

Energy System Modelling Challenges for Synthetic Fuels

Towards net zero systems with synthetic jet fuels

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Long-distance air travel requires fuel with a high specific energy and a high energy density. There are no viable alternatives to carbon-based fuels. Synthetic jet fuel from the Fischer-Tropsch (FT) process, employing sustainable feedstocks, is a potential low-carbon alternative. A number of synthetic fuel production routes have been developed, using a range of feedstocks including biomass, waste, hydrogen and captured carbon dioxide. We review three energy system models and find that many of these production routes are not represented. We examine the market share of synthetic fuels in each model in a scenario in which the Paris Agreement target is achieved. In 2050, it is cheaper to use conventional jet fuel coupled with a negative emissions technology than to produce sustainable synthetic fuels in the TIAM-UCL and UK TIMES models. However, the JRC-EU-TIMES model, which represents the most production routes, finds a substantial role for synthetic jet fuels, partly because underground CO₂ storage is assumed limited. These scenarios demonstrate a strong link between synthetic fuels, carbon capture and storage (CCS) and negative emissions. Future model improvements include better representing blending limits for synthetic jet fuels to meet international fuel standards, reducing the costs of synthetic fuels and ensuring production routes are sustainable.

1. Introduction

In 2015, the global community committed to limiting warming to “well below 2°C” and to pursuing efforts to limit warming to “1.5°C above pre-industrial levels” (1). Global CO₂ emissions must halve by 2030 if we are to have a chance of reaching the 1.5°C target (2). This will require dramatic transformations in all aspects of energy systems around the world. The UK Government, for example, has responded by enacting a new target of net zero greenhouse gas (GHG) emissions by 2050 (3).

Much more stringent climate targets set worldwide has brought renewed attention on the environmental burdens of aviation. The emissions impact of international flying can be 30 times greater than the low-carbon alternative of international rail per passenger kilometre (4). The global aviation industry is responsible for 2% of all anthropogenic CO₂ emissions, but sectoral emissions are set to grow at an annual rate of 4% along increase in international and domestic air travel demands (5), notwithstanding the impacts of the COVID-19 pandemic. In addition, the warming effect of aviation is doubled due to nitrous oxide and water vapour emissions at high altitudes.

While previous decarbonisation efforts for aviation were provided by other sectors *via* carbon offsetting schemes (5), this is more difficult to justify under net-zero futures. Decarbonising aeroplanes *via* new technologies is challenging as high energy density fuel is required for long-distance air travel. Electrification of aircraft has shown some progress as of late, but only for small-scale aircrafts (~20 seats), and it is set to remain focused on short-distance air travel for the foreseeable future (6). Without reliance on early-stage technologies

and heavy infrastructure investments, low-carbon replacement (i.e., 'drop-in') fuels that meet jet fuel specifications are desirable. Bio-based and synthetic jet fuels have strong potential for decarbonisation. These options would have low or zero CO₂ emissions over their lifecycle. Recognising this, ASTM International, USA, has internationally certified several sustainable aviation fuels (SAF) for commercial use.

Table I lists the five alternative jet fuel (AJF) pathways approved so far for commercial airlines. In all cases, neat AJF must be blended with conventional jet fuel (i.e. fossil-based) before it can meet specific properties and molecular components that of standard jet fuel. At this time, the highest possible blend percentage of AJF is 50% by volume. This limit is expected to be increased over time (8), for example through efforts to modify certified routes and pursue enhanced conversion strategies to include additional hydrocarbon products, such as aromatic content, to allow for greater blending volumes of the AJF product (9). Possible feedstocks are of biomass origin, with varying pre-treatment and conversion processes. FT synthetic paraffinic kerosene (FT-SPK) and FT synthetic paraffinic kerosene with aromatics (FT-SPK/A) pathways are the most favourable options in terms of technology maturity and versatility of feedstock, and can take in virtually any carbon based raw material (10).

Many of the AJF pathways involve synthetic products. The term 'synthetic fuels' is widely used as an umbrella definition describing fuels produced from coal, natural gas or biomass through chemical conversion into synthetic crude or synthetic

liquid products. Recently, the term is increasingly associated with relatively clean fuels produced from low-carbon feedstocks. These types of fuels have various potential applications across the energy system in line with net zero ambitions (11), with some organisations envisaging up to 15% of final energy consumption from synthetic fuels in their modelling scenarios (12).

There are many processing options in the production of synthetic fuels. Typically, a carbon source is converted into synthesis gas (syngas, a mixture of carbon monoxide and hydrogen) through gasification. This in turn is synthesised into useful hydrocarbons, which are refined or upgraded for end use. Synthesis is usually *via* either FT synthesis or methanol synthesis. These syngas platforms produce premium alternative fuels that are compatible with existing infrastructure. Much of the current industry and academic focus is on FT synthetic fuels from sustainable feedstocks: biomass (13–15), waste (16–18) and captured CO₂ (19, 20). Therefore, this paper centres on FT jet fuel applications in energy system models.

Energy system models are often used to inform low-carbon energy policies (21). They model the entire energy system from domestic production of fuel resources, commodity processing, to secondary energy carriers and end-use energy service demands across the economy (22). Energy system models balance various interactions, delivering energy services at minimum global cost while meeting GHG targets. Such modelling methods allow for systematic experimentation

Table I Current Options for Alternative Jet Fuel Approved by ASTM International (7)

| Alternative jet fuel | Abbreviated | Possible feedstocks | Maximum blending ratio by volume ^a , % | Year approved |
|---|------------------------|------------------------------------|---|---------------|
| FT synthetic paraffinic kerosene | FT-SPK | Biomass and waste | 50 | 2009 |
| Hydroprocessed esters and fatty acids synthetic paraffinic kerosene | HEFA-SPK | Lipids | 50 | 2011 |
| Hydroprocessed fermented sugars to synthetic isoparaffins | HFS-SIP | Sugars | 10 | 2014 |
| FT synthetic paraffinic kerosene with aromatics | FT-SPK/A | Biomass and waste | 50 | 2015 |
| Alcohol-to-jet synthetic paraffinic kerosene | ATJ-SPK | Starch/sugar or cellulosic biomass | 30 | 2016 |
| Catalytic hydrothermolysis synthetic kerosene | CH-SK or CHJ | Lipids | 50 | 2020 |
| Hydroprocessed hydrocarbons, esters and fatty acids synthetic paraffinic kerosene | HHC-SPK or HC-HEFA-SPK | Algae and lipids | 10 | 2020 |

^aMaximum blending ratio is with conventional fossil-derived jet fuel

of multidimensional variables corresponding to climate, technology, economy and policy (23).

In this paper, we examine whether there is a need to improve the representation of the role of synthetic fuels in energy system models, using three models as case studies: UK TIMES, JRC-EU-TIMES and TIAM-UCL. The paper is organised as follows. Section 2 reviews synthetic jet fuel manufacture through the sequence of gasification and FT processes, including all three sustainable feedstocks that can be processed through this route, i.e. biomass, waste and hydrogen and captured CO₂. Section 3 presents current available technologies in the three models and compares model outputs of jet fuel production in decarbonisation scenarios that are consistent with the Paris Agreement. It outlines the role of synthetic jet fuel in aviation according to the models through to 2050. Section 4 discusses the scenario outputs and recommends improvements in model design and evaluates challenges and opportunities for synthetic fuels in the future of energy systems modelling. We draw conclusions in Section 5.

2. Synthetic Jet Fuel Manufacture

Synthetic jet fuel is produced from biogenic sources (for example, biomass and waste) in three stages. First, syngas is produced through gasification of the feedstock and is cleaned and conditioned. Alternatively, syngas components could be collected from elsewhere, for example by mixing hydrogen from electrolysis with CO₂ from industrial flue gases. Second, middle distillates are produced from the syngas through FT synthesis. Third, the

FT liquids (or 'syncrude') are refined and upgraded to high-quality jet fuel. Syngas from non-biogenic sources are conditioned to suit FT synthesis and subsequently processed through the same steps as the above. **Figure 1** shows the schematic line-up of possible FT routes to synthetic jet fuel.

2.1 Biomass Conversion to Synthetic Fuels

Biomass gasification FT to synthetic fuels is one of the most sought-after and technologically-advanced routes to producing liquid fuels. Owing to the potential to compete with other land uses, particularly food production, globally and in the UK, the production of primary biomass feedstock raises sustainability concerns (24). As the global bioeconomy grows, a relatively wide range of sustainable biomass supply options will be needed. Many studies have evaluated the feasibility of biomass to jet fuel applications from second-generation biomass sources (13, 14).

There are many successful pilot and demonstration scale biomass to liquid (BTL) plants (25). Yet none have been scaled-up to a commercial size (26, 27). One major factor is that BTL plants are only economical at large-scale of greater than 30,000 barrels per day (bpd), so an operator needs to secure substantial biomass resources, which have high transportation costs (15). A company has developed microchannel FT technology to circumvent this issue, which is commercially-viable at production capacities of as low as 1500 bpd (28). The merit of owning several smaller production facilities instead of a single large one has not yet been evaluated.

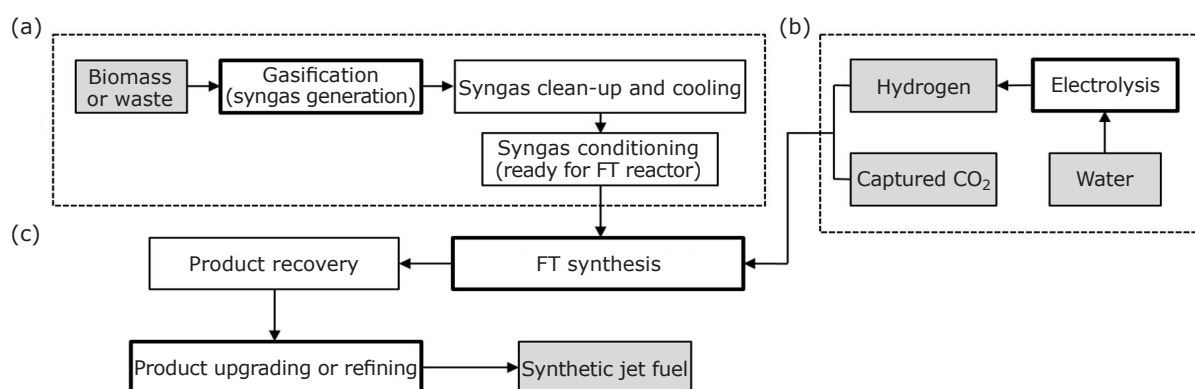


Fig. 1. Schematic of the FT process to produce synthetic jet fuel. First, a syngas is produced by: (a) biomass or waste gasification; or (b) hydrogen generation through electrolysis and combination with captured CO₂; (c) the syngas is converted to longer-chain hydrocarbons *via* FT synthesis and upgraded or refined into synthetic jet fuel. Commodities are in grey and processes are in clear boxes

2.2 Waste Conversion to Synthetic Fuels

Another pathway under investigation is the production of synthetic jet fuel from waste feedstocks (16, 29). In contrast to crop-based feedstocks, waste for alternative fuel production does not require additional land and does not compete directly with food production. In particular, municipal solid waste (MSW) could offer significant environmental advantages by displacing petroleum-derived fuels while also avoiding CO₂ emissions associated with landfill, where waste of biogenic origin decomposes to methane which escapes to the atmosphere.

One of the challenges of using MSW as feedstock comes from its variable composition, which varies from place to place. Reasons include the type and efficacy of local recycling schemes, the culture of the urban population and the time of year, so pose a challenge from a feedstock management standpoint during gasification. For modelling energy generation, MSW is often assumed to contain a 50% organic fraction. Despite the potential advantages of and commercial interest in MSW jet fuels, only three peer-reviewed studies have considered the economic and environmental feasibility for a limited number of pathways (17, 18, 30). There are no studies available that focus on the role of MSW to liquid fuels from the perspective of energy modelling.

2.3 Hydrogen and Carbon Dioxide Conversion to Synthetic Fuels

Hydrogen to synthetic fuels with captured CO₂ as feedstock is another possible pathway to producing synthetic jet fuel. Due to the relative novelty and broad technological coverage, the semantics of hydrogen and captured CO₂ to liquid fuels varies in literature. They are known as electrofuels (e-fuels), power-to-liquids (PtL) or synthetic fuels (31).

There are many variants to producing e-fuels, but all pathways commonly follow three key processing steps: (a) hydrogen production; (b) CO₂ capture; and (c) synthesis (for example, FT or methanol synthesis). In industry, steam methane reforming (using natural gas and steam to produce hydrogen and CO₂) is most commonly used to produce hydrogen. But there would only be an emissions reduction if no CO₂ were produced during hydrogen synthesis. It is therefore most likely that the hydrogen would be produced through electrolysis – splitting water or steam into

its chemical constituents (hydrogen and oxygen) – which has the potential to be deployed in producing low-carbon hydrogen in the near- to mid-term if renewable electricity is used (32). There are three main types of electrolysis technology, differentiated by their cell electrolyte: (a) alkaline electrolysis; (b) proton exchange membrane (PEM); and (c) solid oxide electrolysis cell (SOEC) (33). Sources of electricity will have a big impact on the cost of electrolysis (i.e. intermittent sources will have higher cost). However, in time, electrolysis options are likely to become more commercially viable, as the price of sustainable electricity falls and the technology matures to be more efficient.

CO₂ capture could be from any high-concentration CO₂ source, such as industrial processes or power generation plants. Alternatively, CO₂ could be captured directly from air using direct air capture (DAC) technologies such as amine absorption. However, capture from air requires two to four times more energy compared to from flue gases even with strong bases for scrub (31).

The CO₂ and hydrogen undergo FT synthesis to produce 'e-crude' (a renewable crude oil substitute). A renewable energy-focused company called Sunfire, Germany, operates a facility for the purposes of producing e-crude, which can be refined to generate synthetic jet fuel. The role of hydrogen in the global energy system has been studied extensively but using hydrogen as an intermediate for synthetic fuels is not the focal point in any study due to high cost and difficulties faced in processing (34).

3. Synthetic Fuel in Energy System Models

Although technoeconomic assessments of sustainable synthetic fuels have been performed (9, 35, 36), their role in low-carbon energy systems is not well understood. A recent study (37) touches on the importance of biomass-derived synthetic transport fuels in a global energy system, but is focused on the role of bioenergy and CO₂ removal technologies. A study (38) examined the potential role of FT synthetic fuels in the global energy system as a major alternative energy carrier, but their assumptions on relatively new technologies are outdated or they are not represented at all. European Union (EU) (39) and global (40) energy system modelling studies that focus on the competitiveness of PtL production pathways have model limitations. The global study does not differentiate between synthetic manufacturing

processes (such as FT and methanol synthesis), but instead includes a proxy for all synthetic fuels that does not reflect their varying feedstocks and costs. This model also assumes gasoline, diesel and jet fuels are indistinguishable, yet fuel standards for each of these are quite different in reality. The EU study uses the JRC-EU-TIMES model, whose assumptions are examined in Section 3.1. A national-scale study (41) explores the opportunities for power-to-gas and PtL using an energy system simulation model (EnergyPLAN), but here we examine cost-optimisation models as we aim to understand whether synthetic fuels are likely to be economically-viable in the future.

We examine the role of synthetic fuels in three energy system models operating at different spatial scales: TIAM-UCL (global), JRC-EU-TIMES (EU) and UK TIMES (national). The TIMES Integrated Assessment Model was developed by the International Energy Agency (IEA, France) Energy Technology Systems Analysis Program (IEA-ETSAP). This ETSAP-TIAM model has 15 regions representing global decarbonisation to the year 2100 (42). A version was subsequently developed at University College London (UCL), UK, that included a UK region (TIAM-UCL), as well as a number of improvements particularly around resource availability (43). The JRC-EU-TIMES model represents the 27 EU countries and close neighbours (for example Norway, Switzerland, UK) as separate regions (44). The single-region UK TIMES energy system model is jointly developed by UCL and the UK Government, and has informed a number of UK decarbonisation policies including the Clean Growth Strategy (45).

All three models use TIMES model generator, which is developed by IEA-ETSAP (46). TIMES is a bottom-up (i.e. technology-rich) technoeconomic least-cost optimisation model. It is used to identify decarbonisation pathways for energy systems, over long time horizons that meet all projected energy service demands across the economy.

TIMES includes detailed representations of both current and potential future energy technologies. Technologies are characterised by their efficiency (input and output), cost (capital expenditure and operating expenditure) and lifetime. Energy commodities are produced and consumed by technologies, and can be traded between regions. Commodity shadow prices are endogenously calculated through supply and demand curves (47).

In this section, we first examine which synthetic fuel production technologies are included in each

model and how they are parametrised, in order to identify whether the approaches and data assumptions are consistent. We then examine a comparable decarbonisation scenario in each model to investigate which of these technologies are deployed, in order to understand whether these technologies might have a substantive role in future energy systems. Through these two analyses, we can ascertain whether there is a need to improve the representation of these technologies in these models.

3.1 Representation of Synthetic Fuel Routes

Table II summarises the technologies that are available to produce synthetic fuels. **Figure 2** displays the jet fuel production technologies that are represented in each model.

TIAM-UCL represents FT reactors with or without CCS that produce synthetic fuels from either fossil sources (coal, natural gas) or biomass (agricultural and forestry residues, or energy crops). It does not represent the possibility of using captured CO₂ and hydrogen to manufacture jet fuel.

JRC-EU-TIMES represents a much broader range of FT technologies. It represents jet fuel as a blend of oil-derived kerosene, hydrotreated vegetable oil, FT biodiesel and synthetic kerosene from hydrogen and captured CO₂. The model assumes diesel and kerosene are interchangeable, thus it mixes various types of synthetic diesel and kerosene in any proportions for the blendstock. It is not clear that the flexibility over blends of different fuels in jet fuel that is assumed in the model would meet international fuel quality standards. The FT plants have versions with and without CCS.

The UK TIMES model represents only a single FT plant that produces 50% diesel and 50% kerosene from biomass. There is no carbon capture and utilisation (CCU) route in UK TIMES to produce jet fuel from hydrogen and captured CO₂.

The capital costs of FT plants in TIAM-UCL and JRC-EU-TIMES are similar, while the process efficiency is assumed higher in JRC-EU-TIMES. The UK TIMES FT process has a much lower capital cost and a substantially higher process efficiency. The JRC-EU-TIMES technologies producing synthetic diesel from hydrogen and CO₂ have surprisingly low costs and high efficiencies. TIAM-UCL and UK TIMES assume 30 year plant lifetimes, while JRC-EU-TIMES assumes a lifetime of only 20 years for all plants.

Table II Comparison of Synthetic Fuel Production Technologies in the UK TIMES, JRC-EU-TIMES and TIAM-UCL Energy System Models

| Model | Description | Main feedstock | Capital cost, € PJ ⁻¹ yr ⁻¹ jet fuel | Efficiency ^c , % | Lifetime, years |
|--------------|--|------------------------------------|--|-----------------------------|-----------------|
| UK TIMES | FT diesel and kerosene production | Pellets | 27.0 | 0.75 | 30 |
| JRC-EU-TIMES | FT diesel production | Wood | 132.5 | 0.56 | 20 |
| JRC-EU-TIMES | FT diesel production with CCS | Wood | 132.5 | 0.56 | 20 |
| JRC-EU-TIMES | Hydrotreated vegetable oil production | Oil crop | 4.8 | 0.75 | 20 |
| JRC-EU-TIMES | Diesel production from electricity and captured CO ₂ ^a | Electricity | 32.6 | 0.55 | 20 |
| JRC-EU-TIMES | Diesel production from hydrogen and captured CO ₂ ^b | Hydrogen | 14.4 | 0.78 | 20 |
| JRC-EU-TIMES | Diesel production from electricity and atmospheric CO ₂ | Electricity | 130.4 | 0.33 | 20 |
| TIAM-UCL | FT diesel and kerosene production | Agricultural and forestry residues | 35.5 | 0.50 | 30 |
| TIAM-UCL | FT diesel and kerosene production with CCS | Agricultural and forestry residues | 49.6 | 0.42 | 30 |
| TIAM-UCL | FT diesel and kerosene production | Energy crops | 35.5 | 0.50 | 30 |
| TIAM-UCL | FT diesel and kerosene production with CCS | Energy crops | 49.6 | 0.42 | 30 |

Note: Capital costs are converted to Euros in the year 2018. All costs and efficiencies are projections for the year 2050. Higher heating values are used for all efficiencies.

^aTechnology includes an integrated electrolyser

^bTechnology includes integrated DAC and electrolyser

^cEfficiency is petajoule of fuel produced per petajoule of input (biomass, hydrogen or electricity)

3.2 Economic Viability of Synthetic Fuel Routes in the Long Term

The Paris Agreement aims to keep the global temperature rise well below 2°C compared to pre-industrial levels (1). TIAM-UCL has a climate module that links global temperature with global emissions. We examined a decarbonisation scenario in TIAM-UCL in which emissions are constrained so that the global temperature does not exceed 1.5°C this century. This approach cannot be used for regional models such as JRC-EU-TIMES and UK TIMES. We instead assumed that Europe would adopt a net zero emissions target for the year 2050, as proposed by the European Commission in the European Climate Law. Since JRC-EU-TIMES represents only the energy system, we estimated emissions in 2050 from industrial processes, land use, agriculture and waste, and concluded that these would need to be offset by 400 million tonnes CO₂ equivalent of negative emissions from the

energy system. UK TIMES represents all emissions from these sectors, including mitigation options, so we set a target of net zero GHG emissions in that model. Since every country has agricultural and land use emissions that cannot be mitigated, it is necessary for the energy systems to have net negative emissions in order to meet the overall net zero target (48).

With such challenging emission targets, CCS has important roles in the scenarios from all three models. As these are least-cost optimisation models, synthetic fuels are undermined if it is cheaper to use oil-derived kerosene and offset the emissions using a greenhouse gas removal (GGR) option. Thus, it is important to understand the capacity of captured CO₂ in the models. **Table III** shows the model results of the source of captured CO₂ in each model for 2050. All three models represent negative emission technologies, which sequester atmospheric CO₂ underground, and both DAC and biomass have

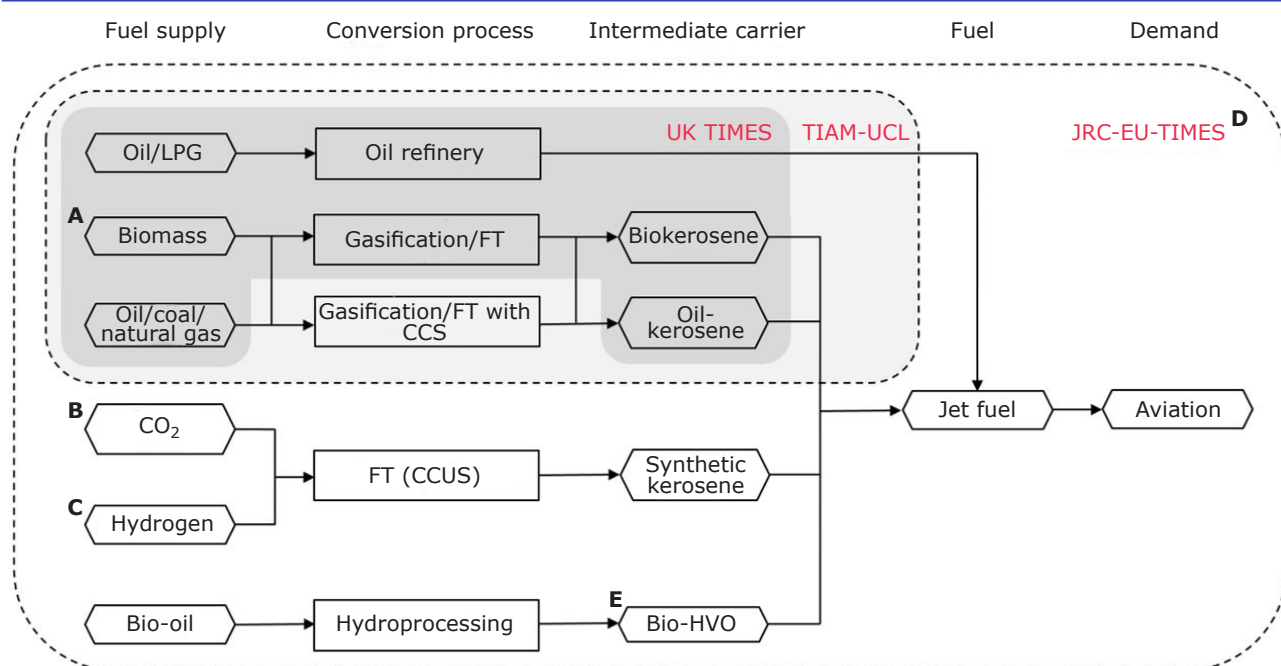


Fig. 2. Simplified technology coverage of jet fuel production in UK TIMES, JRC-EU-TIMES and TIAM-UCL energy system models. **A:** Each model has a unique pre-treatment method and different types of supply feedstock for 'biomass', the latter is listed in the 'Main feedstock' column in **Table II**. **B:** CO₂ is captured and utilised to produce synthetic kerosene in JRC-EU-TIMES, various sources for CO₂ are listed in **Table III**. **C:** Hydrogen is produced or circulated from the centralised medium size alkaline electrolyser, centralised hydrogen tank or centralised hydrogen from underground storage. **D:** Intermediate carriers are blended as described in the text for JRC-EU-TIMES. **E:** hydrotreated vegetable oil (HVO)

Table III Total Captured CO₂ in 2050 Across all Regions Each Scenario, Shares by Type of Capture Technology

| Source of captured CO ₂ | TIAM-UCL | JRC-EU-TIMES | UK TIMES |
|------------------------------------|----------|--------------|----------|
| DAC ^a | 1% | 69% | 49% |
| Biomass ^a | 70% | 25% | 22% |
| Natural gas | 9% | 6% | 27% |
| Waste | 0% | 0% | 0% |
| Industrial processes | 20% | 0% | 1% |

^aOnly DAC and bioenergy with CCS (BECCS) provide negative emissions, while others can provide low carbon mitigation options

substantial roles. Natural gas is also a substantial CO₂ source for UK TIMES. JRC-EU-TIMES reaches a 1000 million tonnes CO₂ sequestration limit in 2050 and this might have prevented higher natural gas CCS. The source of captured CO₂ is important because carbon in jet fuel is released to the atmosphere as CO₂, and if it is from a fossil source then there is a net increase in emissions even though the carbon is recycled.

In each model, there are substantial amounts of captured atmospheric carbon that can be used to produce carbon-neutral jet fuel.

The technologies used to produce jet fuel globally, in Europe, and in the UK, are compared for the three models in **Figure 3**. Despite keeping the global temperature rise below 1.5°C, the TIAM-UCL scenario has a limited role for synthetic fuels in aviation worldwide, comprising less than 5% of the total market for jet fuel by 2050. In contrast, JRC-EU-TIMES uses four different production routes and most jet fuel is low carbon. The synthetic kerosene route using captured CO₂ and hydrogen provides the largest contribution across Europe, yet is not considered as an option in the other two models. UK TIMES uses only fossil-based kerosene in 2050, because biomass availability is very constricted and is generally used by negative emission technologies. This reflects the lack of a FT plant with CCS in UK TIMES, and the assumption that only half of the plant output would be kerosene while the other half would be relatively low-value biodiesel. Under these assumptions, aviation fuel is a less economic market for biomass than alternatives such as biomass electricity generation with CCS.

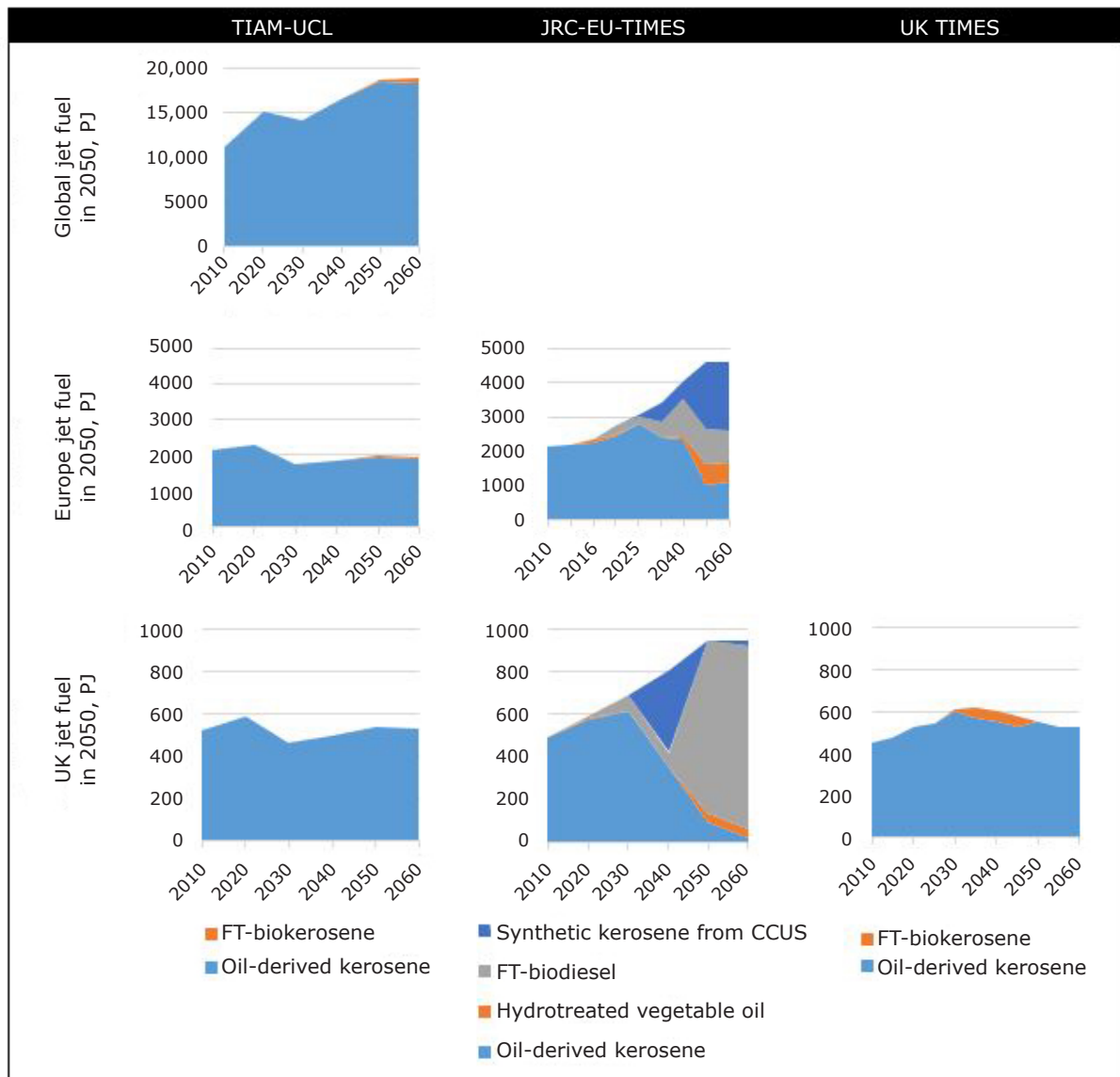


Fig. 3. Global jet fuel production in 2050 (PJ yr^{-1}), from net zero scenarios in the TIAM-UCL, JRC-EU-TIMES and UK TIMES energy system models

JRC-EU-TIMES assumes substantially higher demand for jet fuel by 2050 both across Europe and in the UK. As well as higher demand for air travel, this could reflect a more pessimistic view of the potential for fuel savings through redesigning aircraft and improving the operational efficiency of fleets.

4. Discussion

Synthetic fuels have received little attention in energy system models in the past because of their perceived high costs compared to other decarbonisation approaches, and because there are large uncertainties in the plant cost and performance data. The only exception has been for

technologies using fossil fuels as feedstocks, where there are historical precedents based on energy security needs. As climate science has evolved, decarbonisation targets have become more stringent. While synthetic fuels were expected to have at most a minor role in future energy systems with emissions at 60% or 80% below 1990 levels, the JRC-EU-TIMES scenario in Section 3.2 show that they could make an important contribution to net zero systems.

Yet the choice and level of deployment of these technologies varies substantially between the three models. One reason is that there is uncertainty within the modelling community about which of these technologies is likely to be technically feasible, and about the cost and

performance of the technologies. UK TIMES represents only a single inflexible FT reactor, with only biomass as a feedstock, and with no CCS option. The value of the plant is further reduced by assuming that only 50% of the output can be biokerosene, with lower-value biodiesel comprising the remainder. This technology has no role in 2050 as biomass is more economically used in negative emission plants. In contrast, JRC-EU-TIMES has a range of plants using both biomass and captured CO₂, and with CCS options. In the JRC-EU-TIMES net zero scenario, the CCS versions of both sets of technologies make important contributions. Given the stringent climate targets, in TIAM-UCL synthetic jet fuels are produced exclusively by FT processes with CCS using biomass feedstock (energy crops, and agricultural and forestry residues). Fossil FT processes are not used but kerosene from crude oil is still produced, with the associated emissions offset by 'negative emissions' from bioenergy with CCS (BECCS) electricity generation plants. The availability of other GGR technologies (such as DAC and afforestation) does not reduce pressure on biomass sources but it does change the role of BECCS for climate mitigation (37).

These scenarios suggest a close relationship between negative emissions, CCS and synthetic fuels. This is illustrated by comparing the net zero scenarios in the European and UK models. The JRC-EU-TIMES model assumes that CO₂ sequestration cannot exceed 1000 million tonnes CO₂ per year in 2050, and this limit is reached. For this reason, virtually all sequestration capacity is used for negative emissions and synthetic fuels have an important role. Since the UK has a large CO₂ sequestration capacity compared to the European average, the sequestration limit is not reached in UK TIMES. Natural gas is a substantial source of CO₂, and there is less need for synthetic fuels.

4.1 Improvements to Model Design

Synthetic fuels from hydrogen and captured CO₂ constitutes around 40% of jet fuel production in JRC-EU-TIMES for 2050. It is possible that synthetic fuels would have a similar cost-optimal share of the market in UK TIMES and TIAM-UCL if a wider range of production technologies were available. Despite having electrolyser and CO₂ capture options at various scales, synthetic fuel production from CCU is overlooked in these two models. There is a

need to incorporate a wider range of synthetic fuel technologies in these models.

One of the main bottlenecks in producing synthetic fuels is biomass availability. TIAM-UCL and UK TIMES only consider synthetic fuel production from lignocellulosic biomass, whose supply is expected to be limited by food security and biomass sustainability concerns, and which is better used elsewhere in the energy system such as for BECCS in electricity generation or hydrogen production, as these have higher CO₂ capture rates.

Biomass feedstocks for large-scale gasification plants must have high composition consistency throughout the year. Therefore, it is challenging to use waste as a feedstock, and MSW is implicitly assumed to be a non-viable feedstock by all three models. This is arguably not reflective of the current status quo of FT plant project developments, as a waste-to-fuel plant has been designed to produce 11 million gallons of jet fuel or diesel annually from processing 175,000 tonnes of MSW (49). However, this project does not include CCS, which is a key technology in our model. Further research is needed to understand the role of these types of facilities in climate mitigation and the competitiveness of waste as feedstock for synthetic fuel production.

4.2 Challenges and Opportunities for the Future of Energy Systems Modelling

As explained in Section 1, neat AJF must be blended with conventional jet fuel to meet international standards. This blending percentage stands at maximum of 50% for AJF, but is expected to increase as conversion technologies improve. UK TIMES and TIAM-UCL assume biokerosene has the same effective composition as oil-based kerosene, which does not reflect current limitations. On the other hand, JRC-EU-TIMES limits the proportion of biokerosene to 47% in 2020, increasing to 95% in 2050. However, this model assumes biodiesel and biokerosene are interchangeable, despite there being no precedent of a blend composed of biodiesel and kerosene that can be used as jet fuel. It is unlikely that this type of blend meets the current specification of standard jet fuel (50). The transportation fuel blending approach is based on the IFPEN OURSE model (51), where product specifications are sensibly accounted for by the means of quality control equations under a linear programming framework. However, JRC-EU-TIMES implements an extended production chain in

comparison to that model, and transportation fuel quality is not represented as originally intended. There is a challenge to identify and implement feasible blending combinations that consider the chemical composition of blends to meet jet fuel standards.

Another important challenge is understanding the uncertainty of carbon capture, utilisation and storage (CCUS) in the role of achieving net zero by 2050. Synthetic fuels from CCUS are cost-optimal in a net zero scenario in the JRC-EU-TIMES model. However, using CCUS for fuels does not necessarily contribute towards climate mitigation (52). Captured CO₂-based fuels move carbon through industrial systems over different timescales. Such fuels do not provide net CO₂ removal from the atmosphere, but reduce emissions through industrial CO₂ capture that displace fossil fuel use. The space and time of this pathway is not fully understood and must be analysed to determine its overall impact. On the other hand, CCUS is seen as a stepping stone towards successful implementation of CCS in terms of innovation and reduction of costs, and is a crucial technology to meet net zero targets. CCUS could have a transition role in the aviation sector until electrification or other low-carbon options come into place after 2050. Alternatively, the demand for aviation could reduce if there were a modal shift to transportation modes that are more easily electrified (for example, electric high-speed trains).

There is a general challenge to reduce the cost of synthetic fuels (31), in terms of both the capital cost of production plants and the cost of captured CO₂ and hydrogen. At current cost projections, the UK TIMES and TIAM-UCL results suggest that at present, these options are much more expensive than fossil-based kerosene coupled with negative emission technologies to offset the CO₂ emissions. Further techno-economic assessment is needed to better understand the sensitivity of varying capital cost and cost of the input sources for better comprehension of risks involved in investing in these technologies.

The transparency and validation of assumptions made by the modellers, such as technology costs and performance, are imperative in energy system models (53). Yet we found that model input data sources are poorly documented for key technologies across the models. Detailed documentations for UK TIMES, JRC-EU-TIMES and TIAM-UCL are publicly available but the bulk of the assumptions – especially for technologies that were modelled in the early stages of the models – are

not available. In some cases, reasoning might have been lost when a new model was developed from an existing model (for instance from UK MARKAL to UK TIMES). Lack of documentation is concerning because the cost and efficiency of the equivalent technologies across the models vary significantly, and these technologies appear to have a role in net zero scenarios as discussed in Section 4.

5. Conclusions

Aviation is carbon-intensive and must reduce its emissions to meet current climate goals. Decarbonisation of the sector is challenging, but there are opportunities through switching to low-carbon synthetic jet fuels. Energy system models are valuable for understanding the role of synthetic fuels in climate mitigation. Our evaluation of three models in this paper has identified gaps in technology and input feedstock options for synthetic fuel production. We have identified a variety of potential model improvements to better represent synthetic fuels in the future. This would ideally be coupled with a better understanding of the fuel quality from each production process, and the implications for jet fuel blending.

Model scenario outputs show synthetic jet fuels could make an important contribution to net zero systems. This will mainly rely on improving cost competitiveness compared with conventional jet fuel coupled with negative emissions. Importantly, the scenarios show that there is a close relationship between negative emissions, CCS and synthetic fuels. This means that the share of synthetic fuels in net zero scenarios will also depend on the assumptions made on CCS and negative emissions. Given the stringent climate targets and the long lifetimes of synthetic fuel production plants, further research on synthetic fuels is needed in the context of energy system modelling to fully determine its capabilities in emissions reduction.

Acknowledgements

Seokyoung Kim was supported by an Engineering and Physical Sciences Research Council (EPSRC) Industrial Cooperative Awards in Science & Technology (CASE) studentship (grant EP/R513143/1) and by Johnson Matthey, UK. Paul Dodds and Isabela Butnar were supported by the Natural Environment Research Council (NERC) "Comparative assessment and region-specific optimisation of GGR" project (grant NE/P019900/1).

References

1. "Paris Agreement", United Nations, Bonn, Germany, 2015, 25 pp
2. "Special Report: Global warming of 1.5°C", Geneva, Switzerland, 2018
3. 'Climate Change Act 2008', The Stationery Office, London, UK, 26th November, 2008
4. 'Research and Analysis: Greenhouse Gas Reporting: Conversion Factors 2019', Department for Business, Energy & Industrial Strategy, The Stationery Office, London, UK, 4th June, 2019
5. 'Contribution of the Global Aviation Sector to Achieving Paris Agreement Climate Objectives', Climate Action Network International, Bonn, Germany, 2nd April, 2018
6. A. W. Schäfer, A. D. Evans, T. G. Reynolds and L. Dray, *Nat. Clim. Chang.*, 2015, **6**, (4), 412
7. 'Fuel Qualification', Commercial Aviation Alternative Fuels Initiative (CAAFI): http://www.caafi.org/focus_areas/fuel_qualification.html (Accessed on 4th February 2021)
8. "Sustainable Synthetic Carbon Based Fuels for Transport: Policy Briefing", The Royal Society, London, UK, 16th September, 2019, 46 pp
9. "Alternative Aviation Fuels: Overview of Challenges, Opportunities, and Next Steps", Office of Energy Efficiency and Renewable Energy (EERE), US Department of Energy, Washington, DC, USA, March, 2017, 88 pp
10. M. Wang, R. Dewil, K. Maniatis, J. Wheeldon, T. Tan, J. Baeyens and Y. Fang, *Prog. Energy Combust. Sci.*, 2019, **74**, 31
11. P. Capros, M. Kannavou, S. Evangelopoulou, A. Petropoulos, P. Siskos, N. Tasios, G. Zazias and A. DeVita, *Energy Strateg. Rev.*, 2018, **22**, 255
12. 'A Clean Planet for All: A European Strategic Long-Term Vision for a Prosperous, Modern, Competitive and Climate Neutral Economy', COM/2018/733Final, European Commission, Brussels, Belgium, 28th November, 2018
13. R. C. Baliban, J. A. Elia, C. A. Floudas, B. Gurau, M. B. Weingarten and S. D. Klotz, *Energy Fuels*, 2013, **27**, (8), 4302
14. J. A. Elia, R. C. Baliban, C. A. Floudas, B. Gurau, M. B. Weingarten and S. D. Klotz, *Energy Fuels*, 2013, **27**, (8), 4325
15. A. Lappas and E. Heracleous, 'Production of Biofuels via Fischer-Tropsch Synthesis: Biomass-to-Liquids', in "Handbook of Biofuels Production: Processes and Technologies", 2nd Edn., eds. R. Luque, C. S. K. Lin, K. Wilson and J. Clark, Woodhead Publishing Series in Energy, No. 98, Elsevier Ltd, Duxford, UK, 2016, pp. 549–593
16. 'JM and BP License Waste-To-Fuels Technology to Fulcrum BioEnergy', Johnson Matthey, London, UK, 2018
17. P. N. Pressley, T. N. Aziz, J. F. DeCarolis, M. A. Barlaz, F. He, F. Li and A. Damgaard, *J. Clean. Prod.*, 2014, **70**, 145
18. P. Suresh, R. Malina, M. D. Staples, S. Lizin, H. Olcay, D. Blazy, M. N. Pearlson and S. R. H. Barrett, *Environ. Sci. Technol.*, 2018, **52**, (21), 12055
19. Y. H. Choi, Y. J. Jang, H. Park, W. Y. Kim, Y. H. Lee, S. H. Choi and J. S. Lee, *Appl. Catal. B Environ.*, 2017, **202**, 605
20. 'Syngas: The Renewable Feed Gas', Sunfire GmbH, Dresden, Germany: <https://www.sunfire.de/en/applications/syngas> (Accessed on 4th February 2021)
21. S. Pye, F. G. N. Li, A. Petersen, O. Broad, W. McDowall, J. Price and W. Usher, *Energy Res. Soc. Sci.*, 2018, **46**, 332
22. P. E. Dodds and W. McDowall, *Int. J. Hydrogen Energy*, 2014, **39**, (5), 2345
23. A. Schäfer, 'Introducing Behavioral Change in Transportation into Energy/Economy/ Environment Models', World Bank Policy Research Working Paper No. 6234, The World Bank, Washington, DC, USA, 1st October, 2012, 61 pp
24. T. D. Searchinger, T. Beringer and A. Strong, *Energy Policy*, 2017, **110**, 434
25. R. Rauch, J. Hrbek and H. Hofbauer, *Wiley Interdiscip. Rev. Energy Environ.*, 2013, **3**, (4), 343
26. M. Hogan, 'German Biofuel Firm Choren Declares Insolvency', Reuters, London, UK, 8th July, 2011
27. 'Vapo Oy Freezes the Kemi Biodiesel Project', Vapo Oy, Jyväskylä, Finland, 21st February, 2014
28. 'A Commercially Demonstrated Technology Solution', Velocys, Oxford, UK: <https://www.velocys.com/technology/> (Accessed on 4th February 2021)
29. 'Lakeview Site: Project Summary', Red Rock Biofuels, Fort Collins, USA: <https://www.redrockbio.com/lakeview-site.html> (Accessed on 4th February 2021)
30. A. M. Niziolek, O. Onel, M. M. F. Hasan and C. A. Floudas, *Comput. Chem. Eng.*, 2015, **74**, 184
31. S. Brynolf, M. Taljegard, M. Grahn and J. Hansson, *Renew. Sustain. Energy Rev.*, 2018, **81**, 1887
32. "Options for Producing Low-Carbon Hydrogen at Scale: Policy Briefing", The Royal Society, London, UK, January, 2018, 36 pp
33. "Hydrogen Production by Electrolysis", ed. A. Godula-Jopek, Wiley-VCH Verlag GmbH & Co KGaA, Weinheim, Germany, 2015
34. I. Staffell, D. Scamman, A. Velazquez Abad, P. Balcombe, P. E. Dodds, P. Ekins, N. Shah and K. R. Ward, *Energy Environ. Sci.*, 2019, **12**, (2), 463
35. V. Dieterich, A. Buttler, A. Hanel, H. Spliethoff and S. Fendt, *Energy Environ. Sci.*, 2020, **13**, (10), 3207
36. G. Herz, E. Reichelt and M. Jahn, *Appl. Energy*, 2018, **215**, 309
37. I. Butnar, O. Broad, B. Solano Rodriguez and P. E.

- Dodds, *GCB Bioenergy*, 2020, **12**, (3), 198
38. T. Takeshita and K. Yamaji, *Energy Policy*, 2008, **36**, (8), 2773
39. H. Blanco, W. Nijs, J. Ruf and A. Faaij, *Appl. Energy*, 2018, **232**, 617
40. M. Lehtveer, S. Brynolf and M. Grahn, *Environ. Sci. Technol.*, 2019, **53**, (3), 1690
41. S. Bellocchi, M. De Falco, M. Gambini, M. Manno, T. Stilo and M. Vellini, *Energy*, 2019, **175**, 847
42. R. Loulou, G. Goldstein and K. Noble, "Energy Technology Systems Analysis Programme Documentation for the MARKAL Family of Models", Energy Technology Systems Analysis Programme (ETSAP), International Energy Agency, Paris, France, October, 2004, 389 pp
43. S. Pye, J. Price, J. Cronin, I. Butnar and D. Welsby, "Modelling 'Leadership-Driven' Scenarios of the Global Mitigation Effort", Research Report, UCL Energy Institute, London, UK, May, 2019, 47 pp
44. S. Simoes, W. Nijs, P. Ruiz, A. Sgobbi, D. Radu, P. Bolat, C. Thiel and S. Peteves, "The JRC-EU-TIMES model: Assessing the Long-Term Role of the SET Plan Energy Technologies", JRC Scientific and Policy Reports, No. EUR 26292 EN, European Union, Luxembourg, 2013, 382 pp
45. "The Clean Growth Strategy: Leading the Way to a Low Carbon Future", The Stationery Office, London, UK, 2017, 165 pp
46. R. Loulou, U. Remne, A. Kanudia, A. Lehtila and G. Goldstein, 'Documentation for the TIMES Model: Part I', Energy Technology Systems Analysis Programme (ETSAP), International Energy Agency, Paris, France, April, 2005, 78 pp
47. R. Loulou and M. Labriet, *Comput. Manag. Sci.*, 2007, **5**, (1-2), 7
48. S. Fuss, J. G. Canadell, G. P. Peters, M. Tavoni, R. M. Andrew, P. Ciais, R. B. Jackson, C. D. Jones, F. Kraxner, N. Nakicenovic, C. Le Quéré, M. R. Raupach, A. Sharifi, P. Smith and Y. Yamagata, *Nat. Clim. Chang.*, 2014, **4**, (10), 850
49. 'Sierra Biofuels Plant: Bright Future', Fulcrum BioEnergy Inc, Pleasanton, USA: <http://fulcrum-bioenergy.com/facilities/> (Accessed on 21st July 2020)
50. N. S. Ekaab, N. H. Hamza and M. T. Chaichan, *Case Stud. Therm. Eng.*, 2019, **13**, 100381
51. D. Lorne and S. Tchung-Ming, "The French Biofuels Mandates Under Cost Uncertainty: An Assessment Based on Robust Optimization", Les Cahiers de L'économie No. 87, IFP Energies Nouvelles, Rueil Malmaison, France, September, 2012, 38 pp
52. C. Hepburn, E. Adlen, J. Beddington, E. A. Carter, S. Fuss, N. Mac Dowell, J. C. Minx, P. Smith and C. K. Williams, *Nature*, 2019, **575**, (7781), 87
53. S. Pfenninger, A. Hawkes and J. Keirstead, *Renew. Sustain. Energy Rev.*, 2014, **33**, 74

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