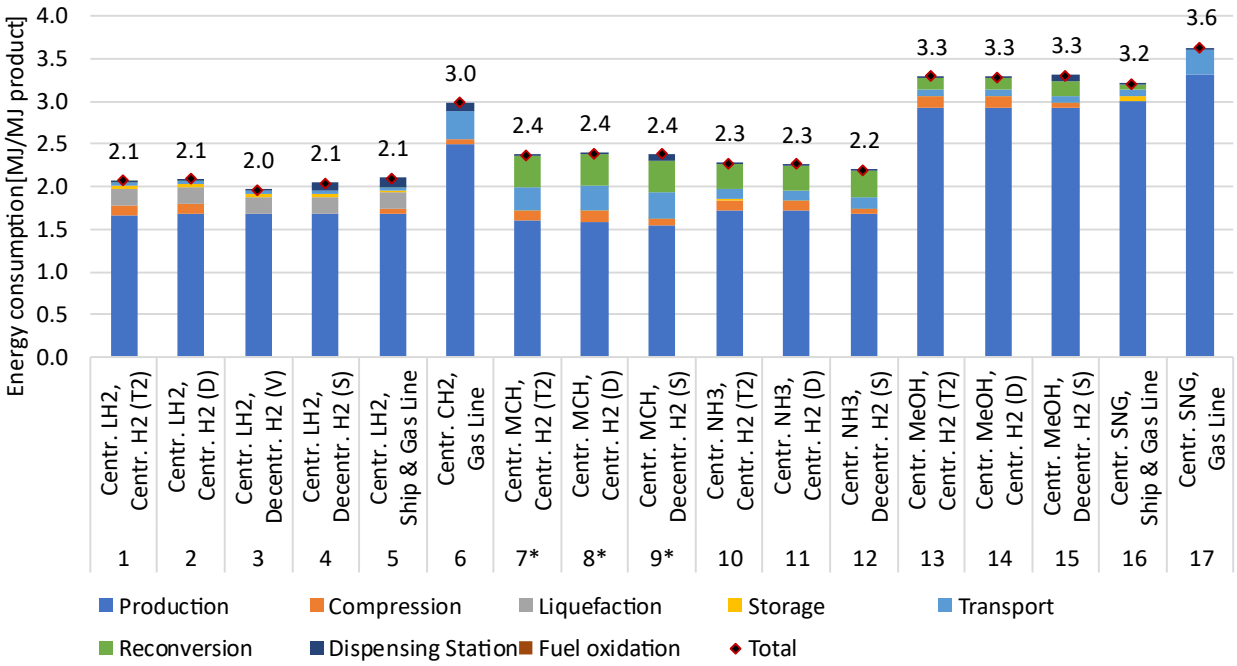

Figure 20: The energy consumption of various gaseous fuel supply chains for the AU to UK route in 2025.

2.3 Supply chain GHG emissions limits for pipeline in transport applications

Table S21: The limits at which pipeline transportation exceeds regulatory standards. Assumed in-situ LCF is used in trans-continental transmission by pipelines due to remote location factors.

H_2 source	**Limit to pipeline length**	**EU Standard of 28.2 gCO_2e/MJ**	
		2025	**2050**
Green H_2	Pipeline length for H_2	20900[a] km	31900[a] km
	Pipeline length for SNG	18400 km	23600[a] km
Blue H_2	Pipeline length for H_2	400 km	4000[b]–6000[c] km
	Pipeline length for SNG	N/A[d]	Up to 2800[c] km

[a] This is a theoretical limit. Earth's antipodal distance is approximately 20,000 km.
[b] Estimates based on an average blue H_2 production emission factor of 2.0 $kgCO_2e/kg\ H_2$ at plant gate in 2050.
[c] Estimates based on IEA blue H_2 production BAT emission factor of 1.5 $kgCO_2e/kg\ H_2$ at plant gate in 2050.
[d] Estimates impractical due to emission at plant gate above the EU emissions limits. This is typically applicable to blue SNG scenarios that require NG (methane) to be converted to blue H_2 to SNG (methane).

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Appendix A5: Supplementary information for Chapter 8: Life cycle assessment of global liquid electro-fuels and chemicals supply chains from technological, geospatial, and temporal perspectives

Supplementary Information (SI) 1

Life cycle assessment of global liquid electro-fuels and chemicals supply chains from technological, geospatial, and temporal perspectives

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1 Methodology

Table S1: Fuel/chemical properties [1], [2], [3], [4].

Fuel/chemical	LHV [MJ/kg]	LHV [MJ/L]	HHV [MJ/kg]	HHV [MJ/L]
Hydrogen	119.950	4.761*	141.880	5.631*
NH_3	18.800	13.160	22.500	15.750
MeOH	20.100	15.959	22.900	18.183
MTG: Gasoline	44.150	32.700	46.940	34.770
MTK: Kerosene	43.690	35.240	45.990	37.100
FT-liquids	42.910	35.940	45.600	38.190
* LHV of H_2 in MJ/L at 70 MPa				

Table S2: Process yield of H_2-related process.

Fuel/chemical	Yield basis				Unrecoverable system loss		Comment/data based on ref.
NH_3	0.010	kg H_2	0.0535	kg NH_3	0.5%	kg H_2	Losses from casing leaks, [3], [5], [6]
MeOH	0.010	kg H_2	0.0502	kg MeOH	32.3%	kg H_2	MeOH formation produces high amount H_2O as a by-product [3]
MTG: Gasoline	0.010	kg H_2	0.0232	kg gasoline	68.6%	kg H_2	See Equation (5) to Equation (8) by-products. Other references: Concawe [3], Kiel [7] and Helton and Hindman [8]
MTK: Kerosene	0.010	kg H_2	0.0227	kg kerosene	68.6%	kg H_2	
FTS: FT-liquids	0.012	kg H_2	0.0232	kg FT-liquids	69.1%	kg H_2	
Drop-in biofuel via hydrothermal liquefaction (HTL)	0.017	kg H_2	0.3084	kg liquid fuel	83.2%	kg H_2	

Table S3: CO_2 capture and N_2 liquefaction material, energy balance, and emission factors data.

Operation	**Net electricity [kWh/kg fuel product]**	**Net heat [MJ/kg fuel product]**	**Embodied emissions [kgCO_2e/kg fuel product]**	**Reference**
DAC w/MeOH, MeOH basis	0.71	6.63	0.004825	[3], [9], [10] and Ecoinvent
DAC w/MeOH/MTG, Gasoline basis	1.61	13.86	0.011034	
DAC w/MeOH/MTK, Kerosene basis	1.63	14.05	0.011186	
DAC w/FTS, FT-liquid basis	1.91	7.31	0.013086	
N_2 liquefaction [for NH_3]	0.26	0.00	0.000206	
Note: The capture energy in the case of decentralised cases was assumed to be zero since CO_2 is obtained at 99 volume percent from bioethanol and biomethane plants.				

Table S4: Rail transportation parameters based on tank cars by Federal Railroad Administration [11].

Rail	**Units**	**as NH_3**	**as MeOH**	**as gasoline/diesel/kerosene**	**Data based on ref.**
Train life (years)	40	40	40	40	
Tank capacity	t (cargo)	31.5	35.7	36.6	[12], [13]
Product stored pressure	bar	1	1	1	[14], [15]
Speed	km/h	69.20	69.20	69.20	[11]
Speed (unloaded)	km/h	80.00	80.00	80.00	
Delivery distance	km	400	400	400	
Travel time (loaded)	h	5.78	5.78	5.78	
Travel time (unloaded)	h	5.00	5.00	5.00	
Numbers of rail cars	h	30	30	30	[11]
Loading/unloading time per rail tank car	h	0.55	0.55	0.55	[16]
Loading/unloading time (total)	h	16.36	16.36	16.36	
Total time	h	22.14	22.14	22.14	
Total time with empty return	h	27.14	27.14	27.14	
Total time with toluene return	h	43.51	43.51	43.51	
Energy consumption	MJ/kg fuel product/km	0.00025	0.00025	0.00025	[11]
Energy consumption with empty return	MJ/kg fuel product/km	0.00036	0.00036	0.00036	
Embodied emissions (single trip basis)	kgCO_2e/kg fuel product	0.00507	0.00507	0.00507	Ecoinvent

Table S5: Ship transportation parameters.

Shipping	**Units**	**as NH_3**	**as MeOH**	**as gasoline/diesel/kerosene**	**Reference**
Capacity	t fuel product (cargo)	53,000	90,402	53,000	[3], [17], [18]
Lifetime	years	35	35	35	
Ship speed	km/h	30	30	30	
Fuel use	MJ/km	2500	5469	5489	
Fuel use	MJ/km/kg cargo (fuel product) transported	0.0000472	0.0000605	0.0000604	
Loading/unloading time	Days	2	2	2	
Embodied emissions (single trip basis)	$kgCO_2e$/ kg fuel product	0.00094	0.00094	0.00094	Ecoinvent

Table S6: Pipeline transportation parameters.

Pipeline	**Leakage rate [per 1000 km]**	**Electricity demand [kWh/kg fuel product/km]**	**Embodied emissions [$kgCO_2e$/kg fuel product/km]**	**Comment/Ref.**
Transport by Pipeline: as NH_3/MeOH/gasoline/diesel/kerosene	0%	0.000003	0.000006	Ecoinvent, [4]

Table S7: Countries and supply chain routes.

Market operation	**Countries**	**Abbreviation**	**Port**
Fuel production	Saudi Arabia	SA	Jeddah
Fuel production	Morrocco	MR	Casablanca
Fuel production	Nigeria	NG	Port Harcourt
Fuel production	Algeria	AL	Skikda
Fuel production	Chile	CL	San Antonio
Fuel production	Australia	AU	Fremantle
Fuel use	United Kingdom	UK	Southampton
Fuel use	Netherlands	NL	Rotterdam

Table S8: Transportation distance parameters.

Location	Transportation mode	Distance [km]	Ref.
Local [Import to distribution terminal]	Any	400	Own assumption
Local [Distribution terminal to station]	Any	150	[19]
SA to UK	Transport by Pipeline	6245	Jeddah to Southampton, Google
SA to UK	Transport by Ship	8,099	Jeddah to Southampton, Ports.com
SA to NL	Transport by Pipeline	5799	Jeddah to Rotterdam, Google
SA to NL	Transport by Ship	8,627	Jeddah to Rotterdam, Ports.com
MR to UK	Transport by Pipeline	2564	Casablanca to Southampton, Google
MR to UK	Transport by Ship	2589	Casablanca to Southampton, Ports.com
MR to NL	Transport by Pipeline	2755	Casablanca to Rotterdam, Google
MR to NL	Transport by Ship	3117	Casablanca to Rotterdam, Ports.com
NG to UK	Transport by Pipeline	7001	Port Harcourt to Southampton, Google
NG to UK	Transport by Ship	8649	Port Harcourt to Southampton, Ports.com
NG to NL	Transport by Pipeline	7192	Port Harcourt to Rotterdam, Google
NG to NL	Transport by Ship	9175	Port Harcourt to Rotterdam, Ports.com
AL to UK	Transport by Pipeline	3635	Google
AL to UK	Transport by Ship	3691	Port.com
AL to NL	Transport by Pipeline	3783	Google, Haumann et al. [20]
AL to NL	Transport by Ship	4219	Port.com
CL to UK	Transport by Pipeline	11780	www.fluentcargo.com, assumes air flight distance
CL to UK	Transport by Ship	17492	Ports.com
CL to NL	Transport by Pipeline	12184	www.fluentcargo.com, assumes air flight distance
CL to NL	Transport by Ship	18020	Ports.com
AU to UK	Transport by Pipeline	14712	www.fluentcargo.com, assumes air flight distance
AU to UK	Transport by Ship	20791	Ports.com
AU to NL	Transport by Pipeline	14443	www.fluentcargo.com, assumes air flight distance
AU to NL	Transport by Ship	21318	Jeddah to Southampton, Google

Table S9: Fuel to electricity parameters.

Turbine for electricity	Efficiency (Gas to Electricity)	Reference
Natural gas turbine	39.10%	[21]
Hydrogen gas turbine	39.82%	
Oil plants	35%	

Table S10: Electricity to motor power and heat parameters.

Electricity to motor power	Efficiency	Reference
Compressors	95%	[22]
Pumps	58%	
Electricity to heat	85%	

Table S11: 2030 to 2050 grid electricity emissions factors by IEA.

Grid electricity	Year	Scenario	Carbon footprint [kg CO_2e/kWh]	Comments
Grid-SA	2030	IEA Sustainable Dev.	0.448669972	
Grid-SA	2050	IEA Sustainable Dev.	0.116710585	
Grid-SA	2030	IEA Stated Policies	0.574577978	
Grid-SA	2050	IEA Stated Policies	0.420475259	
Grid-MR	2030	IEA Sustainable Dev.	0.404840367	
Grid-MR	2050	IEA Sustainable Dev.	0.120239076	
Grid-MR	2030	IEA Stated Policies	0.546549934	
Grid-MR	2050	IEA Stated Policies	0.382524211	
Grid-NG	2030	IEA Sustainable Dev.	0.278911816	Based on IEA estimates of West Africa countries (Cote d'Ivoire, Ghana and Guinea)
Grid-NG	2050	IEA Sustainable Dev.	0.086367623	
Grid-NG	2030	IEA Stated Policies	0.349599830	
Grid-NG	2050	IEA Stated Policies	0.268947265	
Grid-AL	2030	IEA Sustainable Dev.	0.295025159	Based on IEA [23], [24] and [24] energy mix for 2030 and estimates of African countries with similar 2025 numbers (Ghana and Cote d'Ivoire)
Grid-AL	2050	IEA Sustainable Dev.	0.085262241	
Grid-AL	2030	IEA Stated Policies	0.395895157	
Grid-AL	2050	IEA Stated Policies	0.289892067	
Grid-CL	2030	IEA Sustainable Dev.	0.112484157	
Grid-CL	2050	IEA Sustainable Dev.	0.057330125	
Grid-CL	2030	IEA Stated Policies	0.207605549	
Grid-CL	2050	IEA Stated Policies	0.148191653	
Grid-AU	2030	IEA Sustainable Dev.	0.428696645	
Grid-AU	2050	IEA Sustainable Dev.	0.063207333	
Grid-AU	2030	IEA Stated Policies	0.735077279	
Grid-AU	2050	IEA Stated Policies	0.366138846	
Grid-NL	2030	IEA Sustainable Dev.	0.136186901	Based on IEA estimates of neighbouring countries (Belgium, Germany and the UK)
Grid-NL	2050	IEA Sustainable Dev.	0.048270622	
Grid-NL	2030	IEA Stated Policies	0.186353285	
Grid-NL	2050	IEA Stated Policies	0.117268013	

Grid electricity	Year	Scenario	Carbon footprint [kg CO_2e/kWh]	Comments
Grid-UK	2030	IEA Sustainable Dev.	0.134630945	
Grid-UK	2050	IEA Sustainable Dev.	0.048268992	
Grid-UK	2030	IEA Stated Policies	0.194628877	
Grid-UK	2050	IEA Stated Policies	0.136554383	

Table S12: Electricity emissions factors with future grid estimates based on IEA Sustainable Development Policies.

Electricity	Year	Carbon footprint [kg CO_2e/kWh]
Green	2025	0.000
Green	2030	0.000
Green	2050	0.000
Grid-SA	2025	0.593
Grid-SA	2030	0.449
Grid-SA	2050	0.117
Grid-MR	2025	0.644
Grid-MR	2030	0.405
Grid-MR	2050	0.120
Grid-NG	2025	0.459
Grid-NG	2030	0.279
Grid-NG	2050	0.086
Grid-AL	2025	0.468
Grid-AL	2030	0.295
Grid-AL	2050	0.085
Grid-CL	2025	0.325
Grid-CL	2030	0.112
Grid-CL	2050	0.057
Grid-AU	2025	0.590
Grid-AU	2030	0.429
Grid-AU	2050	0.063
Grid-NL	2025	0.268
Grid-NL	2030	0.136
Grid-NL	2050	0.048
Grid-UK	2025	0.183
Grid-UK	2030	0.135
Grid-UK	2050	0.048
HFO	2025	0.792
HFO	2030	0.792
HFO	2050	0.792
Fossil diesel	2025	0.974
Fossil diesel	2030	0.974
Fossil diesel	2050	0.974
e-diesel	2025	0.061
e-diesel	2030	0.041

Electricity	Year	Carbon footprint [kg CO_2e/kWh]
e-diesel	2050	0.031
e-MeOH	2025	0.056
e-MeOH	2030	0.031
e-MeOH	2050	0.021
e-gasoline	2025	0.059
e-gasoline	2030	0.041
e-gasoline	2050	0.031
e-NH_3	2025	0.051
e-NH_3	2030	0.031
e-NH_3	2050	0.021
SNG	2025	0.138
SNG	2030	0.064
SNG	2050	0.037
NG	2025	0.516
NG	2030	0.516
NG	2050	0.516
e-H_2	2025	0.136
e-H_2	2030	0.063
e-H_2	2050	0.036

Table S13: Fuel emissions factors with future grid estimates based on IEA Sustainable Development scenario. E-fuel emission factors obtained from own preliminary analysis and Concawe [3].

Fuel/Heat	Year	Carbon footprint [kg CO_2e/MJ]
Green heat	2025	0.0000
Green heat	2030	0.0000
Green heat	2050	0.0000
Grid-SA to heat	2025	0.1938
Grid-SA to heat	2030	0.1466
Grid-SA to heat	2050	0.0381
Grid-MR heat	2025	0.2104
Grid-MR heat	2030	0.1323
Grid-MR heat	2050	0.0393
Grid-NG heat	2025	0.1498
Grid-NG heat	2030	0.0911
Grid-NG heat	2050	0.0282
Grid-AL heat	2025	0.1529
Grid-AL heat	2030	0.0964
Grid-AL heat	2050	0.0279
Grid-CL heat	2025	0.1062
Grid-CL heat	2030	0.0368
Grid-CL heat	2050	0.0187
Grid-AU heat	2025	0.1927
Grid-AU heat	2030	0.1401

Fuel/Heat	Year	Carbon footprint [kg CO_2e/MJ]
Grid-AU heat	2050	0.0207
Grid-NL heat	2025	0.0877
Grid-NL heat	2030	0.0445
Grid-NL heat	2050	0.0158
Grid-UK heat	2025	0.0599
Grid-UK heat	2030	0.0440
Grid-UK heat	2050	0.0158
HFO	2025	0.0770
HFO	2030	0.0770
HFO	2050	0.0770
Fossil diesel	2025	0.0947
Fossil diesel	2030	0.0947
Fossil diesel	2050	0.0947
e-diesel	2025	0.0059
e-diesel	2030	0.0040
e-diesel	2050	0.0030
e-MeOH	2025	0.0054
e-MeOH	2030	0.0030
e-MeOH	2050	0.0020
e-gasoline	2025	0.0057
e-gasoline	2030	0.0040
e-gasoline	2050	0.0030
e-NH_3	2025	0.0050
e-NH_3	2030	0.0030
e-NH_3	2050	0.0020
SNG	2025	0.0150
SNG	2030	0.0070
SNG	2050	0.0040
NG	2025	0.0560
NG	2030	0.0560
NG	2050	0.0560
e-H_2	2025	0.0150
e-H_2	2030	0.0070
e-H_2	2050	0.0040

Table S14: Key technical specifications of the IEA wind 15-MW turbine.

Parameter	Value	Units	Ref.
Rated power	15	MW	[25]
Cut-in wind speed	3	m/s	
Cut-out wind speed	25	m/s	
Rotor diameter	240	m	
Rotor swept area, A_T	45239	m^2	
Aerodynamic brake	3	blades full feathering	

Parameter	Value	Units	Ref.
Frequency	50/60	Hz	
Hub height	150	m	
Air density, ρ	1.225	kg/m^3	
Power coefficient, C_P	35%		[26]

Table S15: Key technical specifications of utility-grade solar PV.

Parameter	Value	Units	Ref.
Rated power	670	W	[27]
Maximum efficiency, η_{PV}	21.60%		[27], [28]
Dimensions	2384 × 1303	mm	[27]
Area, A_{PV}	3.106352	m^2	
Operational hours	8760	hours	
Performance ratio, PR	85.9%		[29]

Table S16: Emissions of electrolytic H_2 from 50% wind and 50% solar PV (except for NG, which was at 100% solar PV) were calculated using Equations (8)–(10), Ecoinvent, [30], [31] and Smith et al. [32].

H_2 type	Country	Electrolyser/CCUS efficiency	Emission factor [kg CO_2e/kg H_2]	Embodied emission factor [kg CO_2e/kg H_2]
Electrolytic H_2	SA	65.4%	0.0000	0.7167
Electrolytic H_2	SA	75.0%	0.0000	0.6249
Electrolytic H_2	MR	65.4%	0.0000	1.1368
Electrolytic H_2	MR	75.0%	0.0000	0.9913
Electrolytic H_2	NG	65.4%	0.0000	2.0093
Electrolytic H_2	NG	75.0%	0.0000	1.7521
Electrolytic H_2	AL	65.4%	0.0000	0.9442
Electrolytic H_2	AL	75.0%	0.0000	0.8233
Electrolytic H_2	CL	65.4%	0.0000	0.8811
Electrolytic H_2	CL	75.0%	0.0000	0.7683
Electrolytic H_2	AU	65.4%	0.0000	0.7168
Electrolytic H_2	AU	75.0%	0.0000	0.6250

Table S17: Electricity use by processes.

Operation type	**Electricity source, 2025**	**Fuel source, 2025**	**Electricity source, 2030**	**Fuel source, 2030**	**Electricity source, 2050**	**Fuel source, 2050**
Processes occurring at plant location	Green/grid electricity	Green/grid electricity heat	Green/grid electricity	Green/grid electricity heat	Green/grid electricity	Green/grid electricity heat
Processes occurring at terminals	Grid electricity	NG	Grid electricity	NG	Grid electricity	Grid electricity
Processes occurring at terminals (sensitivity analysis)	Synthetic fuel	Synthetic fuel	Synthetic fuel	Synthetic fuel	Synthetic fuel	Synthetic fuel
Transportation: Trucks, rail, local pipeline and ship	Grid electricity	Fossil diesel	Grid electricity	Synthetic fuel	Grid electricity	Synthetic fuel
Processes occurring at stations	Grid electricity	NG	Grid electricity	NG	Grid electricity	Grid electricity

Table S18: Electricity and embodied emission factors of fuel stations. For embodied emissions, a service station with 310,000 m^3 gas sold per year (in 365 days) was used to estimate the embodied emission factors based on Ecoinvent data of NG refuelling station.

Process	**Electricity demand [kWh/kg fuel product]**	**Embodied emissions [$kgCO_2e$/kg fuel product]**	**Reference**
NH_3 Dispensing Station: NH_3	0.004178	0.000002	[3] and Ecoinvent
MeOH Dispensing Station: MeOH	0.004467	0.000002	
Gasoline Dispensing Station: Gasoline	0.041697	0.000002	
Kerosene Dispensing Station: Kerosene	0.041263	0.000002	
Diesel Dispensing Station: Diesel	0.040526	0.000002	

Table S19: Electricity and embodied emission factors of terminals.

Process	**Electricity demand [kWh/kg fuel product]**	**Embodied emissions [$kgCO_2e$/kg fuel product]**	**Reference**
NH_3 Storage: Terminal (Import), NH_3 Product basis	0.003551	0.000755	[3], [17] and Ecoinvent
NH_3 Storage: Terminal (Export), NH_3 Product basis	0.000888	0.000755	
NH_3 Storage: Terminal (Distribution), NH_3 Product basis	0.003551	0.000755	
MeOH Storage: Terminal (Import), MeOH Product basis	0.004690	0.000666	
MeOH Storage: Terminal (Export), MeOH Product basis	0.004690	0.000666	
MeOH Storage: Terminal (Distribution), MeOH Product basis	0.004690	0.000666	
Gasoline, Diesel, Kerosene Storage: Terminal (Import)	0.010012	0.000632	
Gasoline, Diesel, Kerosene Storage: Terminal (Export)	0.010012	0.000632	
Gasoline, Diesel, Kerosene Storage: Terminal (Distribution)	0.010012	0.000632	

Table S20: Emission factors for fuel oxidation in combustion engines and fuel cell vehicles.

Parameter	**Model**	**Embodied emissions [$kgCO_2e$/kg fuel]**	**Oxidation GHG emissions factor [$kgCO_2e$/kg fuel]**	**Data based on ref.**
Road transport appl.: Gasoline	Truck	0.001104	0.01888	[36], Ecoinvent (trailer, agricultural trailer production)
Road transport appl.: Diesel	Truck	0.001104	0.04461	[36], Ecoinvent (trailer, agricultural trailer production)

Rail transport appl.: Diesel	Train	0.017776	0.04461	[36], Ecoinvent (trailer, agricultural trailer production)
Water transport appl.: MeOH	Ship	0.004610	0.00844	[36], Ecoinvent (tanker production for liquefied natural gas)
Water transport appl.: NH_3	Ship	0.004610	0	[36], Ecoinvent (tanker production for liquefied natural gas)
Water transport appl.: Diesel	Ship	0.004610	0.04461	[36], Ecoinvent (tanker production for liquefied natural gas)
Air transport appl.: Kerosene	Aircraft	0.007238	0.00521	[36], Ecoinvent (medium-haul aircraft production)

Table S21: 100-year GWP of GHGs.

GWP	**Value**	**Unit**	**Reference**
H_2	11	CO_2e	[37]
CH_4	28	CO_2e	[38]
N_2O	265	CO_2e	
CO_2	1	CO_2e	

2 Results

2.1 Liquid e-fuel losses in transport applications

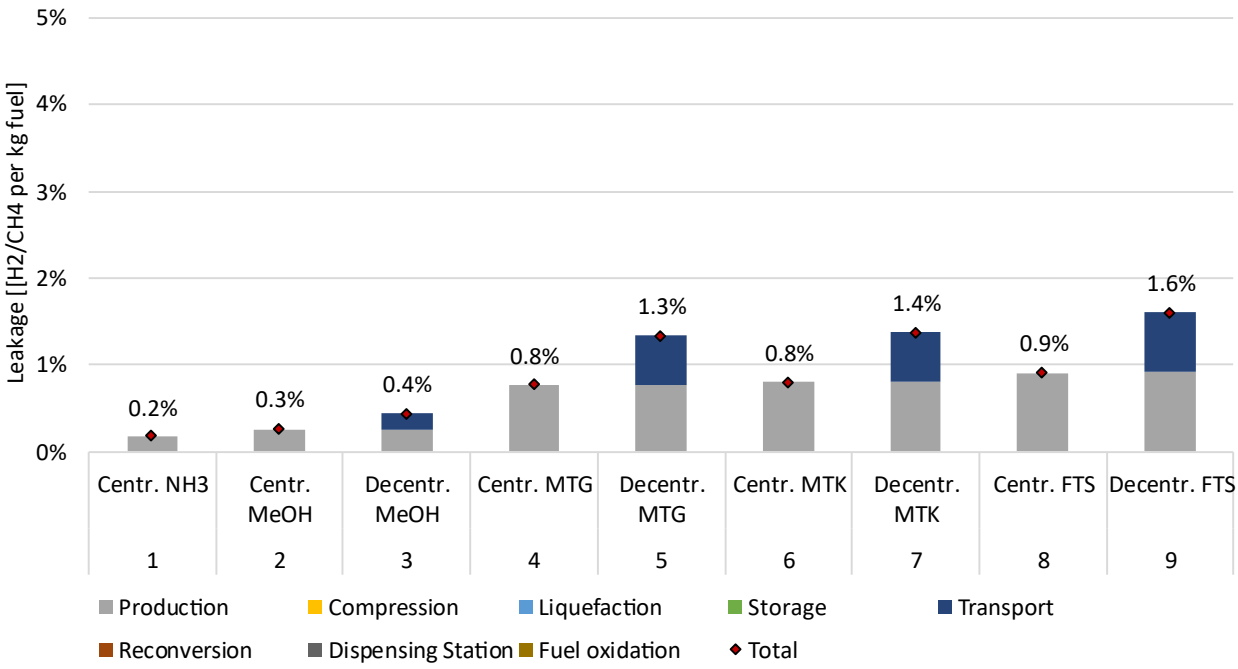

Figure S1: H_2-related losses to the environment for liquid e-fuels from SA to UK.

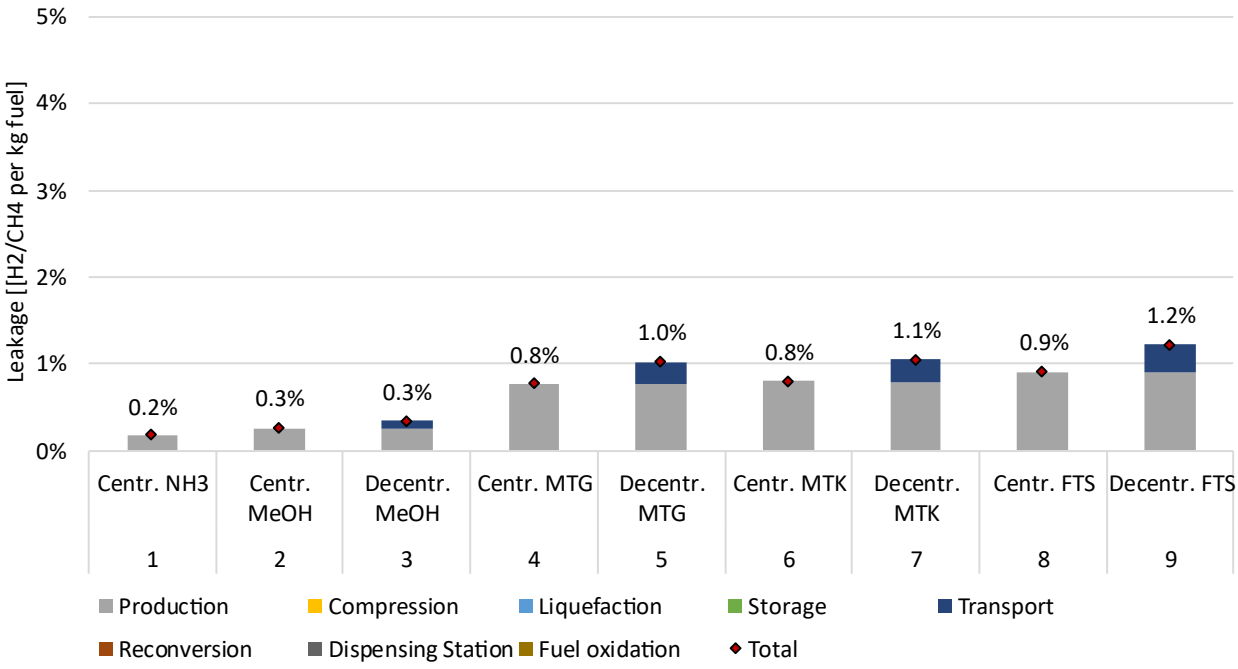

Figure S2: H_2-related losses to the environment for liquid e-fuels from MR to UK.

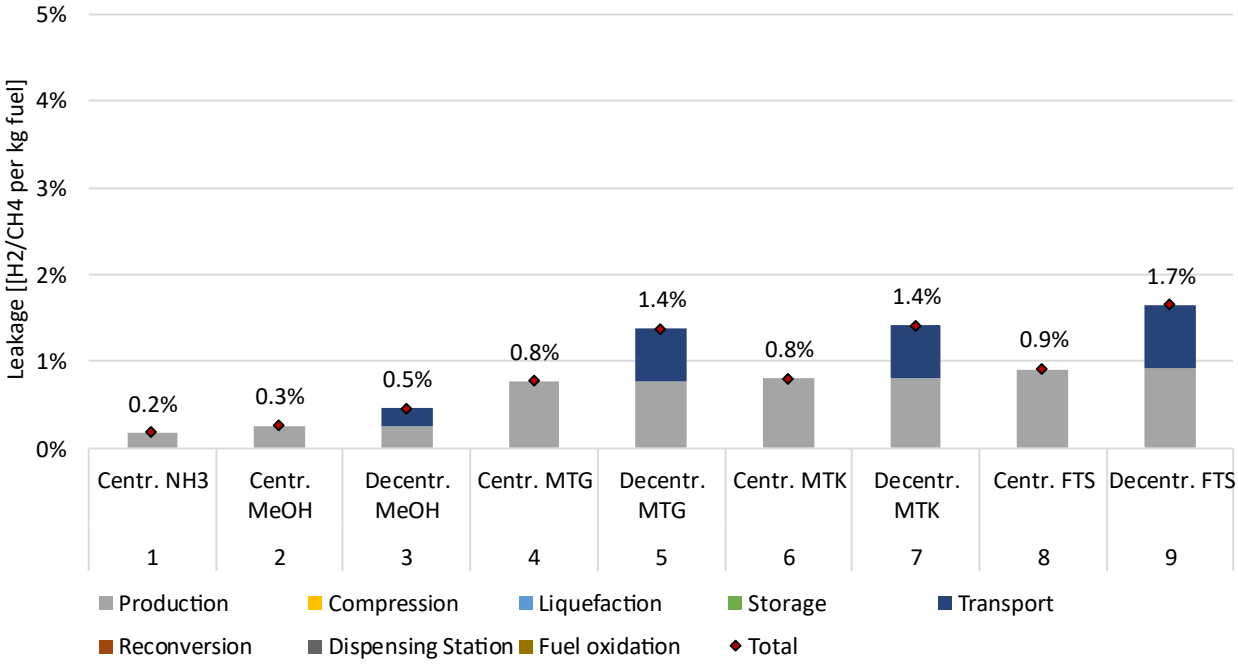

Figure S3: H_2-related losses to the environment for liquid e-fuels from NG to UK.

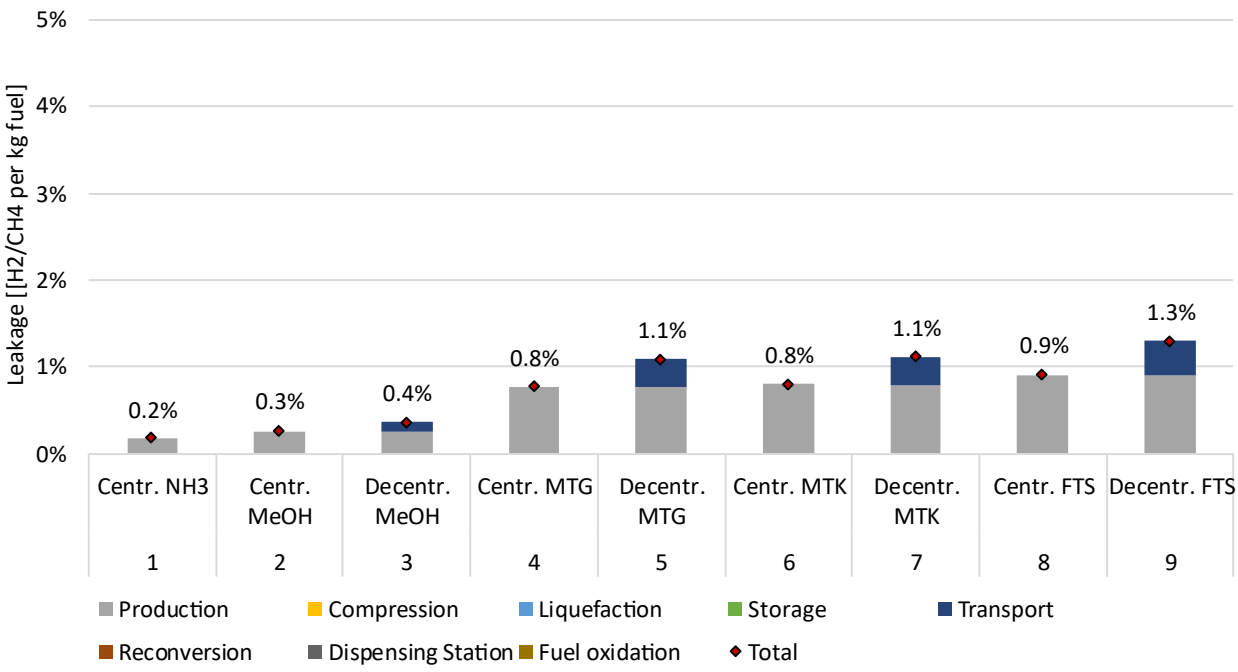

Figure S4: H_2-related losses to the environment for liquid e-fuels from AL to UK.

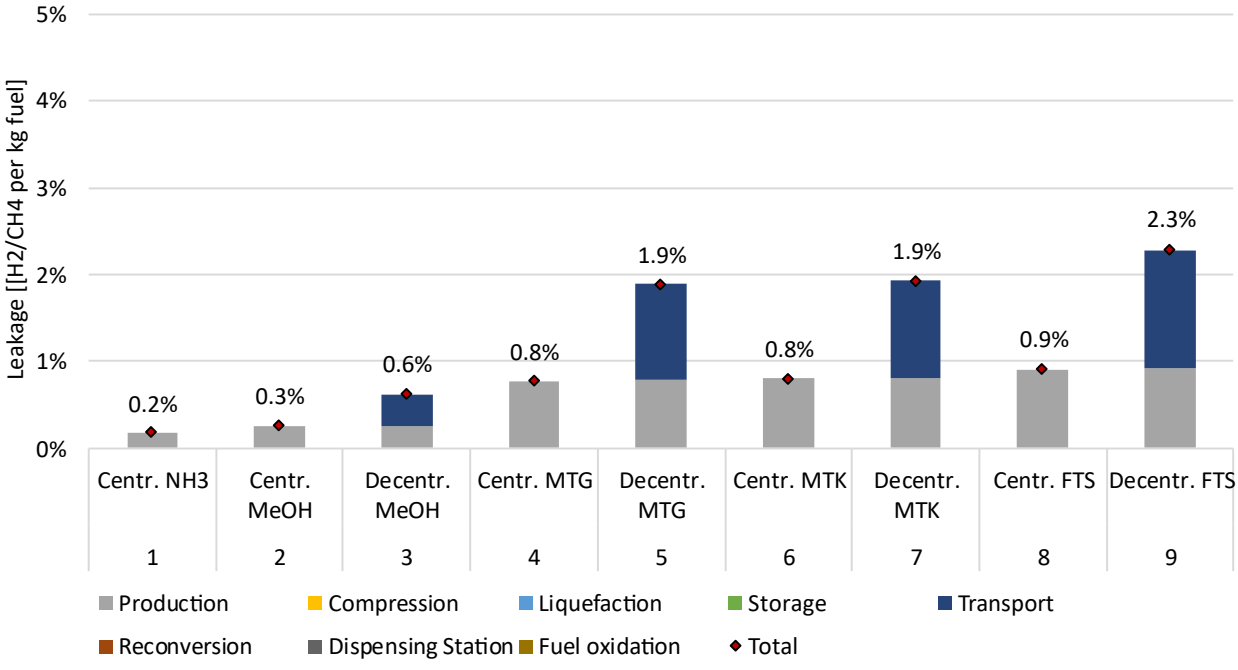

Figure S5: H_2-related losses to the environment for liquid e-fuels from CL to UK.

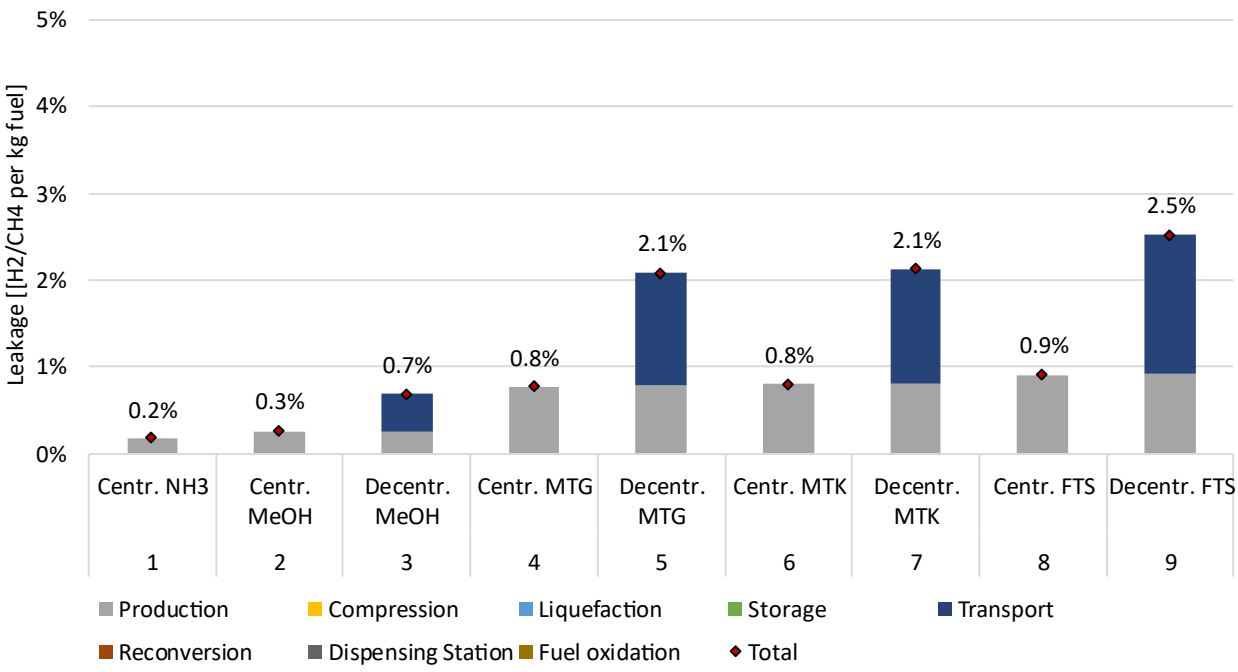

Figure S6: H_2-related losses to the environment for liquid e-fuels from AU to UK.

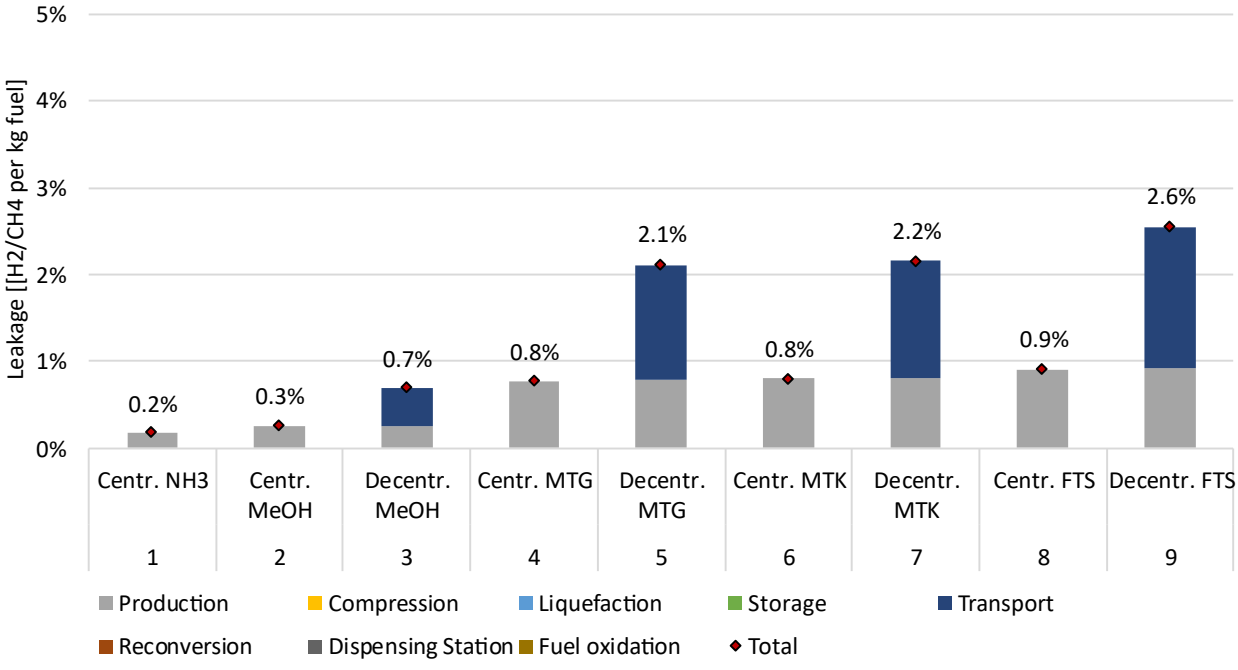

Figure S7: H_2-related losses to the environment for liquid e-fuels from AU to NL.

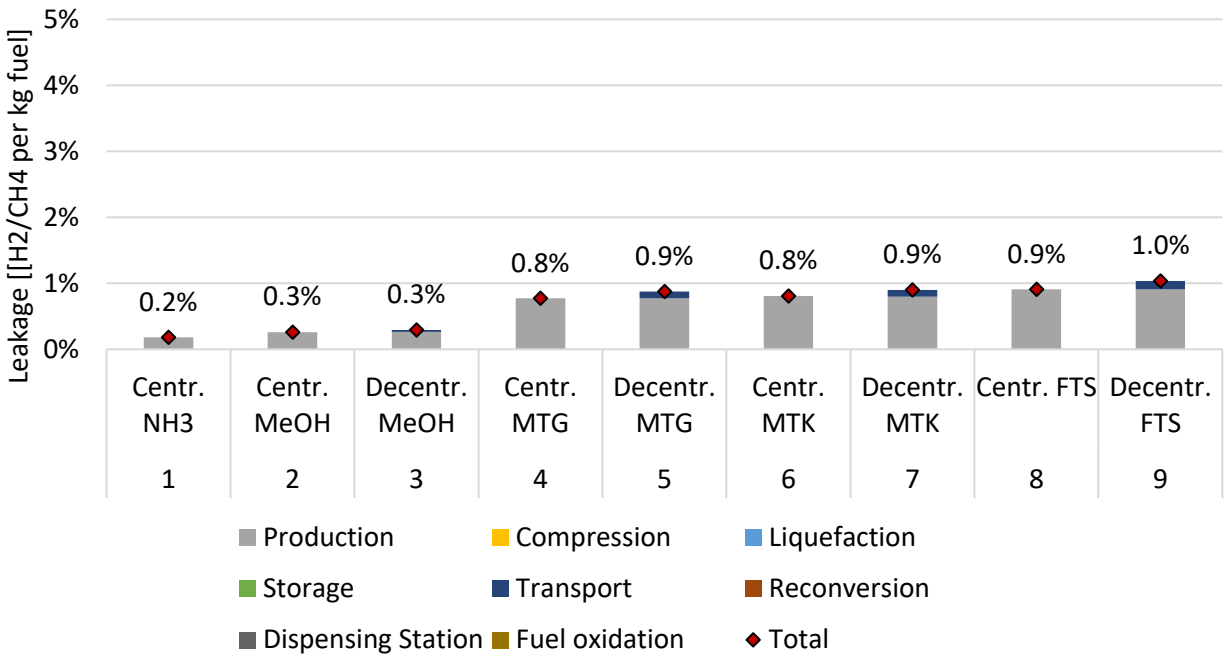

Figure S8: H_2-related losses to the environment for liquid e-fuels from UK to UK.

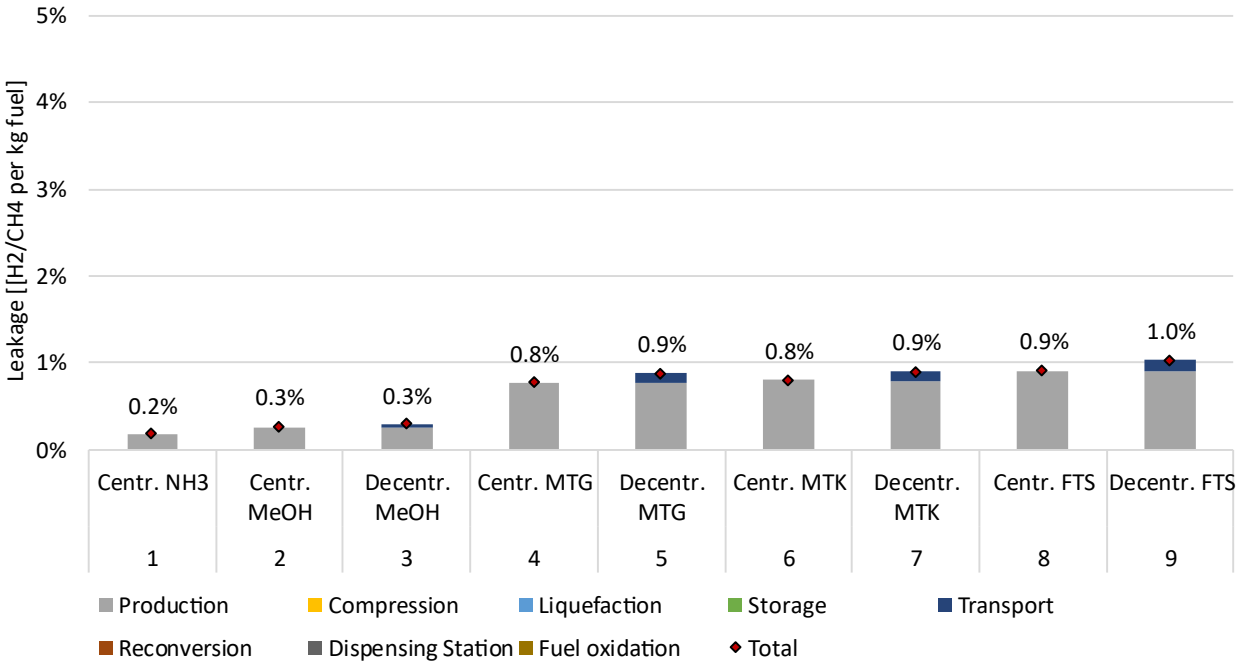

Figure S9: H_2-related losses to the environment for liquid e-fuels from NL to NL.

2.2 Liquid e-fuel energy balance in transport applications

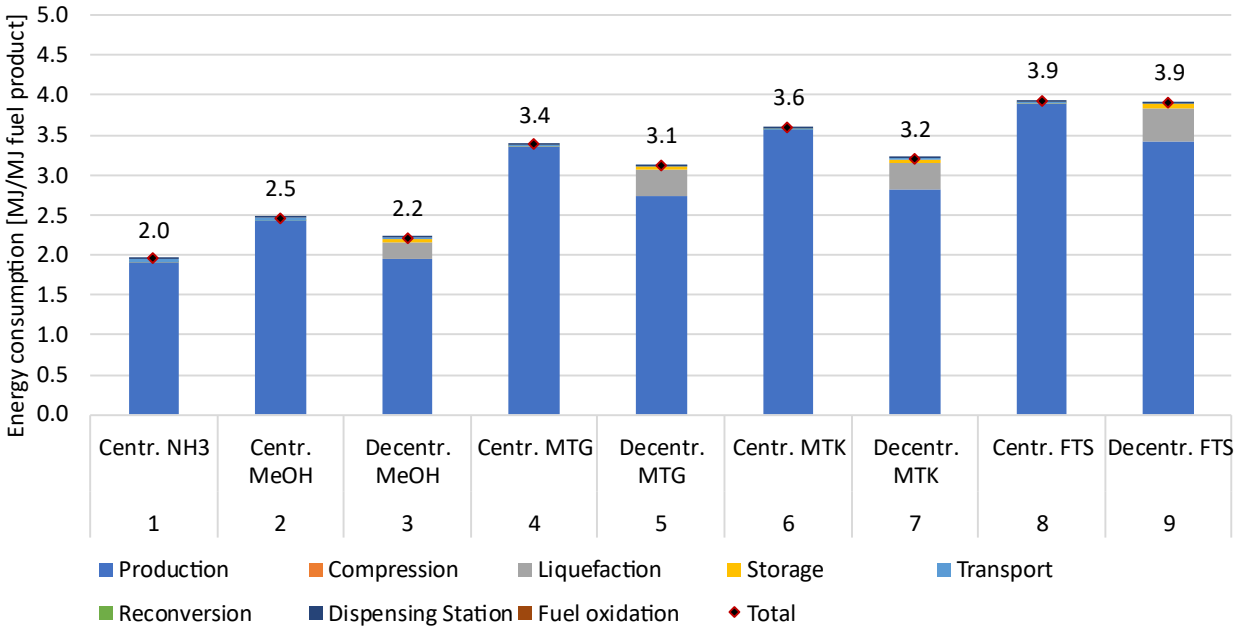

Figure S10: The energy consumption of liquid e-fuel supply chains from the SA to UK.

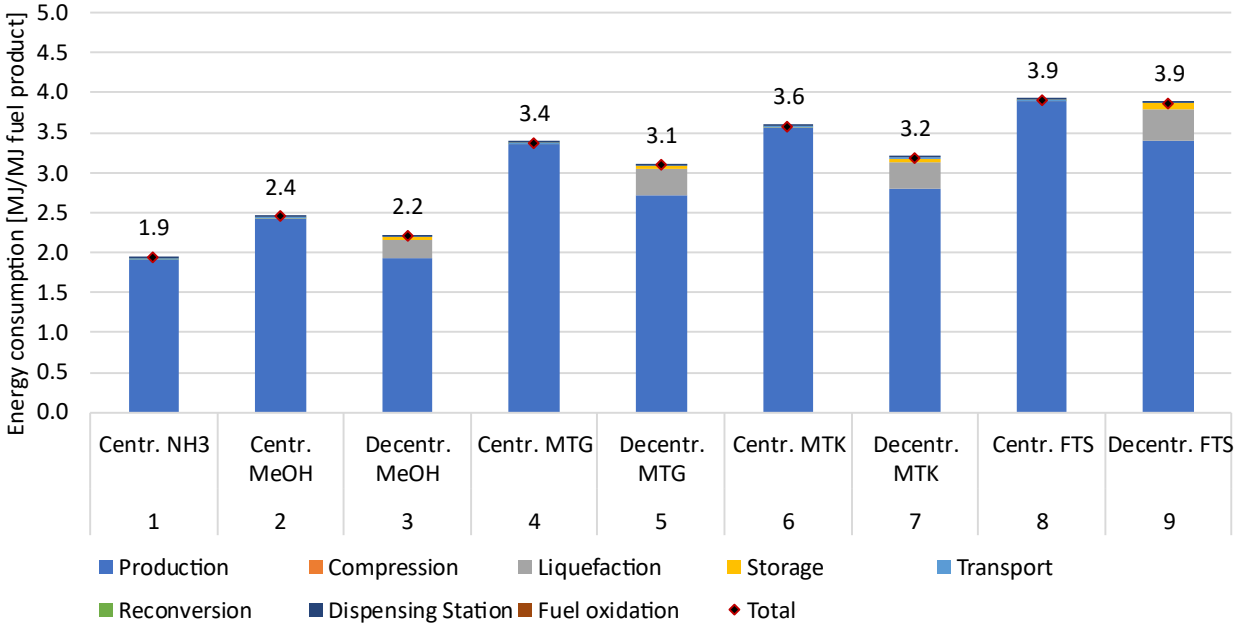

Figure S11: The energy consumption of liquid e-fuel supply chains from the MR to UK.

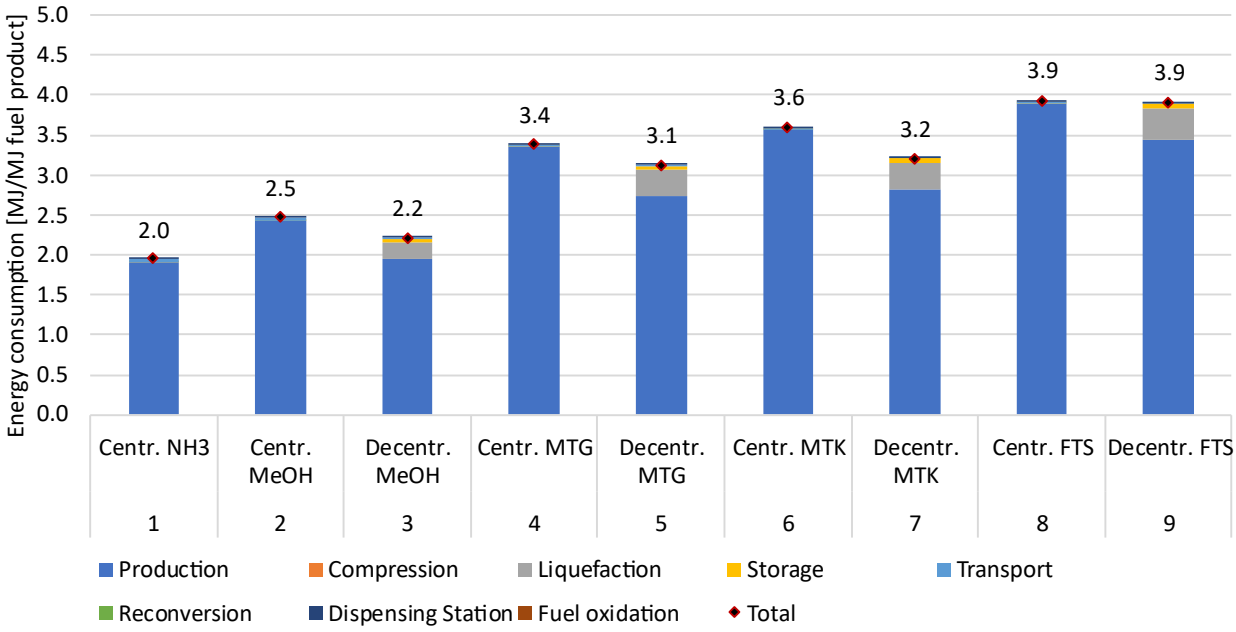

Figure S12: The energy consumption of liquid e-supply chains from the NG to UK.

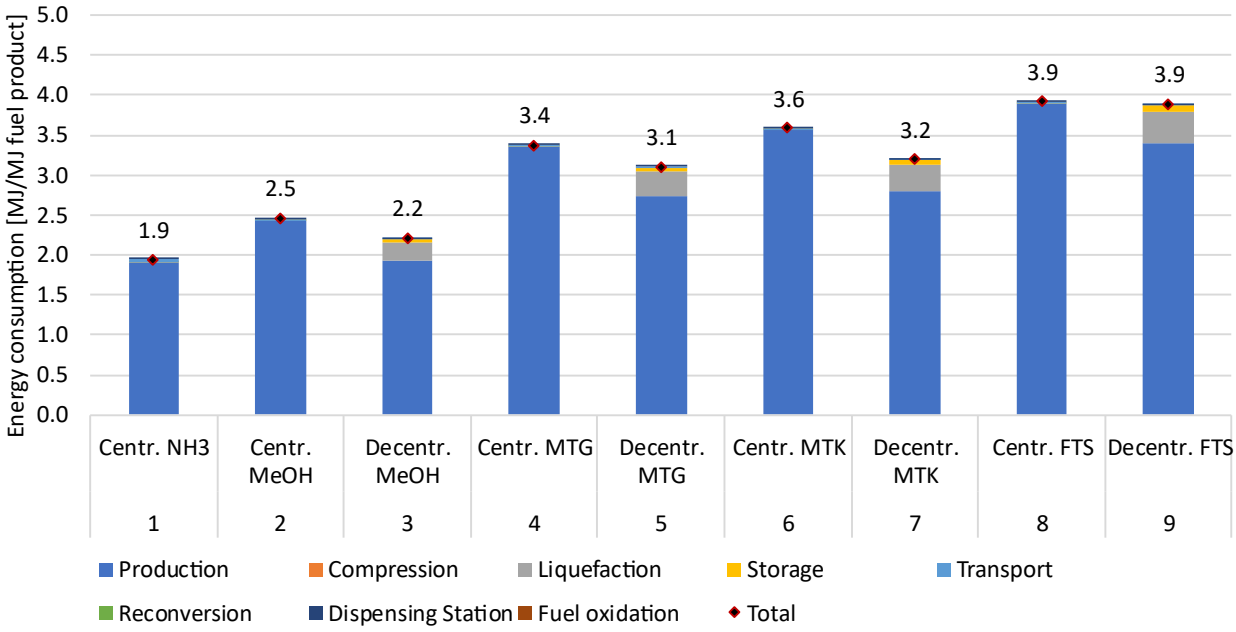

Figure S13: The energy consumption of liquid e-fuel supply chains from the AL to UK.

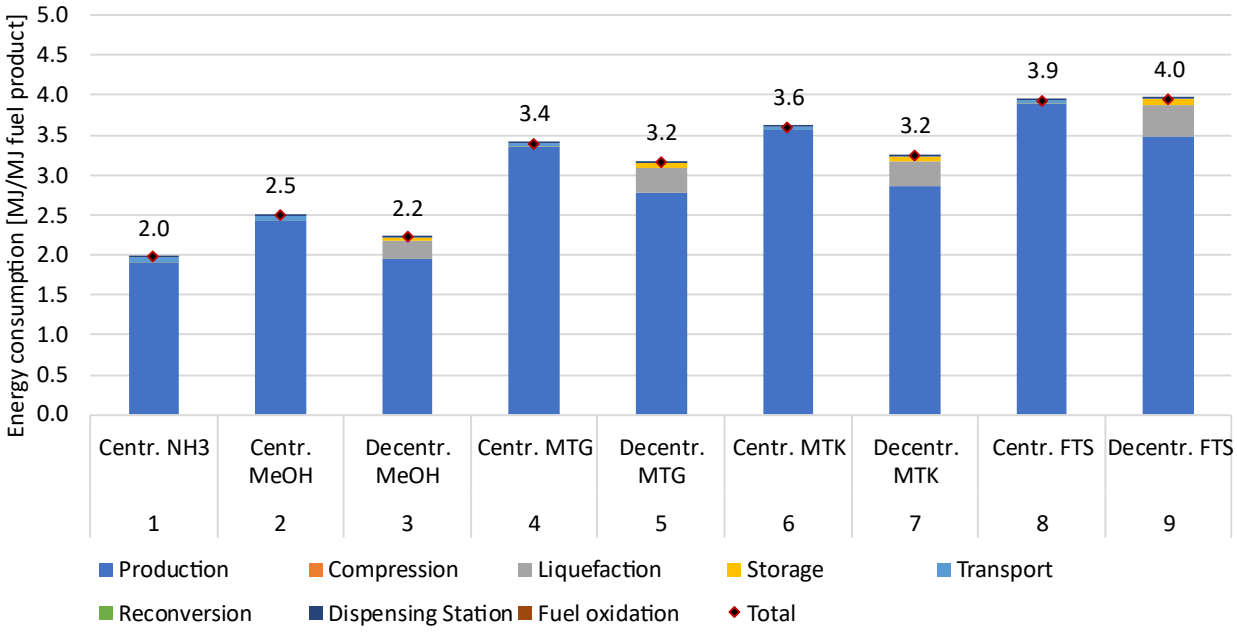

Figure S14: The energy consumption of liquid e-fuel supply chains from CL to UK.

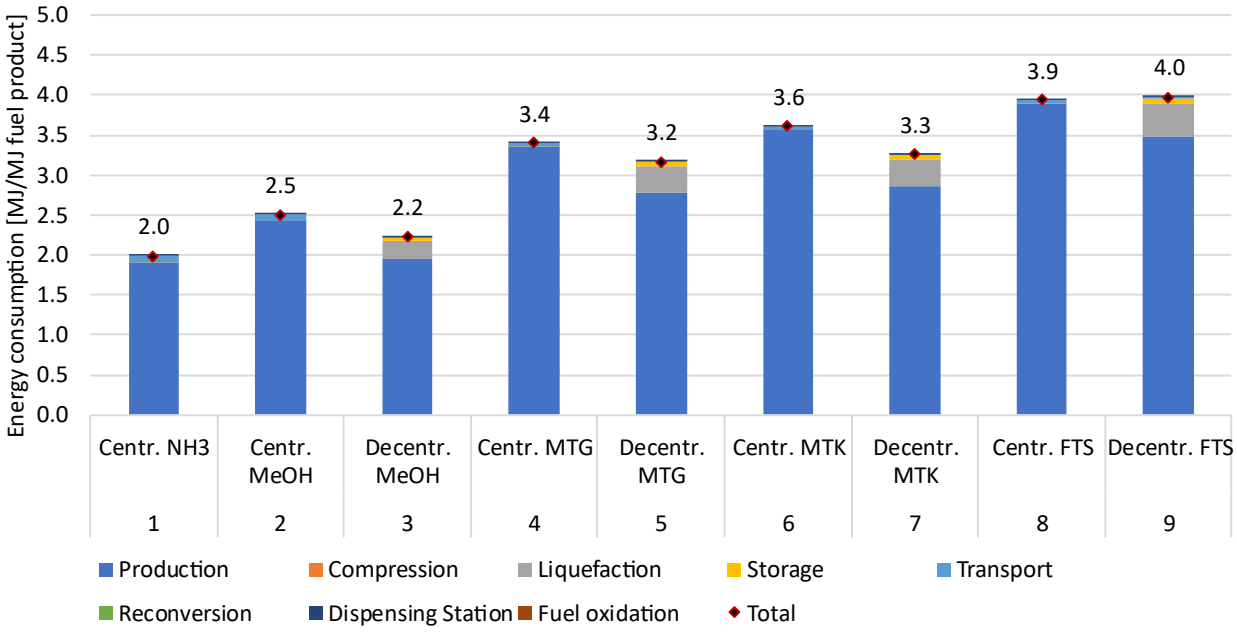

Figure S15: The energy consumption of liquid e-fuel supply chains from AU to UK.

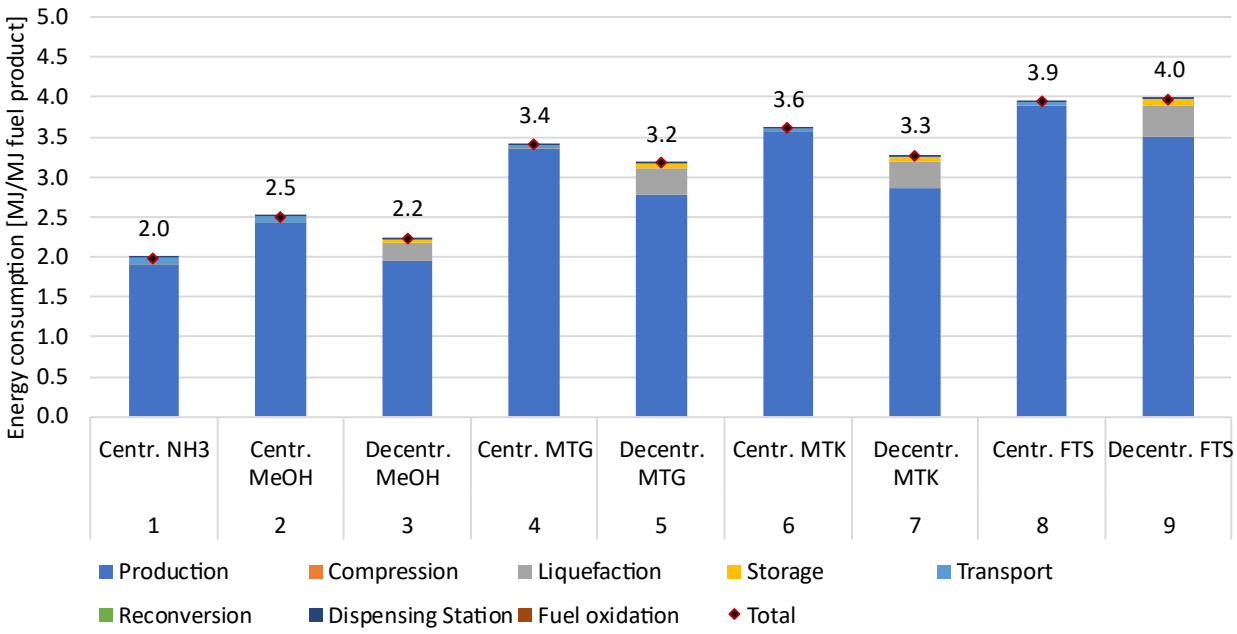

Figure S16: The energy consumption of liquid e-fuel supply chains from AU to NL.

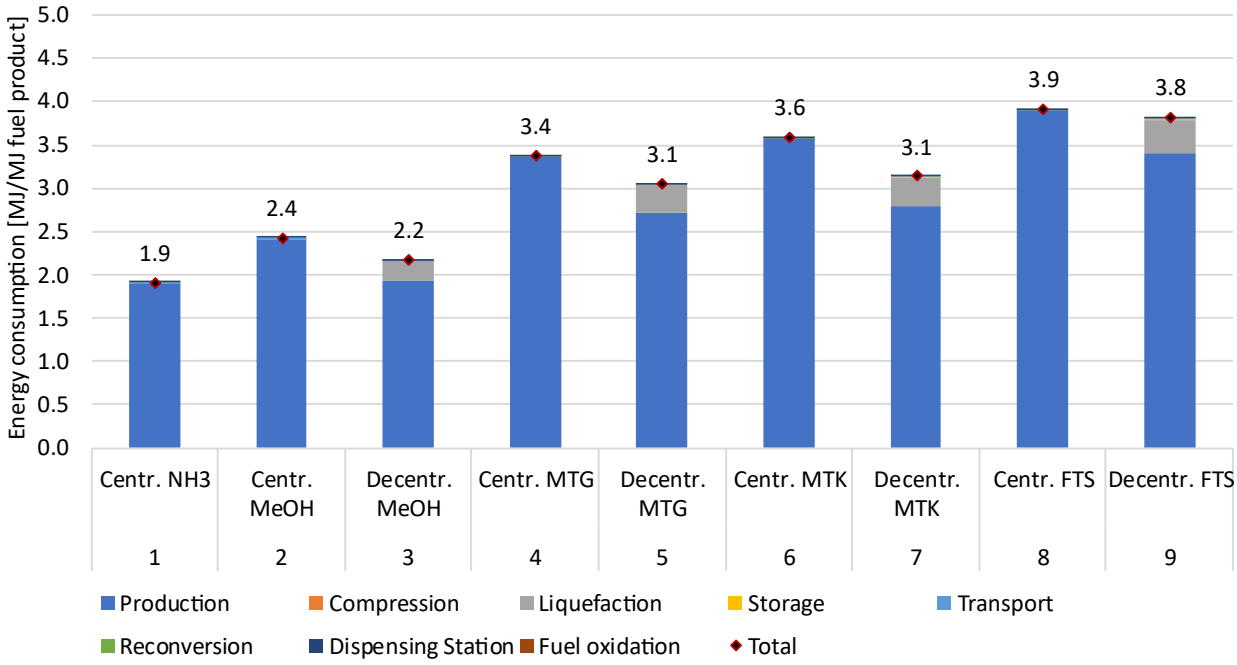

Figure S17: The energy consumption of liquid e-fuel supply chains from UK to UK.

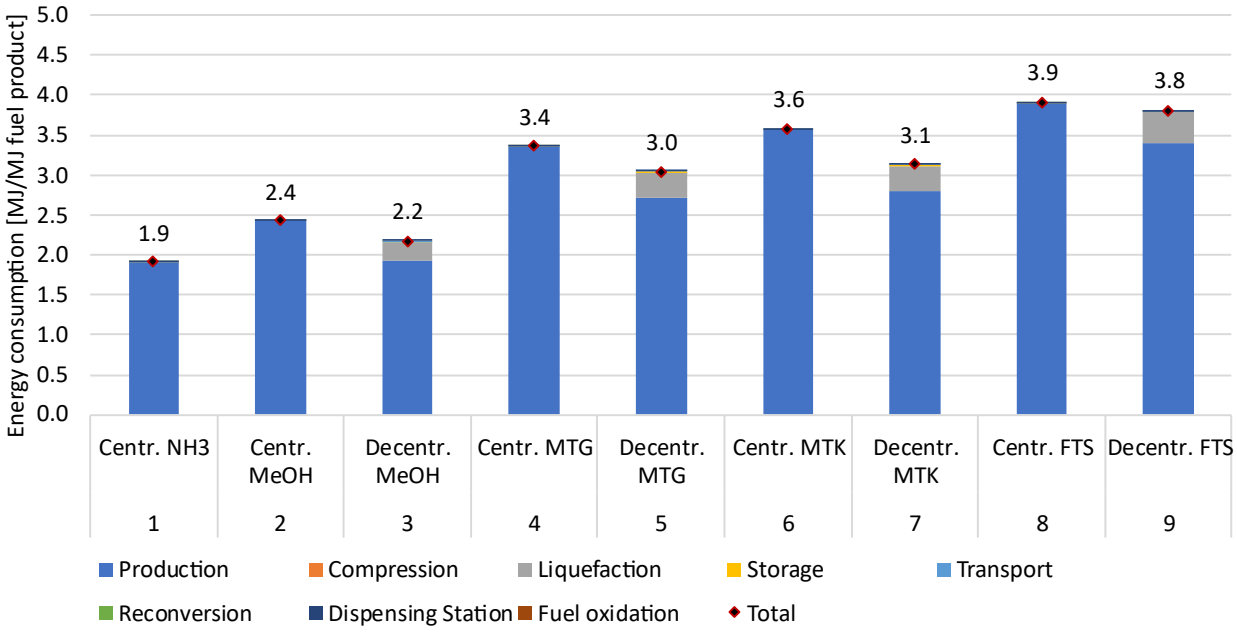

Figure S18: The energy consumption of liquid e-fuel supply chains from NL to NL.

2.3 Liquid e-fuel water consumption

Table S22: Water consumption of liquid e-fuels, based on data from the author's process modelling and [3], [39], [40].

Product	Consumption from electrolysis [kg H_2O/kg fuel]	Production from DAC [kg H_2O/kg fuel]	Production from final fuel synthesis [kg H_2O/kg fuel]	Net water consumption [kg H_2O/kg fuel]	Net water consumption [kg H_2O/MJ fuel]
H_2	9.00–10.00	0.00	0.00	9.00–10.00	0.075–0.083
NH_3	1.60–1.78	0.00	0.00	1.60–1.78	0.085–0.094
MeOH via Centr. MeOH	1.74–1.93	1.26	0.06	0.41–1.93	0.020–0.096
Gasoline via Centr. MTG	3.97–4.41	2.88	0.29	0.80–4.41	0.016–0.010
Kerosene via Centr. MTK	4.12–4.58	2.92	0.31	0.89–4.58	0.021–0.105
FT-liquids via Centr. FTS	4.54–5.04	3.41	0.35	0.77–5.04	0.018–0.118
Note: Upper limits generally assume no water recovery from the DAC and fuel production stages. This could typically hold for decentralised production.					

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