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Comparative Life Cycle Evaluation of Alternative Fuels for a Futuristic Subsonic Long-Range Aircraft

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Abstract: Liquid hydrogen (LH_2) and 100% synthetic paraffinic kerosene (SPK), or sustainable aviation fuel (SAF), represent viable alternatives to conventional Jet-A for long-haul aviation, provided they are produced via pathways enabling net-zero well-to-wake (WTWa) emissions. This study evaluates the WTWa performance, including non-CO_2 emissions, of a blended wing body aircraft (300 passengers, 13,890 km range) powered by either LH_2 or 100% SPK. Use-phase emissions are quantified, and fuel production impacts are assessed using the GREET model. Analysis of over 100 production pathways reveals that LH_2 can achieve net-zero or negative WTWa CO_2-equivalent emissions when produced from biomass or integrated fermentation with carbon sequestration. Non-CO_2 emissions are shown to contribute significantly to WTWa impacts. When miscanthus is used as a feedstock, 100% SPK reduces WTWa CO_2-equivalent emissions by 70–85% compared to Jet-A. A high-level supply analysis indicates that SAF and hydrogen production in 2050 could meet the energy demands of long-haul aviation, assuming a 4% annual traffic growth rate and full adoption of these fuels. These findings provide critical insights to guide R&D investments, fuel cost analyses, and aviation policy development for sustainable long-haul aviation.

Keywords: life cycle assessment; decarbonising long-range aviation; climate neutral aviation; hydrogen aircraft; alternative aviation fuel; sustainable aviation fuel

1. Introduction

Aviation's climate impact stems from both CO_2 and non-CO_2 effects, including soot, aerosols, water vapor, NO_x emissions, and contrail-induced cirrus clouds [1–3]. Currently, aviation contributes 3.5% to anthropogenic radiative forcing, with non-CO2 effects accounting for approximately two-thirds of this impact [1–3]. Despite the pandemic, air travel demand is projected to double over the next two decades (2024–2043) [4], significantly exacerbating aviation's climate footprint. While advancements in aircraft technology and low-carbon fuels could address 80% of the measures needed for carbon-neutral growth [5,6], achieving this goal requires a comprehensive understanding of life cycle emissions.

Life cycle emissions from aviation fuels encompass both operational and production phases, with the former contributing ~70% of total greenhouse gas (GHG) emissions for Jet-A fuel [7]. Current regulatory and technological efforts primarily focus on operational emissions, but a holistic approach is essential to evaluate the sustainability of alternative fuels. Tools like the GREET model [8] enable comprehensive life cycle assessments, revealing that not all alternative fuel pathways have low embodied GHG emissions. For instance, while liquid hydrogen (LH_2) offers zero operational emissions and higher energy density than Jet-A, its life cycle GHG emissions can be 3 times as that of conventional Jet-A fuel, when derived from coal.

Decarbonizing long-haul aviation remains a significant challenge [6,9]. Presently, 100% synthetic paraffin kerosene (SPK) is not permitted for use in the existing aircraft fleet. Approved drop-in fuels for civil aviation use include up to a 50% blend of alcohol-to-jet (ATJ), Fischer-Tropsch (FT), and

hydro-processed renewable or hydro-processed esters and fatty acids (HRJ or HEFA) SPK pathways, as well as a 10% blend of sugar-to-jet (STJ) SPK pathway [10–13]. Among the alternatives, LH_2 and 100% SPK are the only viable options for long-range, large twin-aisle (LTA) aircraft, whether tube-wing or blended wing body designs [6,14–16]. However, existing studies on SPK and LH_2 often focus solely on operational impacts, neglecting embodied emissions from fuel production [17,18]. A holistic evaluation framework is therefore critical to identify sustainable fuel pathways and assess their life cycle performance.

This study adopts a life cycle approach to evaluate fuel feedstock and production pathways for LH_2 and 100% SPK, aiming to enable climate-neutral long-range flights for LTA aircraft. By integrating operational and embodied emissions, this work contributes to the development of a methodological framework for sustainable aviation, addressing gaps identified in recent reviews [19–21]. The analysis focuses on combustion-based LTA aircraft, providing insights into the potential of LH_2 and 100% SPK as alternatives to conventional Jet-A fuel.

Numerous studies have conducted life cycle or well-to-wake (WTWa) emissions analyses for SPK and LH_2 fuels across various aircraft range applications. These include fossil fuel-based SPK [22], bio-jet fuel e.g., [23–26], power-to-liquid (PtL) or electro-fuel e.g., [27,28], and LH_2 (e.g., [29,30]. However, none of these studies comprehensively examine the combination of feedstocks and manufacturing pathways required to achieve climate-neutral long-range flights for LTA aircraft powered by LH_2 and 100% SPK (bio-jet and PtL fuels). Additionally, many of these analyses exclude non-CO_2 emissions in their WTWa assessments, limiting their applicability to sustainable aviation goals.

Key findings from recent reviews highlight the potential of alternative fuels to reduce WTWa GHG emissions. For instance, Lau et al. [31] report that HEFA and alcohol-to-jet (ATJ) bio-jet fuels can reduce WTWa GHG emissions by 19–42% and 20–65%, respectively. Braun et al. [25] find that Fischer-Tropsch (FT) SPK fuel derived from miscanthus, agricultural residues, and municipal solid waste can achieve up to 100% reduction in WTWa GHG emissions, with regional variations exceeding 125%. Ansell [32] notes that bio-jet fuel and renewable hydrogen can reduce WTWa CO_2 emissions by 68% and ~80%, respectively, assuming a fully renewable grid. However, these studies do not account for non-CO_2 emissions, which are critical for a holistic assessment of aviation's climate impact.

Afonso et al. [23] and Song et al. [33] demonstrate that bio-jet fuels can reduce WTWa GHG emissions by up to 80% (including non-CO_2 emissions) and 41–89% (excluding non-CO_2 emissions), depending on feedstock and production pathways. Despite these advancements, existing research often focuses on limited or selective feedstocks, leaving gaps in understanding the full potential of alternative fuels for decarbonizing long-haul aviation.

For further details on manufacturing pathways, fuel properties, operability issues, and other aspects of alternative fuels, readers are directed to comprehensive reviews by Su-ungkavatin et al. [34]), Cabrera and Sousa [35], Ansell [32], and Braun et al. [25]. A detailed review of selected studies is also provided in Supplementary Information (SI) file SI §1.

Kolosz et al. [22] compare WTWa performance metrics for blended/drop-in SPK fuels, including fossil fuel-based SPK (derived from coal, oil sands, oil shale, and natural gas) and bio-jet fuels (first, second, and third generation). Similarly, Wei et al. [36], Pavlenko et al. [37], and De Jong et al. [24] assess WTWa emissions for bio-jet fuels but focus on limited biomass feedstocks. Studies by the International Civil Aviation Organization [38] and Prussi et al. [39] explore bio-jet fuels using feedstocks listed in the CORSIA database, while Van Der Sman et al. [40] review WTWa emissions for SPK fuels (bio-jet and PtL) within the EU region. Saad et al. [41] estimate a ~50% reduction in WTWa emissions for PtL and bio-jet fuels but limit their analysis to Switzerland. Notably, none of these studies account for non-CO_2 emissions from aircraft operations in their WTWa analyses.

Grim et al. [42] report that PtL fuels can reduce WTWa GHG emissions by 66–94% (excluding non-CO_2 effects). In the study by Grim et al., the wide range of 66–94% reduction is attributable to the variability in the sourcing of (carbon) feedstock (direct air capture or point based carbon

sourcing). while Sacchi et al. [43] find reductions of 65–100% (including non-CO_2 effects) for PtL derived from direct air capture and carbon storage. Micheli et al. [44] and Papantoni et al. [45] highlight the role of renewable energy in PtL production, with Micheli et al. [44] reporting WTWa GHG reductions of 27.6–46.2% (with non-CO_2 effects) and 52.6–88.9% (without non-CO_2 effects) for PtL produced using wind power in Germany. Papantoni et al. [45] observe reductions of 32% (solar) and 42% (wind) when non-CO_2 emissions are included. Klenner et al. [46] find that PtL and LH_2 produced using wind power in Norway reduce WTWa GHG emissions by 48% and 44%, respectively, for short flights (<200 km), with higher reductions (52% for PtL and 54% for LH_2) for longer flights. VanLandingham [47] and VanLandingham and Hall [48] report WTWa GHG reductions of 43% (PtL) and 61% (LH_2) for a Boeing 737, while Prashanth et al. [49] estimate reductions of 84–93% (PtL) and 91–98% (LH_2) depending on the renewable energy source (solar or wind). Studies by the German Environment Agency (2016) and Schmidt et al. [28] project near-100% WTWa GHG reductions for PtL in Germany's future energy mix. However, these analyses are often limited to specific energy landscapes or feedstocks, and the life cycle GHG performance of PtL and LH_2 depends heavily on CO_2 sourcing (direct air capture vs. point sources) and the electricity mix used in production.

Delbecq et al. [27] evaluate the WTWa performance of bio-jet fuel, PtL, and hydrogen at the aviation system level for a small aircraft. However, the individual WTWa GHG reduction potential of each fuel remains unclear, and the feedstock sourcing for bio-jet fuel is unspecified, while PtL and hydrogen are limited to renewable energy. Fantuzzi et al. [50] assess alternative aviation fuels but focus on limited feedstocks/pathways for bio-jet fuel (HEFA and ATJ), PtL, and hydrogen (steam methane reformation [SMR] and electrolysis), achieving up to 70% WTWa GHG savings (excluding non-CO_2 emissions). Their analysis is restricted to the UK energy landscape. [51] provide a detailed evaluation of alternative fuels, including bio-jet fuel (ATJ, HEFA, FT), PtL (using direct air capture), and hydrogen (electrolysis with renewable power), considering non-CO_2 emissions. They project an 89–94% reduction in WTWa GHG emissions by 2050, accounting for efficiency improvements and contrail avoidance, despite a 2–3x increase in demand. However, their study examines limited feedstocks for each fuel.

Quante et al. [52] report WTWa GHG reductions (excluding non-CO_2 emissions) of 85% (FT SPK), 100% (PtL), 54% (HEFA SPK), 62% (ATJ SPK), 61% (STJ SPK), and 80% (hydrogen), though specific bio-jet fuel feedstocks are unspecified. Penke et al. [53] find WTWa GHG reductions (excluding non-CO_2 emissions) of 77% (PtL), 30% (HEFA from soy oil), and 95% (renewable hydrogen). Kossarev et al. [54,55] focus on renewable hydrogen, algae-based HEFA, and hydrogenated vegetable oil, achieving WTWa GHG reductions (including non-CO_2 emissions) of 59.5%, 35.8%, and 112%, respectively. These studies are limited to specific energy landscapes or feedstocks, restricting their broader applicability.

Studies on hydrogen as an aviation fuel [56–58] frequently exclude non-CO_2 emissions, a critical oversight. Similar limitations are found in other prior studies [30,50,52,59,60]. Additionally, many studies [56,57,61] limit feedstock/pathway selection to renewable power, neglecting other potential sources. These similar limitations are observed in other previous literature [30,58,62,63]. The impact of aircraft use-phase energy consumption and emissions on WTWa performance is significant, yet studies often fail to account for the poor volumetric energy density of LH_2, which penalizes aircraft energy performance.

Koroneos et al. [61] examine LH_2 for an A320-type aircraft, considering realistic design effects, but their analysis is outdated and limited in LH_2 production methods. Mukhopadhaya and Rutherford [30] project ~100% WTWa GHG reductions (excluding non-CO_2 emissions) for PtL and LH_2 from renewable electrolysis. Tveitan [57] reports a 58% WTWa GHG reduction (excluding non-CO_2 emissions) for green hydrogen, while Chan et al. [58] find that green hydrogen and bio-jet fuel (feedstock unspecified) can achieve up to 88% WTWa GHG reductions. However, these studies often omit non-CO_2 emissions, limiting their comprehensiveness.

Miller [64] and Miller et al. [65] expand on previous studies by evaluating a broader range of feedstocks and pathways for LH_2 and bio-jet fuels, incorporating contrail-cirrus effects in their WTWa

analysis. However, their work excludes PtL or electro-fuels and the STJ pathway, and their results are limited to smaller, shorter-range aircraft, unlike the LTA aircraft focus of this study. The FlyZero report [66] addresses performance penalties from cryogenic tank installation and includes non-CO_2 emissions in its WTWa analysis of LH_2, PtL, and bio-jet SPK fuels for small to mid-size aircraft. Nevertheless, it examines only a limited number of feedstocks and manufacturing pathways for these fuels.

A critical gap in the existing literature is the lack of comprehensive WTWa analyses that include non-CO_2 emissions and explore diverse feedstock and manufacturing pathway combinations for achieving climate-neutral long-range flights using LH_2 and 100% SPK (bio-jet and PtL fuels). While studies such as Afonso et al. (2023), Ansell (2023), and others provide valuable insights, they often focus on specific energy landscapes, limited feedstocks, or exclude non-CO_2 effects. Furthermore, none of these studies consider fuel production routes that integrate carbon capture and storage (CCS), except for Fantuzzi et al. [50], who demonstrate that CCS in SMR-based LH_2 production can reduce WTWa GHG emissions by 60% (median value). Pavlenko and Searle [67] highlight hydrogen's critical role in SPK fuel production, emphasizing that green hydrogen can significantly reduce WTWa GHG emissions. However, the sensitivity of hydrogen production to SPK life cycle emissions remains unexplored.

According to the International Air Transport Association [68], achieving net-zero CO_2 emissions by 2050 will require a combination of strategies: sustainable aviation fuels (SAF) contributing 65%, new aircraft technologies (e.g., electric and hydrogen) 13%, operational efficiencies 3%, and offsets/carbon capture 19%. Carbon removal is identified as a key strategy, yet its integration into fuel production pathways is underexplored. Additionally, none of the reviewed studies estimate the energy demand for long-haul aviation in 2050 or assess whether this demand can be met entirely with 100% SPK (or SAF) and/or LH_2.

The limitations in existing literature motivate this study, which aims to address critical gaps in understanding the life cycle or WTWa GHG performance of long-range LTA aircraft powered by LH_2 and 100% SPK, including bio-jet and PtL fuels. This work evaluates over 100 feedstocks and manufacturing pathways, some incorporating CCS, while accounting for non-CO_2 emissions. Additionally, it investigates the sensitivity of hydrogen sourcing to SPK production, biomass sourcing for hydrogen pathways, and the impact of energy mix transitions (2020 vs. 2050). The study also estimates future (2050) energy demand and supply for long-haul aviation using 100% SPK (or SAF) and LH_2, providing novel contributions to the field.

In the authors' previous work [15,16], the engine and operational energy performance of a 2030+ (N+2 timeframe) blended wing body (BWB) LTA aircraft powered by LH_2 and 100% SPK was conducted while incorporating penalties from cryogenic tank installation for LH_2. These prior studies based on conceptual design/low order modelling enable estimation of use-phase GHG emissions in the present work, which, combined with manufacturing-phase emissions, facilitates comprehensive WTWa or life cycle emissions analysis. Because the prior studies were conducted using low order modelling, the use phase emission estimation in this work is of low fidelity level. Over 100 production pathways for LH_2, PtL, and bio-jet SPK are examined, including those employing CCS. The primary objectives of this work are:

1. Develop a database of energy, emissions, and materials inventory for alternative fuels produced via various pathways.

2. Assess sensitivities of hydrogen sourcing to SPK production and biomass sourcing for hydrogen pathways.

3. Evaluate aircraft operational-phase emissions, including non-CO_2 effects.

4. Estimate future energy demand and supply (2050) for 100% SPK (or SAF) and LH_2 in long-haul aviation.

In addition to quantifying CO_2-equivalent emissions, this study evaluates unintended effects of LH_2 and 100% SPK use, such as fossil fuel consumption, water use, and other emissions. The GREET model [8], CORSIA default values, and literature are used to create an inventory of manufacturing-phase CO_2-equivalent emissions for over 100 fuel production pathways. Use-phase emissions are modeled for a 2030+ BWB aircraft powered by LH_2 and 100% SPK, incorporating non-CO_2 emissions from literature to estimate WTWa CO_2-equivalent emissions. Further details are provided in the Supplementary Information (SI) document.

2. Methodology

The WTWa emissions or performance of any fuel is the summation of emissions during the fuel manufacturing stage (from raw material extraction stage to its transportation and storage at fuel pump) and the operational phase of the aircraft. The fuel manufacturing stage is referred to as well-to-pump (WTP) and operational phase of aircraft is referred to as pump-to-wake (PTWa). In this work, it is assumed that for all fuels the pump to aircraft tank emissions and/or leakages are zero. Figure 1 shows the schematic of WTWa emissions calculation process from WTP and PTWa emissions, used in this work. Referring to Figure 1, WTWa CORSIA default values (2021), are available directly from literature and these are listed in Table SI 5 (in SI §1). It is to be noted that the CORSIA default values are limited to a few feedstocks and/or pathways for bio-jet fuel. The methodology for WTWa emissions calculation is split into WTP and PTWa as separate models, or estimation procedures are required. The methodology for estimating WTP and PTWa is discussed separately in §2.1 and §2.2, respectively. It is to be noted that for both 100% SPK and LH_2, all feedstocks and manufacturing pathway combinations that are available in GREET model are explored in this work. The latest version of the GREET model is available both in .NET framework and as Excel Spreadsheet from resource [69]. The version of the GREET model used in this work is available in resource [70] [email registration is required before it can be downloaded] and it is also provided as a supplementary information file.
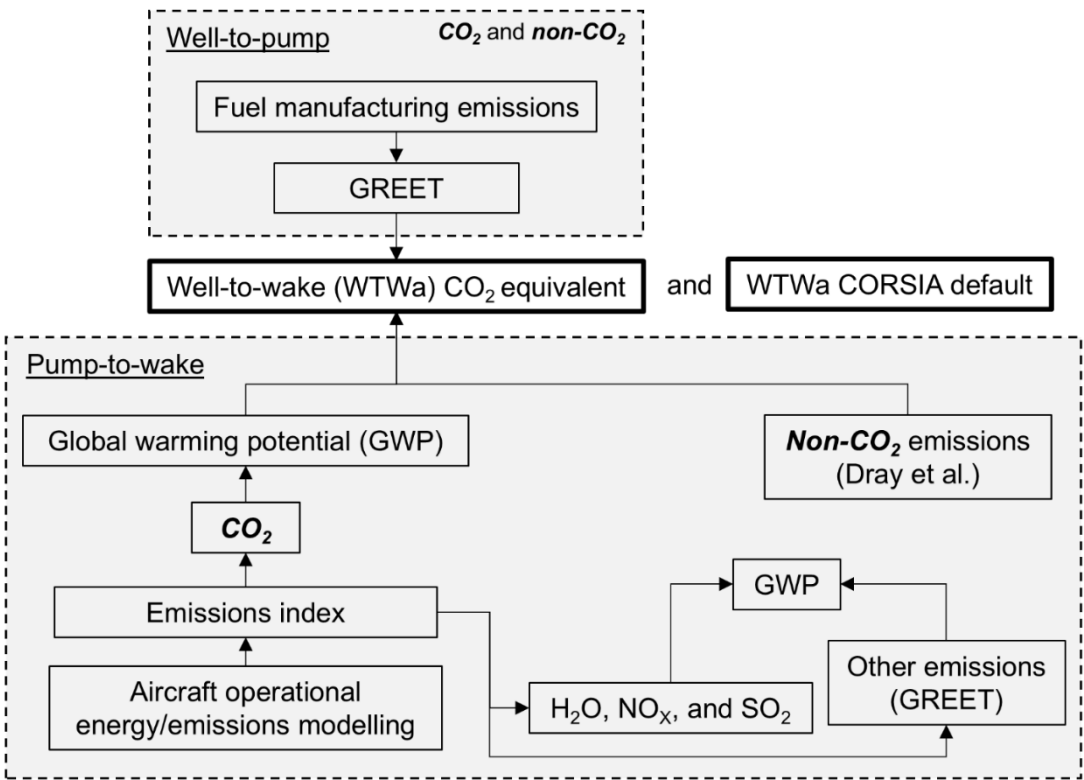

Figure 1. Schematic of WTWa emissions calculation process from WTP and PTWa emissions.

2.1. Well to Pump Emissions

Referring to Figure 1, the GREET model is used for making a database of fuel manufacturing phase emissions for LH_2 and 100% SPK (bio-jet fuel and PtL). The different processes of manufacturing LH_2 and 100% SPK routes are reviewed/discussed in SI §2. The GREET model is documented extensively in literature (report, articles, manual, etc.) and the list of publications can be found in resource [71]. It is to be noted that the GREET model is USA specific, and thus is a limitation of this work. For both LH_2 and 100% SPK, a wide range of manufacturing pathways and/or feedstocks are examined. For a fuel under consideration, not all feedstocks and/or pathways are considered for whole WTWa analysis. Most feedstocks and/or pathways are screened out based on their WTP performance for computational compactness and ease. Additionally, a few parameters are identified from literature to which the WTP emissions are sensitive, and these parameters are varied in GREET, for each fuel type under examination, and these are detailed next. It is to be noted that GREET model includes all emissions in WTP phase including transportation of products/raw materials and indirect emissions (land use change).

2.1.1. Liquid Hydrogen

Table 1 lists the different feedstock and/or pathways for producing hydrogen at centralised manufacturing unit with or without carbon sequestration facility and type of liquefication used. There are in total 59 different ways to produce LH_2 from centralised manufacturing units in the USA as simulated, using GREET model [8].

There are two assumptions/models for hydrogen production in GREET: (a) H2A model of National Renewable Energy Lab, USA (b) Industry data. 59 cases (and Jet-A) are simulated for both hydrogen production assumptions, wherever applicable and available. For example: Industry data assumptions are applicable/available in GREET for all 59 cases except four cases: (a) North American natural gas (NANG) with carbon sequestration (w CS) and hydrogen liquefaction using US mix electricity (LUSME); (b) renewable natural gas (RNG) w CS LUSME; (c) NANG w CS and liquification using power from natural gas combined cycle (LNGCC); (d) RNG w CS LNGCC. Similarly, H2A model assumptions are applicable/available in GREET for all 59 cases except 18 cases: six feedstocks each (willow, poplar, switchgrass, corn stover, forest residue, and miscanthus) for biomass manufacturing plant type w CS for both LUSME type and hydrogen liquefied using electricity from biomass integrated gasification combined cycle (LBIGCC), and six feedstocks (same as above) with integrated fermentation manufacturing plant type w CS.

In the results section (§3), for each of the 59 manufacturing cases, the sensitivity of the selection of model assumptions (H2A or industry data) is reflected as a range of values. This is the first sensitivity parameter. Additionally, each of the 59 manufacturing cases (and Jet-A) with respective manufacturing model assumptions is simulated for year 2020 and 2050. This is essentially to check the sensitivity of US energy mix, the second sensitivity parameter, on LH_2 WTWa emissions. The energy mixes for both 2020 and 2050 are listed in Table 2. According to Table 2, the USA energy mix in 2050 is expected to be dominated by more renewable energy sources, especially solar energy (photovoltaics [PV]). The objective of this work is to find (fuel) feedstock and pathway combinations that enable climate neutral long-range flight. Thus, after examining 59 cases, only LH_2 manufacturing options that provide near-zero and/or negative CO_2 equivalent emissions are considered for further WTWa analysis.

Table 1. List of different feedstocks and/or pathways of producing hydrogen at centralised manufacturing unit with or without carbon sequestration facility and type of liquefication used.

Type of LH_2	Pathways/Feedstock	Carbon sequestration (CS)	Liquefication type
Grey	Coal	Without (w/o) CS	Liquefied using US mix electricity (LUSME) Liquification using electricity from coal

	Feedstock	Biomass subtype	CS	Process
Blue	Coke oven gas (COG)		With (w) CS	integrated gasification combined cycle (LCIGCC)
				LUSME LCIGCC
			-	LUSME LCIGCC LUSME
	North American Natural Gas (NANG)		w/o CS	Liquefication using power from natural gas combined cycle (LNGCC)
				LUSME LNGCC
			w CS	LUSME LNGCC
	H$_2$ as a by-product of natural gas liquid (NGL) steam cracking (SC)		-	LUSME
	Renewable natural gas (RNG)		w/o CS	LUSME LNGCC
			w CS	LUSME LNGCC
			-	LUSME
	Solar photovoltaics (PV)		-	Liquefication using electricity from solar energy (L-Solar)
	Nuclear thermochemical cracking of water (TCCW)		-	Liquefication using electricity from nuclear energy (L-Nuclear)
	Nuclear high temperature gas reactor (HTGR)		-	LUSME L-Nuclear
Green	Biomass	Willow Poplar Switchgrass Corn stover Forest residue Miscanthus	w/o CS	LUSME
	Biomass	Willow Poplar Switchgrass Corn stover Forest residue Miscanthus		Liquification using electricity from biomass integrated gasification combined cycle (LBIGCC)
	Biomass	Willow Poplar Switchgrass Corn stover Forest residue Miscanthus	w CS	LUSME
	Biomass	Willow Poplar Switchgrass Corn stover Forest residue Miscanthus		LBIGCC
	Integrated fermentation (IF) (Biomass)	Willow Poplar Switchgrass Corn stover Forest residue Miscanthus	w/o CS	LUSME
		Willow Poplar Switchgrass Corn stover Forest residue Miscanthus	w CS	

High temperature electrolysis with solid oxide electrolysis cell (HTE SOEC) using electricity from Nuclear HTGR for electrolysis	-	
HTE SOEC using electricity from natural gas combined cycle (NGCC) for electrolysis		LUSME
H_2 produced as a by-product of chlorine manufacturing plant (By-product Cl plant)		

Table 2. US energy mix in 2020 and 2050 – share of different energy sources for electricity production (stationary use).

2020 USA energy mix [8]				2050 USA energy mix [72]			
Source	%	Others source	%	Source	%	Others source	%
Residual oil	0.4	Hydroelectric	38.1	Residual oil	0.0%	Hydroelectric	13.0%
Natural gas	39.6	Geothermal	2.1	Natural gas	36.0%	Geothermal	2.0%
Coal	20.0	Wind	45.9	Coal	11.0%	Wind	34.0%
Nuclear power	20.4	Solar PV	11.4	Nuclear power	11.0%	Solar PV	47.0%
Biomass	0.3	Miscellaneous	2.5	Biomass	0.0%	Miscellaneous	4.0%
Others	19.4			Others	42.0%		

2.1.2. 100%. Synthetic Paraffin Kerosene

2.1.1.1. Preliminary Shortlisting of Feedstocks and Pathways

In this section, four SPK fuel pathways are examined using the GREET model, where the 100% SPK fuel is produced from different feedstocks and manufacturing schemes. These are ATJ, STJ, HRJ or HEFA, and FT. For each of the four SPK fuel pathways, different feedstocks and manufacturing schemes are evaluated. Table 3 and Table 4 list different feedstocks and manufacturing schemes for 100% SPK produced from ATJ (18 cases) and STJ (24 cases), and FT (eight cases) and HEFA (four cases each of food and non-food crops) pathways, respectively.

For HEFA, though there are eight feedstocks in total that are considered purely as an academic exercise in Table 4, only four non-food crops will be considered as feedstocks for fuel production in this work for further consideration. This arises from social concerns of using food crops for fuel production. In total there are 54 different ways (58 ways if food crops are included) in which 100% SPK can be produced using the above four pathways and feedstock combinations. These 54 manufacturing options are examined and only the options that provide lowest or negative CO_2 equivalent emissions for each of the four pathways are considered for sensitivity analysis (discussed next) and further WTWa analysis.

Table 3. List of different feedstocks and manufacturing schemes for 100% SPK produced from ATJ and STJ pathways.

ATJ schemes and feedstocks (18 cases)		STJ schemes and feedstocks (24 cases)	
Feedstocks in standalone (S.) scheme	Feedstocks in distributed (D.) scheme	STJ manufacturing schemes	Feedstocks for each of the four STJ manufacturing schemes
Corn with dry mill (CDM)	Corn US mix (CUSM)	Biological plant type (B.)	Poplar
Poplar	Corn dry mill without extraction (CDMWOE)	Catalytic with external H_2 plant type (CWEH.)	Forest residue
Forest residue	Corn dry mill with extraction (CDMWE)	Catalytic with in-situ H_2 plant type (CWIH.)	Miscanthus
Miscanthus	Corn wet mill (CWM)		Switchgrass
Switchgrass	Poplar		Willow
Willow	Forest residue	Catalytic with H_2 from biomass gasification plant type (CWHBG.)	
	Miscanthus		
	Switchgrass		
Corn stover	Willow		Corn stover
	Corn stover		
	Solid waste		

Table 4. List of different feedstocks and manufacturing schemes for 100% SPK produced from FT and HEFA pathways.

FT feedstocks (8 main cases)	HEFA feedstocks (8 cases)
North American (NA) natural gas (NANG),	Food-crops
Non-NA natural gas (non-NANG)	Soybean
Non-NA flared gas (non-NAFG)	Palm FFB (fresh fruit bunch)
Biomass*	Canola
Coal	Corn oil
Coal (50%) + biomass* (50%) (share by mass)	Non-food feedstocks
Natural gas (50%) + biomass* (50%) (share by mass)	Algae
Electro-fuel (or PtL)	Camelina
*Poplar, forest residue, miscanthus, switchgrass, willow, corn stover	Jatropha
	Carinata

2.1.2.2. Manufacturing Emissions Sensitivity to Identified Parameters

According to the study by Pavlenko et al. [67], hydrogen is one of the important component required in the SPK fuel manufacturing process and therefore it contributes significantly to the life cycle GHG emissions of SPKs, especially for HEFA and STJ pathways. Additionally, the use of green hydrogen for producing SPKs could be useful to reduce the life cycle greenhouse gas emissions [67]. From the exercise on LH_2 discussed in §2.1.1, the feedstocks/pathways that enable a near-zero or negative emissions fuel production are used for this sensitivity analysis. For example, if solar-PV and biomass routes of hydrogen production are shortlisted via the approach detailed in §2.1.1, then these routes will be used for producing the required hydrogen in the manufacturing process of a given SPK pathway. In the results section (§3), for each of the shortlisted SPK fuel manufacturing case, the sensitivity of the hydrogen production route for manufacturing SPK fuel, is reflected as a range of values. The hydrogen production route for manufacturing SPK fuel is the first sensitivity parameter.

Additionally, similar to the exercise for LH_2, the WTP emissions for SPKs are simulated for year 2020 and 2050 (more renewable energy sourcing), and this is useful in the estimation of the sensitivity of US energy mix, the second sensitivity parameter, on 100% SPK WTWa emissions.

2.2. Pump to Wake Emissions

In the authors' previous studies [15,16], the engine (ultrahigh bypass ratio geared turbofan) and aircraft operational energy performance modelling of a 2030+ (N+2 timeframe) BWB LTA aircraft powered by Jet-A, LH_2, and 100% SPK (separately) are conducted. For the LH_2 aircraft, the penalties due cryogenic tank installation are modelled. The Jet-A, LH_2, and 100% SPK aircraft operational performance enables the estimation of emissions in the aircraft use-phase. Additionally, the engine cycle parameters required for PTWa emissions modelling are known for the aircraft from authors' previous study [15]. The PTWa emissions estimation process for the BWB aircraft (Jet-A, 100% SPK, and LH_2) modelled in [15,16] is considered next. It is to be noted that these prior studies model the engine and aircraft using low order modelling methods, therefore the emission modelling would be at a low fidelity level. The reader is advised to explore studies [73–76] for high order modelling of non-volatile particulate matter, NO_x, carbon monoxide, and hydrocarbon emission, especially for Jet-A fuel.

2.2.1. Oxides of Nitrogen

In the authors' previous study [15], the use of the lean direct injection (LDI) combustor type in the BWB aircraft (Jet-A, 100% SPK, and LH_2) is discussed. In terms of oxides of nitrogen (NO_x) emission modelling for this combustor, the emission index (EI) estimation process for NO_x is known from the study by Marek et al. [77], which is based on experiments conducted by NASA. The $EI_{NOx,Jet-A}$ (grams NO_x per kg fuel) i.e., emissions index for Jet-A LDI combustor is given by equation 1 (source [77]),

$$EI_{NOx,Jet-A} = A'(143P_3)^{0.594}e^{\left((T_3-255)/194\right)}\left(\frac{f}{a}\right)^{1.6876}\left(100\frac{\Delta P}{P}\right)^{-0.56}, \tag{1}$$

where A', P_3 (MPa), T_3 (K), $\frac{f}{a}$, and $\frac{\Delta P}{P}$ (%) are correlation constant for emission index based on Jet-A fuel, combustor inlet pressure, combustor inlet temperature, fuel to air ratio, and fuel injector air flow pressure drop ratio, respectively. A' is 14 for advanced LDI technology, and P_3, T_3, and $\frac{f}{a}$ are known from authors' previous study [15] (GasTurb engine modelling for engines powered by different fuels). A nominal value of 4% for $\frac{\Delta P}{P}$ is used for the combustor design (for both Jet-A and hydrogen) as reported by Marek et al. [77] and is used in this work for NOₓ modelling. It is assumed in this work that equation 1 is also applicable to 100% SPK, and respective P_3, T_3, and $\frac{f}{a}$ are used (known from authors' previous study [15]).

For hydrogen, C4 type of LDI combustor configuration (please refer to authors' previous study [15] for details about all configurations) is used in this work for emissions modelling, as according to Marek et al. [77], it was the only configuration that performed the best from a low NOₓ and durability criteria. For hydrogen, NOₓ is estimated in terms of parts per million (ppm) i.e. ppm_{NOx}, in the study by Marek et al. [77]. The calculation of ppm_{NOx} for hydrogen LDI combustor is given by equation 2 (source [77]),

$$ppm_{NOx} = A(143P_3)^a\left(\phi_{H_2}\right)^b(\tau)^c e^{\left((1.8T_3-460)/d\right)}\left(\frac{\Delta P}{P}\right)^e, \tag{2}$$

where A, a, b, c, d, and e are correlation constants for emission index based on hydrogen data, and ϕ_{H_2} and τ are hydrogen equivalence ratio and combustor residence time, respectively. For C4 configuration, the values of A, a, b, c, d, and e are known to be 9.355, 0.275, 4.12, 0.455, 211, and -0.288, respectively. ϕ_{H_2} is calculated from the fuel to air ratio according to the definition in authors' previous study [15]. The fuel to air ratio and τ are known from authors' previous study [15] (GasTurb engine modelling). The generic equation for the estimation of EI_{NOx} from ppm_{NOx} is given by equation 3 (source [77]),

$$EI_{NOx} = \frac{1}{1000}\,\frac{MW\ of\ NO_2}{MW\ of\ combustion\ products}\,\frac{(1+f/a)}{f/a}\,ppm_{NOx} \tag{3}$$

where MW is the molecular weight for respective species. The MW of NO_2 is 46 and for the combustion products it is calculated using the 'major species' combustion model as described in authors' previous study [15]. Therefore, once ppm_{NOx} is calculated using equation 2, the EI_{NOx} can be estimated using equation 3 for a given fuel case where the f/a is known.

It is to be noted that equations 1 and 2 that estimate NOₓ are applicable to typical temperature and pressure combination during cruise, according to Marek et al. [77]. Therefore, using equation 1, and equations 2 – 3 the cruise EI_{NOx} for Jet-A (and 100% SPK) and LH₂ aircraft can be calculated, respectively.

For estimating EI_{NOx} at other points in the flight mission, the 'DLR fuel flow correlation' method [78] is used which is dependent on pressure, temperature, and Mach number, for respective flight segment. After calculating cruise EI_{NOx}, the EI_{NOx} at sea level static (SLS) ($EI_{NOx,SLS}$) point can be calculated using the DLR method, where both EI_{NOx} are related by parameters that depend on flight altitude, ambient pressure and temperature, and flight Mach number. Thus, now knowing the $EI_{NOx,SLS}$, the EI_{NOx} at other flight points like engine start and warm up, taxi out, take-off, climb, descent and approach, loiter, landing, taxi in, and shutdown, can be calculated knowing the respective flight altitude, ambient pressure and temperature, and flight Mach number. The relation between $EI_{NOx,SLS}$ and EI_{NOx} at other flight points is given by equation 4,

$$EI_{NOx} = EI_{NOx,SLS}\,\delta_{total}^{0.4}\,\theta_{total}^3 e^H, \tag{4}$$

$$\text{where } \delta_{total} = \frac{p_{total}}{101325\ Pa}, \tag{5}$$

$$\theta_{total} = \frac{T_{total}}{288.15\ K}, \tag{6}$$

$$H = -19\left(-0.00634 + 0.001\ e^{-0.0001426\left(h'-12900\right)}\right), \tag{7}$$

$$p_{total} = p_{amb}\left(1 + \frac{(\Upsilon-1)}{\Upsilon}M^2\right)^{\Upsilon/(\Upsilon-1)},\ \text{and} \tag{8}$$

$$T_{total} = T_{amb}\left(1 + \frac{(\Upsilon-1)}{\Upsilon}M^2\right). \tag{9}$$

p_{amb}, p_{total}, T_{amb}, T_{total}, M, Υ, δ_{total}, θ_{total}, $EI_{NOx,SLS}$, H, and h' are ambient pressure (in Pa), total pressure (in Pa), ambient temperature (in K), total temperature (in K), flight Mach number, specific heat ratio (1.4 for air), pressure correction factor, temperature correction factor, NO_x emission index at SLS, humidity correction factor, and flight altitude (in feet), respectively.

The breakdown of mission fuel burn or block fuel ($W_{F,block}$, in kg) for Jet-A, 100% SPK, and LH_2 (case 3) is known from the authors' previous study [16] at different flight segments such as engine start and warm up, taxi out, take-off, climb, cruise descent and approach, loiter, landing, taxi in, and shutdown. After calculating EI_{NOx} for these segments, the quantity of NO_x (kg) emitted can be calculated. Table SI 6 (in SI §3) lists the engine parameters required to estimate EI_{NOx} during cruise (in equations 1 – 3) for different fuel cases. Table SI 7 (in SI §3) provides the operational conditions and fuel burn for different fuels at various flight segments needed for estimating EI_{NOx} (using equations 4 – 9). For estimating the speed of the aircraft during taxi out (20 knots [79]), take-off (150 knots [80,81]), descent (average descent 250 knots [80]), and landing (155 knots approach-landing speed [80,82]), the speed of present-day LTA aircraft are used (values in SI system in Table SI 7 (in SI §3)).

2.2.2. Carbon Dioxide, Water Vapour, Sulphur Dioxide, Other Emissions, and Contrails

Table SI 8 (in SI §3) lists the emission index of different species and contrails for the three fuels under consideration. CO_2, H_2O, and sulphur dioxide (SO_2) emission vary linearly with fuel burn. The production of species like volatile organic compounds (VOC), carbon monoxide (CO), particulate matter 10 and 2.5 (PM_{10} and $PM_{2.5}$ respectively), oxides of sulphur (SO_x) (total), black carbon (BC), organic carbon (OC), methane (CH_4), and nitrous oxide (N_2O), after Jet-A and 100% SPK fuel combustion is not linearly dependent on fuel burn and its estimation requires detailed combustion physics-based modelling. It is to be noted that the impacts of non-CO_2 emissions, especially contrails, vary by region, altitude, humidity, time of the day, etc. Non-CO_2 emissions are uncertain, and difficult to quantify, and depend on type of technology and fuel used – they are not linearly dependent on the fuel burn.

Future LDI combustors are expected to have significantly lower emission indices for these species. In this work, it is assumed that the emission index for these species in the future (N+2 timeframe) BWB remains similar to the present-day emission index listed in Table SI 8 (in SI §3) for LTA aircraft. Similarly, contrail modelling requires detailed physics-based simulation which should capture the effects of nucleation particles and/or lubrication oil from the aircraft engine acting as nuclei for ice formation, presence of nucleation particles in atmosphere (concentration expected to vary with time), and interaction of engine wake and wing-tip vortices. In this work, for aircraft's operational phase (PTWa) though all non-CO_2 emissions are calculated except for contrails, the CO_2 equivalent for the total non-CO_2 emissions (in g/MJ) for Jet-A, 100% SPK or SAF, and LH_2 reported by Dray et al. [51] is used directly. The CO_2 equivalent of the total non-CO_2 emissions during aircraft's operational phase for Jet-A, 100% SPK or SAF, and LH_2 are 9.4 – 54 g/MJ, 6 – 47 g/MJ, and 11 – 68 g/MJ, respectively [51].

2.3. Global Warming Potential

Table SI 9 (in SI §3) lists the global warming potential (GWP) of NO_x and H_2O at different mission segments. The GWP of NO_x increases from a negative value at zero altitude to a positive value at 11 km altitude [83]. A study by Svensson [83] provides the variation of GWP of NO_x and H_2O with altitude. The GWP of H_2O is zero until 9 km (from zero altitude) and increases thereafter. For cruise, the most recent GWP values for NO_x and H_2O from the study by Lee et al. [2] are used in this work and are listed in Table SI 9 (in SI §3). At zero and low altitudes (< 2 km), the GWP of NO_x provided by GREET model [8] is used here. For altitude between 2 km and 10.67 km (cruise), the NO_x GWP provided in a study by Svensson [83], is used in this work. Table SI 10 (in SI §3) provides the GWP of all emissions in the WTP and PTWa phase.

2.4. Other Unintended Environmental and Social Impacts

In addition to the CO_2 and non-CO_2 effects of aircraft on climate, there are other metrics that should be considered and quantified. These include the use of fossil fuels, water consumption, and WTWa emissions that affect air-quality. The emissions that are considered include VOC, CO, NO_x, PM_{10}, $PM_{2.5}$, SO_x, BC, and OC. These emissions affect both the environmental and human health. It is assumed that the emission index for VOC, CO, PM_{10}, $PM_{2.5}$, SO_x, BC, and OC for the future (N+2 timeframe) BWB remains similar to the present-day emission index listed in Table SI 8 (in SI §3) for LTA aircraft. The use of fossil fuels (natural resource) has an environmental impact, and water consumption has both environmental and social impact. The WTWa data for VOC, CO, PM_{10}, $PM_{2.5}$, SO_x, BC, and OC is directly obtained from GREET model. WTWa NO_x is calculated from WTP NO_x obtained from GREET, and PTWa NO_x calculated from methodology described in §2.2.1. The data for use of fossil fuels and water consumption is directly obtained from GREET model.

2.5. Future Worldwide Energy Demand and Supply of Sustainable Aviation Fuel and Green Hydrogen

The total Jet-A fuel consumption for 2024/25 is known to be 14.04 EJ from IATA [84] and Boeing's CASCADE tool [85]. Long-haul aviation contributes to 37% [86] – 43% [87] of the total aviation fleet CO_2 emissions. Therefore, the energy demand for long-haul aviation is presently 37% – 43% of 14.04 EJ. In this work, the energy demand for long-haul aviation in 2050 is calculated for two traffic growth rate cases i.e. 3% and 5% compound annual growth rate (CAGR). For this calculation, it is assumed that the share of energy demand of long-haul aviation to total aviation energy demand will stay constant in future (i.e. 37% – 43%).

The quantification of future supply potential of SPK or SAF is conducted using data available from Boeing SAF dashboard [88] and Air Transport Action Group (ATAG) report [89]. Boeing SAF dashboard provides global SAF supply potential until 2035, and it provides data for operational manufacturing unit along with other plant types such as planned, aspirational, final investment decision, under construction, and pending final investment decision. ATAG report provides global SAF supply potential for 2050, for three supply scenarios.

Similarly, the quantification of future supply potential of green hydrogen is carried out using data available from the International Energy Agency (IEA) hydrogen dashboard [90], McKinsey report [91], and ATAG report [89]. The IEA hydrogen dashboard provides hydrogen supply until 2030 for different manufacturing plant types, where low-carbon hydrogen is produced from electrolysis, fossil fuel with carbon capture, utilization and storage, and other routes. These manufacturing plant types include conceptual, demonstration projects, feasibility study, under construction and operational plants. McKinsey report provides four supply scenarios. Lastly, ATAG report provides global hydrogen supply potential for 2050, for three supply scenarios. It is to be noted that the effect of different supply scenarios of SAF and hydrogen is considered in this work via a range of energy supply values for each fuel.

3. Results and Discussion

3.1.1. Well to Wake Emissions for Liquid Hydrogen

Figure 2 shows the WTWa comparison of different LH$_2$ feedstocks and/or pathways (59 manufacturing cases) for 2020 and 2050 US energy mix (with only CO$_2$ emissions in PTWa phase). In this figure, for the WTP stage all greenhouse gas emissions are considered but for PTWa only CO$_2$ emissions are included. The non-CO$_2$ emissions are included later in §3.1.3. As discussed in §2.1.1, sensitivity to two parameters is analysed. For each of the 59 manufacturing cases, the sensitivity of the selection of model assumptions (H2A or industry data) is reflected as a range of values. This is the first sensitivity parameter.

Additionally, each of the 59 manufacturing cases (and Jet-A) with respective manufacturing model assumptions is simulated for both 2020 and 2050 to check the sensitivity of US energy mix - the second sensitivity parameter, on LH$_2$ WTWa emissions.

It can be observed from Figure 2 that grey and blue hydrogen WTWa emissions are of the similar magnitude as that of Jet-A or more, regardless of the hydrogen production assumptions used or the energy mix type. Additionally, not all green hydrogen manufacturing cases have near zero or sub-zero WTWa CO$_2$ equivalent emissions. Certain manufacturing schemes like IF w/o CS, HTE SOEC – NGCC, and By-prod Cl plant have higher WTWa CO$_2$ equivalent emissions than Jet-A. This can be attributed to the low manufacturing efficiency resulting in higher WTWa GHG emissions.
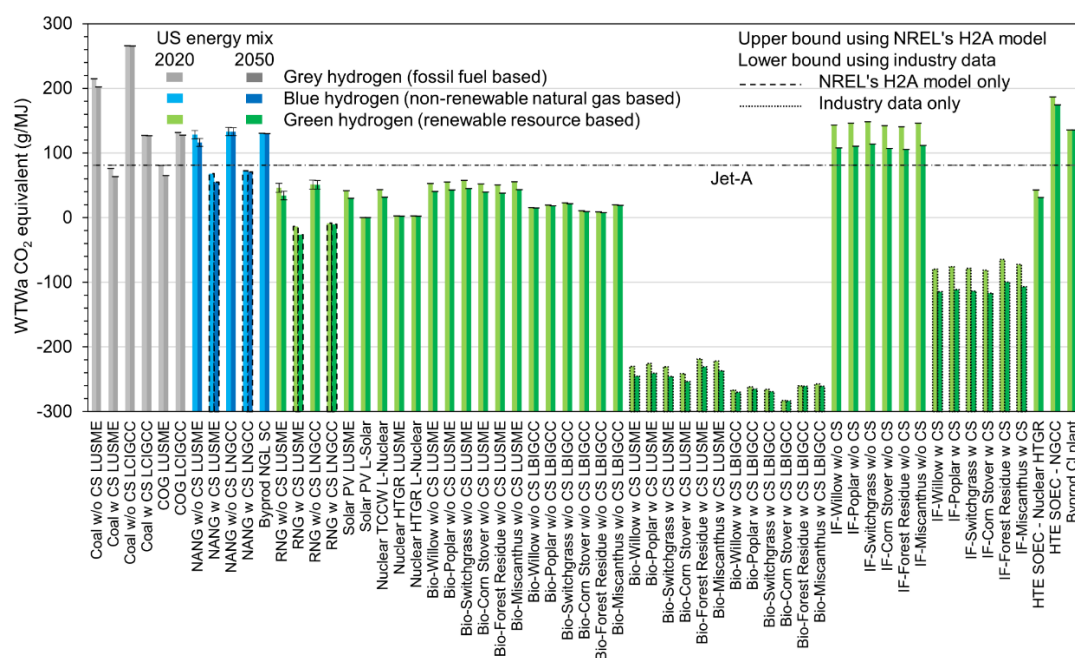

Figure 2. WTWa comparison of different LH$_2$ feedstocks and pathways for 2020 and 2050 (with only CO$_2$ emissions in PTWa phase). **[w/o: without; w: with; CS: Carbon sequestration; LUSME: liquification using US mix of electricity; COG: Coke oven gas; LCIGCC; Liquification using electricity from coal integrated gasification combined cycle; NANG: North American natural gas; LNGCC: Liquification using power from natural gas combined cycle; NGL: Natural gas liquid; SC: Stream cracking; RNG: Renewable natural gas; L-liquification; PV: Photovoltaic; TCCW: Thermochemical cracking of water; HTGR: high temperature gas reactor; LBIGCC: Liquefied using electricity from biomass integrated gasification combined cycle; IF: Integrated fermentation; HTE: High temperature electrolysis; SOEC: Solid oxide electrolysis cell; NGCC: Natural gas combined cycle].**

As discussed in §2.1.1, only the LH$_2$ manufacturing options that provide near-zero and/or negative CO$_2$ equivalent emissions are considered for further WTWa analysis (including non-CO$_2$ emissions in PTWa). The LH$_2$ manufacturing cases that have near-zero and/or negative CO$_2$ equivalent emissions are RNG w CS LUSME, RNG w CS LNGCC, solar PV L-solar, nuclear HTGR LUSME, biomass w/o CS LBIGCC, biomass w CS LUSME, biomass w CS LBIGCC, and IF w CS. These

eight cases will be considered for further WTWa analysis in §3.1.3, which includes non-CO_2 emissions in PTWa.

3.1.2. Well to Wake Emissions for 100% Synthetic Paraffin Kerosene

3.1.2.1. Preliminary Shortlisting of 100% Synthetic Paraffin Kerosene Feedstocks and Pathways
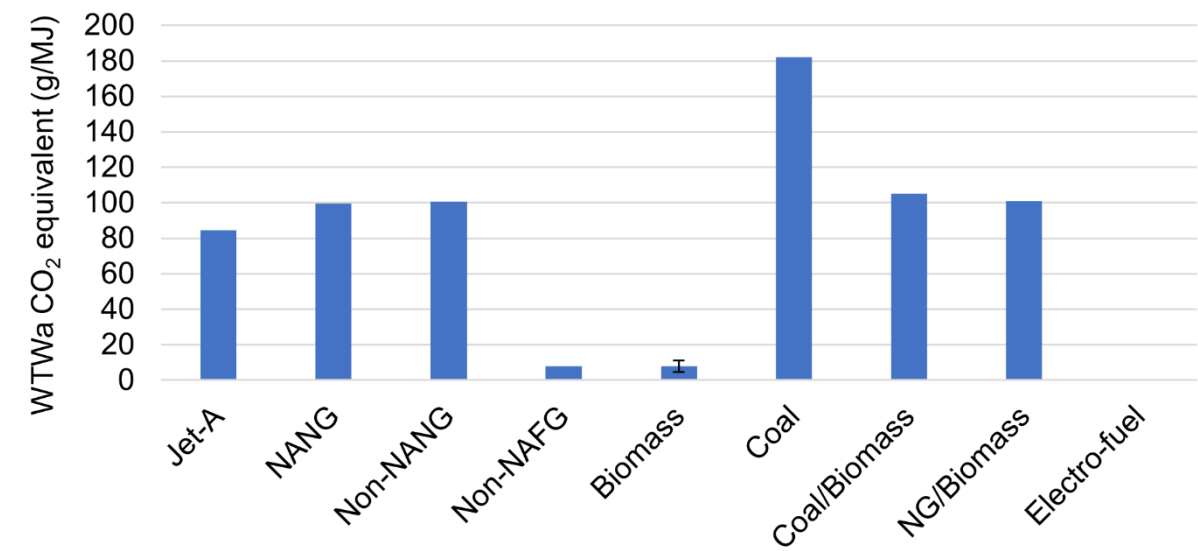

Figure 3. WTWa CO_2 equivalent emission comparison of different FT feedstocks for 2020 (with only CO_2 emissions in PTWa phase). **[NANG: North American natural gas; NAFG: North American flared gas].**
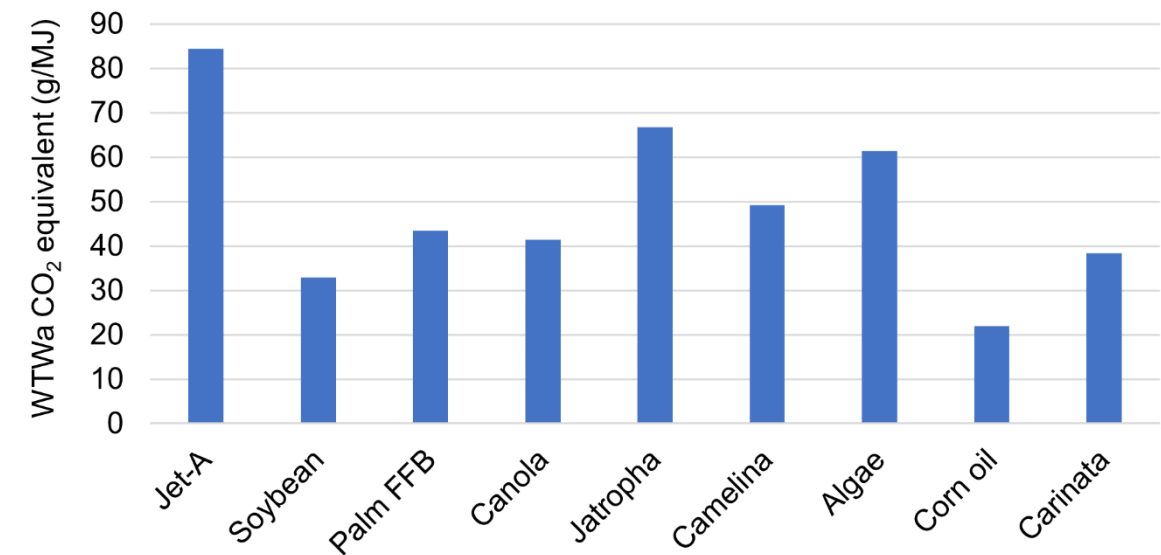

Figure 4. WTWa CO_2 equivalent emission comparison of different HEFA feedstocks for 2020 (with only CO_2 emissions in PTWa phase).
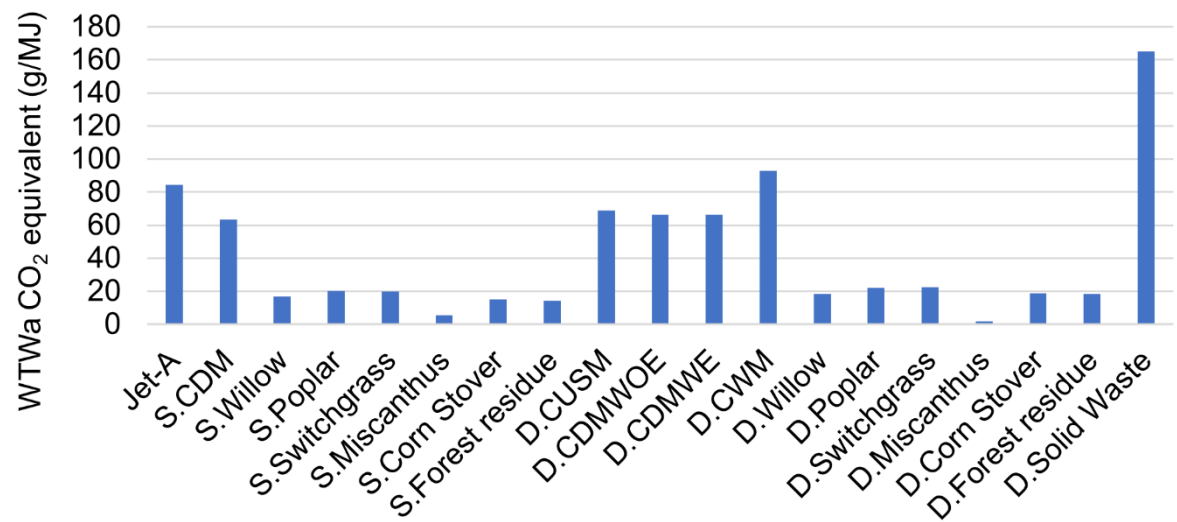
Figure 5. WTWa CO₂ equivalent emission comparison of different ATJ feedstocks for 2020 (with only CO₂ emissions in PTWa phase). **[S; Standalone; CDM: Corn with dry mill; D: Distributed; CUSM: Corn US mix; CDMWOE: Corn dry mill without extraction; CDMWE: Corn dry mill with extraction; CWM: Corn wet mill]**.
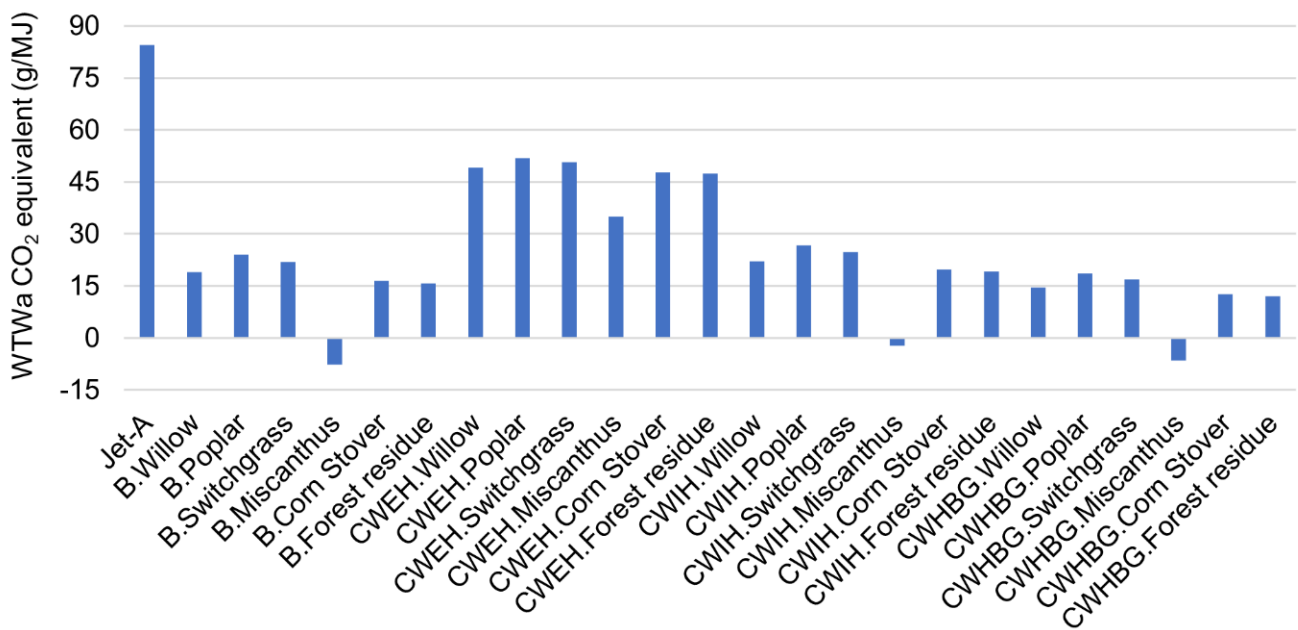

Figure 6. WTWa CO₂ equivalent emission comparison of different STJ feedstocks for 2020 (with only CO₂ emissions in PTWa phase). **[B: Biological; CWEH: Catalytic with external H₂ plant type; CWIH: Catalytic with in-situ H₂ plant type; CWHBG: Catalytic with H₂ from biomass gasification plant type]**.

Figure 3, Figure 4, Figure 5, and Figure 6 provide the WTWa comparison of different FT, HEFA, ATJ, and STJ feedstocks, respectively, for 2020 (with only CO₂ emissions in PTWa phase). It can be observed from Figure 3 that electro-fuel (E-fuel) or PtL, and biomass are the two feedstocks/routes that have lowest (almost zero) WTWa CO₂ equivalent emissions and are shortlisted for further analysis. For the biomass case, six feedstocks are considered that include willow, poplar, switchgrass, miscanthus, corn stover, and forest residue. This is included as a range in Figure 3. Switchgrass has a poor performance whereas forest residue provides a greater reduction in WTWa CO₂ equivalent emissions and is thus considered as the default FT biomass-based feedstock for further analysis.

Similarly, it can be seen from Figure 4 that Carinata is the only non-food crop that has lowest WTWa CO_2 equivalent emissions of all HEFA feedstocks and is thus considered for further analysis. Ideally, corn oil has the lowest emissions but as discussed in §2.1.2 only non-food crops are considered for analysis (due to the social impacts).

Referring to Figure 5, Miscanthus is the feedstock which provides lowest WTWa CO_2 equivalent emissions in both standalone and distributed ATJ production schemes (S.Miscanthus and D.Miscanthus) and are therefore shortlisted for further analysis. Similarly, it can be observed from Figure 6 that Miscanthus provides negative WTWa CO_2 equivalent emissions in three STJ production schemes – biological, catalytic with in-situ H_2 plant type, and catalytic with H_2 from biomass gasification plant type (B.Miscanthus, CWIH.Miscanthus and CWHBG.Miscanthus, respectively), and are thus considered for further analysis. It is to be noted that the above shortlisting of FT, HEFA, ATJ, and STJ feedstock/pathways (for further analysis) also takes into consideration WTWa CORSIA default values (2021) which are included in Table SI 5 (in SI §1). The feedstock/pathways shortlisted from analysis in Figure 3, Figure 4, Figure 5, and Figure 6 have significantly lesser WTWa than the CORSIA data.

3.1.2.2. Manufacturing Emissions Sensitivity to Identified Parameters

From §3.1.1, RNG w CS, Solar PV, Nuclear HTGR, Biomass, and IF (biomass) LH_2 production pathways are found to provide near-zero or sub-zero WTWa CO_2 equivalent emissions. For each of the shortlisted 100% SPK fuel manufacturing cases in §3.1.2.1, the sensitivity of selection of the hydrogen production route (discussed above) and the US energy mix type (year) for manufacturing SPK fuel on the WTWa CO_2 equivalent emissions is analysed.

Figure 7 provides the WTWa comparison of low-carbon 100% SPK feedstocks and pathways for 2020 and 2050 US energy mix scenarios using hydrogen produced from less carbon intense scheme (with only CO_2 emissions in PTWa phase). It can be observed that HEFA (Carinata), miscanthus STJ biological production type, and both ATJ distributed and standalone schemes using miscanthus, are sensitive to the hydrogen manufacturing route. This is because hydrogen input to the production of these 100% SPK routes are greater than other routes for fuel production (i.e., greater dependency on hydrogen), in GREET. Also, it can be observed that for ATJ distributed and standalone schemes using miscanthus, and miscanthus STJ biological production type, the WTWa CO_2 equivalent emissions increase between 2020 to 2050, opposite to the trend observed for other 100% SPK cases. This is primarily due to the higher use of fossil fuels via these routes, and the increased need for fossil fuels in the 2050 US energy mix which otherwise has a greater share of renewable energy as discussed in §2.1.1. The effect of use of fossil fuels is further detailed in SI §4.
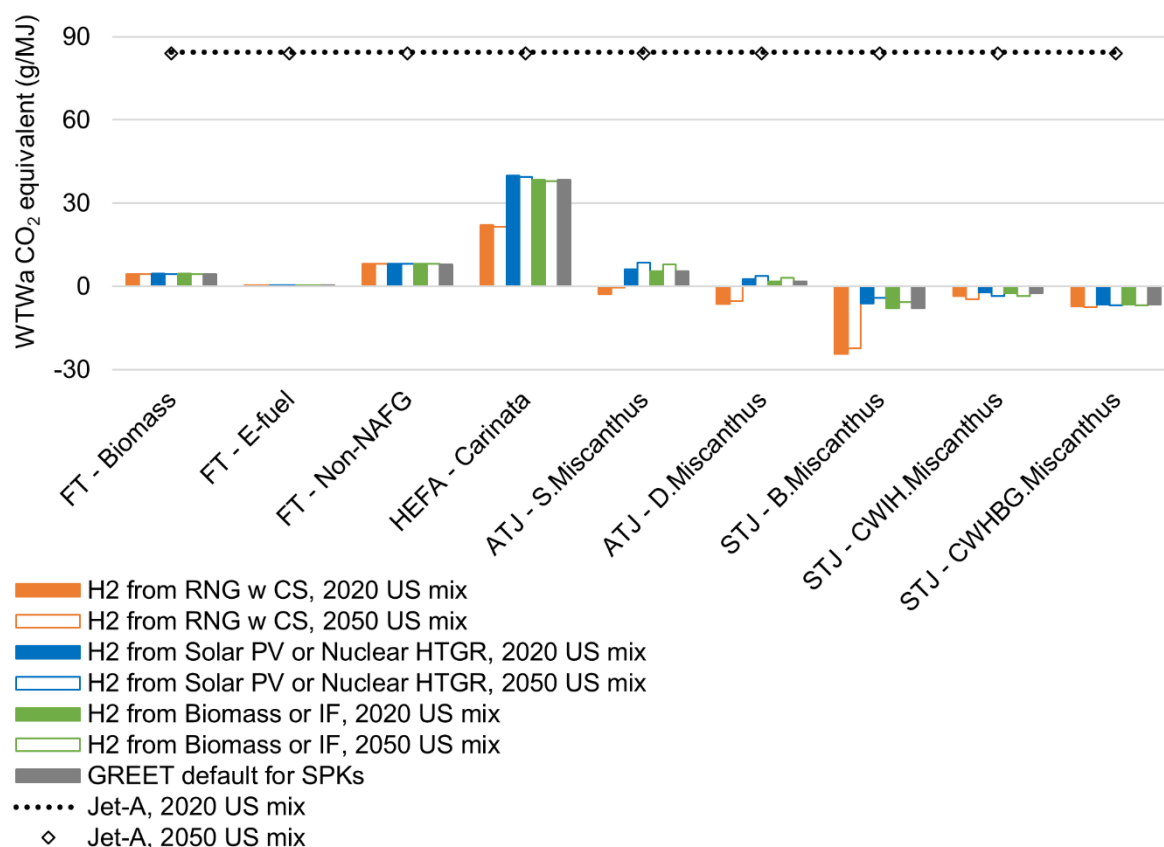
Figure 7. WTWa CO₂ equivalent emission comparison of low-carbon 100% SPK feedstocks and pathways for 2020 and 2050 US energy mix scenarios using hydrogen produced from less carbon intense scheme (with only CO₂ emissions in PTWa phase). **[FT: Fischer Tropsch; NAFG: North American flared gas; D: Distributed; S: Standalone; ATJ: Alcohol to jet; STJ: Sugar to jet; CWIH: Catalytic with in-situ H₂ plant type; Catalytic with H₂ from biomass gasification plant type; RNG: Renewable natural gas; CS: Carbon sequestration; PV: Photovoltaics; HTGR: High temperature gas reactor; IF: Integrated fermentation; SPK: Synthetic paraffin kerosene]**.

3.1.3. Comparative Well to Wake Analysis with Non-CO₂ Emissions

A comparative analysis of PTWa (CO₂ equivalent) NOₓ, H₂O, SO₂ and other emissions (VOC, CO, BC, OC, CH₄ and N₂O) for Jet-A, LH₂ and 100% SPK is provided in Figure SI 13. It is observed that by using an LDI combustor, there is a significant drop in PTWa NOₓ emissions (CO₂ equivalent) for N+2 BWB Jet-A (and 100% SPK) and LH₂ aircraft, compared to present-day LTA aircraft. N+2 BWB (using LDI combustor) Jet-A, 100% SPK, and LH₂ aircraft in use phase (PTWa) show 52%, 54%, and 96% reduction in NOₓ emissions (CO₂ equivalent), respectively, compared to present-day LTA aircraft.

Figure 8 shows the WTWa CO₂ equivalent emission comparison for different LH₂ and 100% SPK feedstock and pathways for 2020 and 2050 US energy mix scenarios with non-CO₂ effects (including contrails). Referring to Figure 8, the error bars in WTP phase reflect a range of values to accommodate a significant variability (in the life cycle emissions) for any given pathway, especially due to the carbon intensity of the sourced feedstock. Also, the error bars in PTWa phase reflect the variability due to non-CO₂ emissions. For LH₂ cases, the error bars in WTP show a range of values arising from the use of different biomass feedstocks. Similarly, for 100% SPK cases, the error bars in WTP phase show a range of values due to the sensitivity because of using hydrogen produced from different low-carbon source for producing 100% SPK (see Figure 7 and discussion).
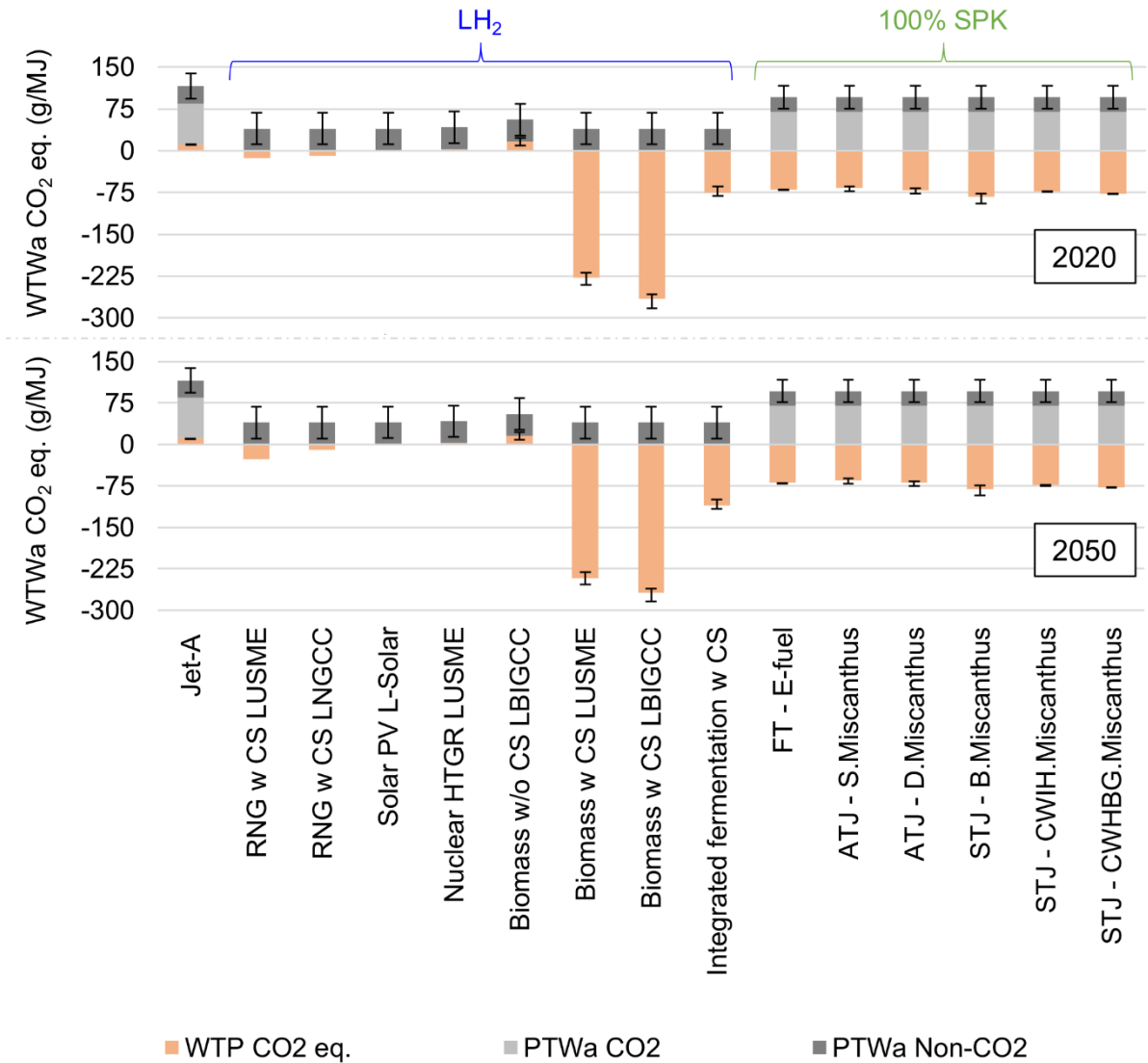
Figure 8. WTWa CO₂ equivalent emission comparison for different LH₂ and 100% SPK feedstock and pathways for 2020 and 2050 US energy mix scenarios including non-CO₂ effects. **[w: with; w/o: without; CS: Carbon sequestration; RNG: Renewable natural gas; LUSME: liquification using US mix of electricity; PV: Photovoltaics; HTGR: High temperature gas reactor; LNGCC: Liquification using power from natural gas combined cycle; LBIGCC: Liquefied using electricity from biomass integrated gasification combined cycle; FT: Fischer Tropsch; D: Distributed; S: Standalone; ATJ: Alcohol to jet; STJ: Sugar to jet; B: Biological; CWIH: Catalytic with in-situ H₂ plant type; CWHBG: Catalytic with H₂ from biomass gasification plant type]**

Table 5 provides a summary of Figure 8 in terms of WTWa GHG emissions (CO₂ equivalent) reduction potential of different LH₂ and 100% SPK feedstock and pathways for 2020 and 2050. It can be observed from Figure 8 and Table 5 that all listed feedstock and pathways of producing LH₂ and 100% SPK could make aviation climate neutral (while considering highest reduction for any case). Particularly, LH₂ fuel can enable net zero or negative WTWa CO₂ equivalent emissions long-range flight of 300 passengers where LH₂ fuel is produced from Biomass w CS LUSME (260.8% – 266.1% reduction), Biomass w CS LBIGCC (296.2% – 302.6% reduction), and/or integrated fermentation (IF) w CS (96.2% – 150.7% reduction), relative to Jet-A. It is to be noted that though the GHG reduction potentials could increase in 2050 (as observed from Table 5), the comparison is made with 2020 numbers.

Table 5. WTWa GHG emissions (CO_2 equivalent) reduction potential of different LH_2 and 100% SPK feedstock and pathways for 2020 and 2050.

Manufacturing route	% reduction relative to Jet-A	
	2020	2050
LH2		
RNG w CS LUSME	41.5 – 101.7	55.7 – 111.3
RNG w CS LNGCC	36.3– 98.2	38.0 – 99.3
Solar PV L-Solar	26.8 – 91.8	26.8 – 91.8
Nuclear HTGR LUSME	24.1 – 90.0	24.6 – 90.3
Biomass w/o CS LBIGCC	2.8 – 85.6	3.6 – 86.1
Biomass w CS LUSME	260.8 – 266.1	274.1 – 275.6
Biomass w CS LBIGCC	296.2 – 302.6	297.4 – 306.2
Integrated fermentation w CS	96.2 – 150.7	133.6 – 176.6
100% SPK		
FT - E-fuel	49.2 – 95.4	49.3 – 95.4
ATJ - S.Miscanthus	43.1 – 97.7	40.5 – 96.0
ATJ - D.Miscanthus	46.9 – 100.3	45.7 – 99.6
STJ - B.Miscanthus	56.4 – 113.3	54.1 – 111.8
STJ - CWIH.Miscanthus	52.1 – 92.1	53.4 – 99.0
STJ - CWHBG.Miscanthus	56.7 – 100.9	57.0 – 101.1

Additionally, the effect of carbon sequestration on LH_2 WTWa emissions can be observed from Table 5. In 2020, biomass LBIGCC without and with carbon sequestration show 2.8% – 85.6% and 296.2% – 302.6% reduction in WTWa GHG emissions, which is a significant impact. The of low carbon fuels and carbon capture which are few of IATA's decarbonization strategies, are observed to be simultaneously employed in the case of Biomass w CS LUSME.

Moreover, it can be observed from Figure 8 that on an average the WTWa CO_2 equivalent emissions of 100% SPK long-range (BWB) flight of 300 passengers can be reduced by 70% – 85% if the fuel is produced from Miscanthus (depending on manufacturing route such as ATJ/STJ, standalone/distributed, etc.). This is similar to the observations made by Afonso et al. [23] and Song et al. [33] bio-jet fuel can reduce WTWa GHG emissions by up-to 80% (with non-CO_2 emissions), compared to Jet-A. The authors acknowledge that life cycle emissions for any given fuel and manufacturing pathway could vary significantly, particularly due to the carbon intensity of the feedstock used.

As summarised in §1 via a literature review, the non-CO_2 emissions contribute significantly to WTWa GHG emissions. If these effects are ignored in this work, then all the feedstocks/pathways shortlisted for LH_2 fuel can enable a net negative carbon emission (according to Figure 8). For Jet-A and 100% SPK cases, the PTWa non-CO_2 emissions (g/MJ) are of similar magnitude as that of PTWa CO_2 effects. Moreover, for LH_2 fuel cases, the contribution of non-CO_2 emissions to WTWa emissions are significant, though the net WTWa CO_2 equivalent emission is significantly lesser than Jet-A. The use of only advanced technology and low-carbon fuel (like LH_2) enable near-zero WTWa CO_2 equivalent emissions long-range flight, but these are insufficient strategies to reduce the effect of non-CO_2 emissions such as contrails. Similar to Jet-A aircraft, for LH_2 powered aircraft, operational strategies such as avoiding ice-supersaturated regions to prevent contrail formation could be used [92,93].

The perspective used to select three feedstock and/or pathways for LH_2 fuel identified above only take into consideration the WTWa CO_2 equivalent emissions. However, for commercial aviation, the fuel cost, and the resulting direct operating cost (inclusive of carbon tax exemption) are significant aspects which should be accounted for identifying fuel manufacturing pathways for both LH_2 and 100% SPK. In this work, cost analysis is not conducted. The accuracy of fuel cost analysis depends primarily on the accuracy of simulation of the fuel manufacturing process, year of simulation, government incentives and market penetration of a fuel, and scale of fuel manufacturing and/or fuel manufacturing process technology readiness level. Additionally, there are fuel cost fluctuations due to externalities. For example: economic uncertainties due to pandemic like COVID-19, instability in

Middle Eastern countries, and events such as the 2022 Eastern European conflict directly affect the global energy cost. The aspect of fuel production capacity is addressed in SI §3 (Table SI 11). Additionally, the other unintended environmental and social impacts (fossil fuel use, water consumption, air-quality, etc.) are addressed in SI §4. Overall, the success of LH_2 powered aviation requires appropriate: airport infrastructure, aircraft design, air-traffic or operations management, safety, fuel supply chain/manufacturing efficiency and capacity to meet the required fuel demand, fuel cost and direct operating cost, and policy.

3.1.4. Future Energy Demand for Long-Haul Aviation and Supply of SAF and Green Hydrogen

It is to be noted that the production capacities and supply estimates of different feedstocks and pathways explored in this work for SAF and hydrogen, are not available in literature. In this sub-section, a high-level demand and supply aspect is explored as a feasibility check for the alternative fuels considered in this work.

Figure 9 shows the energy demand forecast for long-haul aviation and supply of SAF. It is to be noted that this analysis (in Figure 9) assumes that all long-haul aviation will be powered by SAF. It can be observed from Figure 9 that the supply of SAF in 2050, considering the uncertainties, would satisfy a 3% CAGR in air-traffic and it might just be enough to support the energy demand for a 5% CAGR in air traffic. It is to be noted that the present air traffic growth rate is 4% [4]. Additionally, the SAF supply is expected to be dominated by PtL and advanced feedstocks as per ATAG.
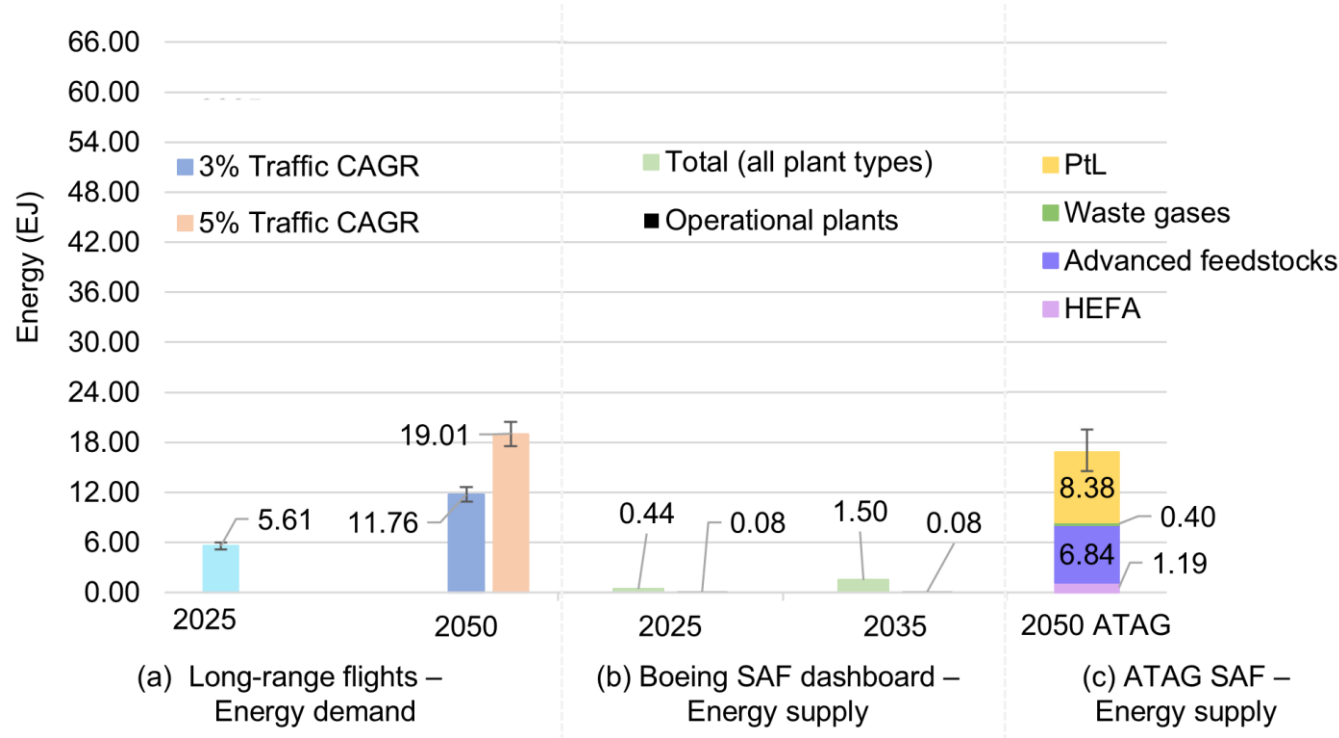

Figure 9. Energy demand forecast for long-haul aviation and supply of SAF. **[HEFA: Hydro-processed esters and fatty acids; PtL: Power to liquid fuel; CAGR: Compound annual growth rate]**

Figure 10 shows the energy demand forecast for long-haul aviation and supply of green hydrogen. It is to be noted that this analysis (in Figure 10) assumes that all long-haul aviation will be powered by hydrogen. It can be observed from Figure 10 that the supply of hydrogen in 2050, considering the uncertainties, would satisfy a 3% CAGR in air-traffic according to ATAG and McKinsey (MK) green hydrogen supply estimates. However, for a 5% CAGR in air traffic, ATAG 2050 supply estimates for hydrogen would support the required energy demand but for MK supply estimates the energy demand might be met with at least current trajectory and/or accelerated production capacities (scenarios are part of the uncertainty band). Furthermore, it is extremely

important to note that these estimates are global estimates and there would be other sectors competing with aviation for hydrogen.

Considering the high-level analysis in this sub-section, the forecasted SAF and hydrogen supply in 2050 can meet the energy demand of long-haul aviation with the present air traffic CAGR of 4% if flights are completely powered by either of the two fuels. An increase in air traffic CAGR (to 5%) and other competing sectors, necessitates ramping up of production capacities, especially for hydrogen. Alternatively, some of the long-haul flights could be powered with SAF and some with hydrogen, such that the energy supply easily meets the required energy demand while the energy demand from other sectors are satisfied simultaneously. In any scenario, to enable a climate neutral long-haul aviation, the production capacities of SAF and hydrogen should be increased than the existing production trajectories.
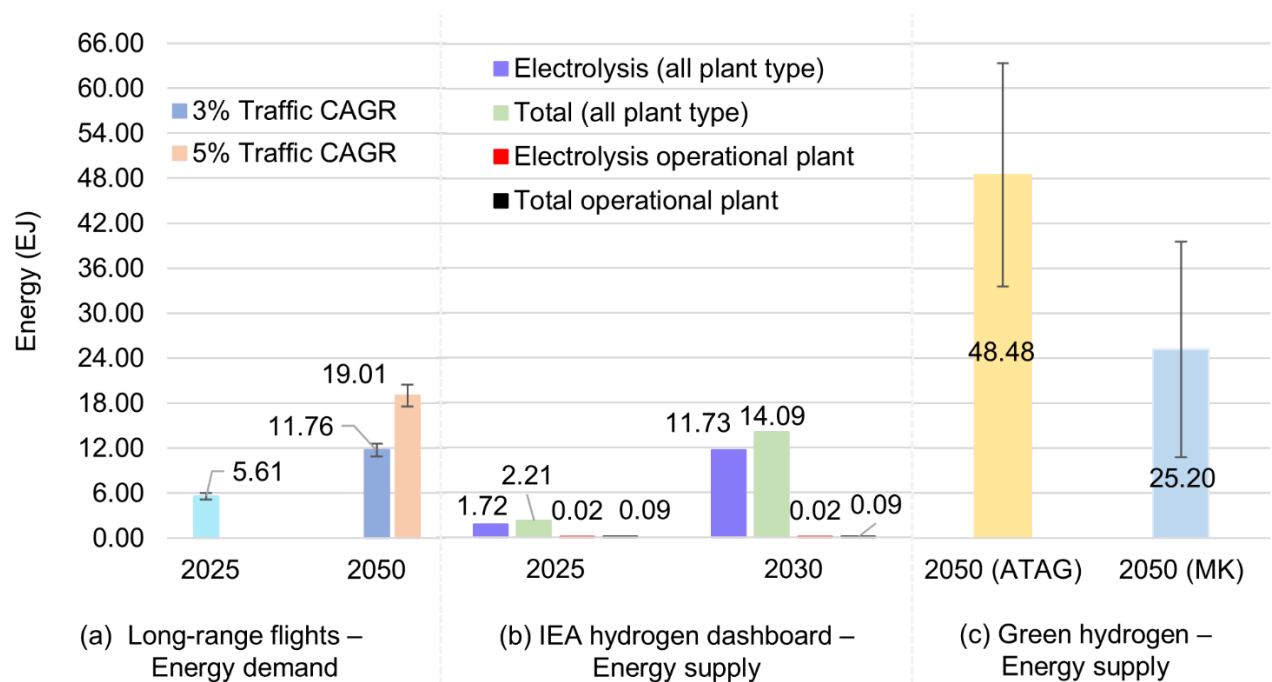

Figure 10. Energy demand forecast for long-haul aviation and supply of green hydrogen. **[ATAG: Air Transport Action Group report; MK: McKinsey report; CAGR: Compound annual growth rate]**.

3.1.5. Limitations of the Present Work

The fuel WTP emissions database used in this work is primarily based on the GREET model which is US specific. The WTP emissions are sensitive to country's energy mix, availability of raw materials (according to the location) and the number of such locations in the country (determines the transportation emissions), transportation mode used (emissions and efficiency, viz. rail vs trucks, electricity/battery vs diesel, etc.), transportation network and its efficiency (direct connectivity between two points, terrain type of the transportation network, etc.), and fuel manufacturing plant efficiency. Additionally, for LH_2 fuel it is assumed that the pump to tank emission is zero. This assumption is simplistic and there could be some emissions associated in terms of energy/emission required to maintain the cryogenic temperature and pressure while filling LH_2 fuel in the aircraft tank, transportation used (depending on the location of the fuel storage at or away from airport), and fuel losses while filling LH_2 fuel in aircraft tank. Also, NO_x estimation in this work is based on a simplified (multi-segment) mission where the energy consumption in smaller flight segments is calculated using the modifications to Roskam's fuel fraction. Moreover, the quantification of net non-CO_2 emissions used in this work for use-phase emissions (including contrails) are based on literature. The errors from those studies will add up in the results of this work. Lastly, this work does not

conduct cost analysis for aircraft mission powered by different fuels produced from various feedstocks and/or pathways.

4. Conclusions

Liquid hydrogen and 100% synthetic paraffin kerosene could serve as alternatives to Jet-A for long-haul aviation, provided they are produced from feedstocks and/or processes that ensure zero life cycle well-to-wake emissions. In this work, the life cycle or well-to-wake performance is evaluated for long-range large twin aisle aircraft powered by liquid hydrogen and 100% synthetic paraffin kerosene or SAF (separately) manufactured from different feedstocks and/or pathways. The GREET model is used for making a database of fuel manufacturing phase emissions for liquid hydrogen and 100% synthetic paraffin kerosene (bio-jet and power-to-liquid fuel), and the use-phase emissions are quantified separately in this work. In this work, the sensitivity of hydrogen sourcing to SPK production, and of biomass sourcing for some hydrogen production pathways, are addressed. Similarly, this work addresses the sensitivity of energy mix to alternative fuel production.

After examining over 100 different ways in total for producing liquid hydrogen and 100% synthetic paraffin kerosene, it is observed that liquid hydrogen fuel can enable net zero or negative well-to-wake CO_2 equivalent emissions for long-range (blended wing body aircraft) flight of 300 passengers where liquid hydrogen fuel is produced from Biomass (liquefaction is done using US electricity mix and manufacturing unit employing carbon sequestration) ($260.8\% - 266.1\%$ reduction), Biomass (liquefaction is done using electricity from biomass integrated gasification combined cycle and manufacturing unit employing carbon sequestration) ($296.2\% - 302.6\%$ reduction), and/or integrated fermentation with carbon sequestration ($96.2\% - 150.7\%$ reduction). This aligns with the decarbonization strategies of the International Air Transport Association of use of alternative fuel and carbon capture. Also, it is found that non-CO_2 emissions are significant to the net well-to-wake CO_2 equivalent emissions, and operational strategies need to be employed for reducing contrail formation. It is to be noted that the quantification of non-CO_2 effects (such as contrails) from hydrogen aircraft in literature is relatively at a nascent stage and more research work is required. The well-to-wake CO_2 equivalent emissions of 100% synthetic paraffin kerosene long-range (blended wing body aircraft) flight of 300 passengers can be reduced (on an average) by $70\% - 85\%$ (depending on SAF manufacturing pathways), using miscanthus as a feedstock, compared to Jet-A. It is to be noted that there could be a significant variability in the life cycle emissions for any given fuel and the manufacturing pathway, especially due to the carbon intensity of the sourced feedstock.

Based on the high-level analysis in this work, the projected SAF and hydrogen supply in 2050 can meet the energy demand of long-haul aviation with the current air traffic CAGR of 4%, assuming all flights are powered solely by one of these two fuels. However, if the air traffic CAGR increases to 5% and other sectors also compete for energy, production capacities, especially for hydrogen, will need to be scaled up. Alternatively, a mix of SAF and hydrogen could be used for long-haul flights, ensuring the energy supply meets the demand while also satisfying the needs of other sectors. In any case, achieving climate-neutral long-haul aviation will require boosting the production capacities of SAF and hydrogen beyond current projections.

The perspective used to select three feedstock and/or pathways for liquid hydrogen fuel identified in this work, only take into consideration the well-to-wake CO_2 equivalent emissions. However, for commercial aviation the fuel cost and the resulting direct operating cost (inclusive of carbon tax exemption) are significant aspects which also needs to be accounted for identifying fuel manufacturing pathways for both liquid hydrogen and 100% synthetic paraffin kerosene, which are not considered in this work. The fossil-fuel based energy consumption in fuel manufacturing phase should be reduced by increasing the share of renewables in the energy mix and improving the energy efficiency of the fuel manufacturing process and supply chain, for making SAF and/or liquid hydrogen an environmentally and socially benign aviation fuels. This work will inform: (i) research and development investments aimed at increasing production capacities for identified fuel manufacturing processes; (ii) assessments of fuel costs; and (iii) the formulation of aviation policies.

Lastly, the success of liquid hydrogen powered aviation requires appropriate airport infrastructure, aircraft design, air-traffic or operations management, safety, and fuel supply chain/manufacturing capacity and energy efficiency, to meet the required fuel demand, fuel cost and direct operating cost, and policy.

More information:

First author's other research work can be found in [6,10–16,26,94–118].

Nomenclature

Abbreviations

ATAG	Air Transport Action Group	LNGCC	Liquification using power from natural gas combined cycle
ATJ	Alcohol-to-jet	LTA	large twin aisle
B.	Biological plant type	LUSME	Liquefaction using US mix electricity
BC	Black carbon	L-Nuclear	Liquefaction using electricity from nuclear energy
BWB	Blended wing body	L-Solar	Liquefaction using electricity from solar energy
By-product Cl plant	H_2 produced as a by-product of chlorine manufacturing plant	M	Flight Mach number
CAGR	Compound annual growth rate	MK	McKinsey
CDM	Corn with dry mill	MW	Molecular weight
CDMWE	Corn dry mill with extraction	NAFG	North American flared gas
CDMWOE	Corn dry mill without extraction	NANG	North American natural gas
CH_4	Methane	NGCC	Natural gas combined cycle
CO	Carbon monoxide	NGL	Natural gas liquid
CO_2	Carbon dioxide	NO_x	Oxides of nitrogen
COG	Coke oven gas	N_2O	Nitrous oxide
CORSIA	Carbon offsetting and reduction scheme for international aviation	N+2	2030+ timeframe
CS	Carbon sequestration	OC	Organic carbon
CUSM	Corn US mix	PM	Particulate matter
CWEH	Catalytic with external H_2 plant type	PtL	Power-to-liquid
CWHBG	Catalytic with H_2 from biomass gasification plant type	ppm_{NOx},	parts per million of oxides of nitrogen
CWIH	Catalytic with in-situ H_2 plant type	PTWa	Pump-to-wake
CWM	Corn wet mill	PV	Photovoltaics
D.	Distributed	RNG	Renewable natural gas
FFB	Fresh fruit bunch	SAF	Sustainable aviation fuel
FT	Fischer–Tropsch	SC	Steam cracking
GHG	Greenhouse gas	SI	Supplementary information
GREET	Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies	SLS	Sea level static
GWP	Global warming potential	SMR	Steam methane reformation
HEFA	Hydro-processed esters and fatty acids	SOEC	Solid oxide electrolysis cell
HRJ	Hydro-processed renewable jet fuel	SO_x	Oxides of sulphur
HTE	High temperature electrolysis	SO_2	Sulphur Dioxide
HTGR	High temperature gas reactor	SPK	Synthetic paraffinic kerosene
IATA	International Air Transport Association	STJ	Sugar-to-jet fuel
IF	Integrated fermentation	S.	Standalone
LBIGCC	Liquefied using electricity from biomass integrated gasification combined cycle	TCCW	Thermochemical cracking of water
LCIGCC	Liquification using electricity from coal integrated gasification combined cycle	VOC	Volatile organic compound
LDI	Lean direct injection	w CS	With carbon sequestration
LH_2	Liquid hydrogen	WTP	Well-to-pump

WTWa   Well-to-wake
w/o CS   Without carbon sequestration

Symbols

$A, a, b, c, d,$ and e Correlation constants for emission index based on hydrogen data

$A^{'}$	Correlation constant for emission index based on Jet-A fuel
EI	Emission index
f/a or FAR	Fuel air ratio
$h^{'}$	Flight altitude (in feet)
H	Humidity correction factor
p_{amb}	Ambient pressure (in Pa)
p_{total}	Total pressure (in Pa)
P_3	Combustor inlet pressure (in MPa)
T_{amb}	Ambient temperature (in K)
T_{total}	Total temperature (in K)
T_3	Combustor inlet temperature (in K)
$W_{F,block}$	Block fuel weight
δ_{total}	Pressure correction factor
Υ	Specific heat ratio (1.4 for air)
$\Delta P/P$	Fuel injector air flow pressure drop ratio
Φ	Equivalence ratio
ϕ_{H_2}	Hydrogen equivalence ratio
τ	Combustor residence time
θ_{total}	Temperature correction factor

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