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Pimchanok Su-Ungkavatin. Assessing the environmental performance of future sustainable aviation systems : methodological development and evaluation by life cycle assessment. Chemical and Process Engineering. INSA de Toulouse, 2022. English. NNT : 2022ISAT0036 . tel-04416268

HAL Id: tel-04416268

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THÈSE

**En vue de l'obtention du
DOCTORAT DE L'UNIVERSITÉ DE TOULOUSE**
Délivré par l'Institut National des Sciences Appliquées de
Toulouse

**Présentée et soutenue par
Pimchanok SU-UNGKAVATIN**

Le 14 décembre 2022

**Évaluation des performances environnementales des futurs
systèmes d'aviation durables : développement méthodologique et
évaluation par l'analyse du cycle de vie**

Ecole doctorale : **MEGEP - Mécanique, Energétique, Génie civil, Procédés**

Spécialité : **Génie des Procédés et de l'Environnement**

Unité de recherche :

TBI - Toulouse Biotechnology Institute, Bio & Chemical Engineering

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Évaluation des performances environnementales des futurs systèmes d'aviation durables : développement méthodologique et évaluation par l'analyse du cycle de vie

Assessing the environmental performance of future sustainable aviation systems: methodological development and evaluation by life cycle assessment

Pimchanok Su-ungkavatin

PhD thesis

14 December 2022





ABSTRACT

This PhD work proposes and applies a methodology to compare and anticipate, by life cycle assessment (LCA), the environmental consequences of investments into four key emerging alternatives aviation systems to fossil kerosene. This includes biofuels (from waste cooking oil (WCO) or forestry residues), electrofuels (from atmospheric/industrial CO₂, combined with renewable H₂), electric battery, and H₂ systems (either combustion or within fuel cells). This work focuses on commercial aviation (passengers and cargo), this representing 88% of the CO₂ emissions from global aviation.

Four pathways for biofuels (hydroprocessed esters and fatty acids (HEFA) with WCO, biomass gasification followed by either Fischer-Tropsch (FT) or syngas fermentation and alcohol upgrading (Ethanol-to-Jet), and sugar fermentation and alcohol upgrading (as Isobutanol-to-Jet), two for electrofuels (carbon capture technologies based on liquid or solid sorbent), four for Li-based batteries, and two for water-splitting H₂ production have been studied. Full electric systems are considered only for the domestic segments (19 passengers plane). Hybridization with fossil kerosene is considered for the international segments. The comparisons are made based on the following functional unit: “Ensuring the annual global supply in 2035 of 6 trillion revenue passenger kilometres (RPK) of domestic flight and 9 trillion RPK of international flight”, itself based upon forecasts of International Civil Aviation Organization (ICAO).

The comparative framework built within this PhD work covers essential issues typically disregarded in previous analyses, including the fact that: i) under current framework conditions, liquid fuel alternatives require blending with fossil kerosene; ii) residual biomasses, when mobilized for aviation, are diverted from another use (counterfactual use); iii) fuels may affect the type and number of aircraft needed to supply the service described by the functional unit, among others because of an induced mass penalty; iv) some of the systems imply additional infrastructure, including for the end-of-life, and v) a fair comparison requires considering non-CO₂ climate forcers such as NO_x, induced cloudiness, water vapour, black carbon, sulfate.

Two-time scopes are considered (near- and long-term). The main differences are: (i) the long-term assumes that blending with fossil kerosene will no longer be required, and (ii) natural gas is used as a heat source in the near-term while heat is fully electrified in the long term.

In total, 16 impacts were quantified, and six were studied more finely, including climate change, photochemical ozone formation, particulate matter, freshwater eutrophication, marine eutrophication, and water scarcity.

All scenarios perform better than fossil kerosene, with some exceptions. These include (i) HEFA owing to induced heat generation (having worse performance than fossil kerosene in climate change for near-term, particulate matter and freshwater eutrophication for the long-term scenarios; (ii) Electricity intensive systems including electrofuels and H₂ because of electricity consumption during water electrolysis (worse impacts observed in particulate matter, freshwater eutrophication and water scarcity, irrespective to assessed time scopes).

Biofuels and electrofuels are heavily penalized by the blending requirements with fossil kerosene in the near-term; this also applies to hybrid electric battery systems (international segments, both time horizons). Biofuels derived from forestry residues have demonstrated the most environmentally performant systems. This is explained by the significant amount of counterfactual use of forestry residue (translating into avoided CH₄ emissions). However, the field measurement is further required to narrow the uncertainty ranges of their emissions. Full electric systems are proven as environmentally preferable approaches for the domestic segment.

Keywords: Batteries (Electric); Biofuels; Electrofuels; Energy Transition; Hydrogen (H₂); Life Cycle Assessment (LCA); Sustainable Aviation Fuels (SAF); Sustainable Aviation

RESUME

Ce travail propose et applique une méthodologie permettant de comparer et d'anticiper, par l'analyse du cycle de vie (ACV), les conséquences environnementales d'investissements dans quatre systèmes d'aviation alternatifs au kérosène fossile. Il s'agit des biocarburants de deuxième génération, des électrocarburants (à partir de dioxyde de carbone, CO₂, atmosphérique/industriel, combiné à de l'hydrogène renouvelable, H₂), de l'aviation électrique (batteries) et des systèmes à H₂ (soit par combustion, soit dans des piles à combustible). L'emphase de cette thèse porte sur l'aviation commerciale (passagers et fret).

Ce travail étudie quatre voies pour les biocarburants : (i) esters et acides gras hydrotraités (HEFA) avec des huiles usagées, (ii) gazéification de la biomasse suivie soit de Fischer-Tropsch (FT), (iii) soit de la fermentation du gaz de synthèse avec valorisation de l'alcool (Ethanol-to-Jet), et (iv) fermentation du sucre et valorisation de l'alcool (Isobutanol-to-Jet). A ceci s'ajoutent deux voies pour les électrocarburants avec des technologies de capture du carbone basées sur un sorbant liquide ou solide, quatre voies pour les batteries, et deux voies pour la production d'H₂ par l'électrolyse de l'eau. Les systèmes entièrement électriques ne sont envisagés que pour les segments domestiques (avion de 19 passagers) ; pour les segments internationaux, un système hybride avec le kérosène fossile est considéré.

Le cadre comparatif bâti par cette étude couvre des questions essentielles généralement négligées dans les analyses précédentes, notamment le fait que : i) dans les conditions actuelles, les carburants liquides de substitution doivent être mélangés au kérosène fossile ; ii) les biomasses résiduelles, lorsqu'elles sont mobilisées pour l'aviation, sont détournées d'une autre utilisation (utilisation contrefactuelle) ; iii) les carburants peuvent affecter le type et le nombre d'avions nécessaires pour fournir le service décrit par l'unité fonctionnelle, notamment en raison d'une pénalité de masse induite ; iv) certains des systèmes impliquent des infrastructures supplémentaires, y compris pour la fin de vie, et v) une comparaison équitable nécessite la prise en compte des facteurs de forçage du climat autres que le CO₂, tels que les NO_x, la nébulosité induite, la vapeur d'eau, le noir de carbone et les sulfates.

Deux horizons temporels ont été considérés : court terme 2035 et long terme 2045. Les principales différences sont les suivantes : (i) le long terme suppose que le mélange avec le kérosène fossile ne sera plus nécessaire pour les carburants liquides, et (ii) le gaz naturel est utilisé comme source de chaleur à court terme alors que la chaleur est entièrement électrifiée à long terme.

Au total, 16 impacts ont été quantifiés, et six impacts ont été étudiés plus finement, dont celui sur les changements climatiques. Tous les systèmes considérés présentent de meilleures performances que le kérosène fossile à l'exception de (1) HEFA en raison de la production de chaleur induite (les impacts dont la performance est pire que le kérosène fossile sont: changement climatique pour le court terme, matières particulaires et eutrophisation des eaux douces pour le long terme) et (2) Systèmes électro-intensifs incluant les électrocarburants et H₂ en raison de la consommation d'électricité lors de l'électrolyse de l'eau (les impacts dont la performance est pire que le kérosène fossile sont: matières particulaires, eutrophisation des eaux douces et utilisation des ressources en eau, pour le court et le long terme). Les biocarburants dérivés des résidus forestiers se sont avérés les plus performants sur le plan environnemental. Toutefois, ce résultat dépend hautement de la (mauvaise) performance environnementale, largement incertaine et peu mesurée sur le terrain, de la dégradation de ces résidus en forêt. Les systèmes entièrement électriques sont démontrés comme approche favorable à l'environnement pour le segment domestique.

Mots-clés: Analyse du cycle de vie (ACV); Aviation électrique; Biocarburants ; Carburants d'aviation durables (SAF); Electrocarburants ; Hydrogène; Systèmes d'aviation durable (SA) ; Transition Énergétique ; Aviation Net Zero

ACKNOWLEDGMENT

This dissertation is a product of my research as a doctoral candidate at Toulouse Biotechnology Institute (TBI), the Institut National des Sciences Appliquées de Toulouse (INSA Toulouse), France, between October 2019 and December 2022. My gratitude extends to those who have contributed to and supported me during these periods.

It was an unbelievable period that I stayed here (in Toulouse) for about three years. The journey began when I submitted an email to the supervisor working on the interesting project posted on the Campus France page. She promptly replied to me one day later, and we had a virtual meeting the next day (such an active schedule with the particulate matter intensive day in Bangkhuntien, Bangkok). It was a pleasure to discuss the project and prepare for the Campus France application (two weeks left before its deadline).

First of all, I would like to present my sincere gratitude to the whom made me interviewed on that day, Dr. Lorie Hamelin. Thank you for your continuous trust in me working on this challenging topic from the first day until now. She is a very calm, active professor and always open and listening. She is the first LCA teacher who patiently gives me numerous innumerable suggestions and tireless supervision on this work. I appreciate every moment of her dedicated time working with me, anytime she is available for discussions. Although I often ask her repeating questions, she always smiles and politely responds. I would also like to thank my co-advisor: Professor Dr. Ligia Tiruta-Barna, for always favoring me, teaching, and giving me constructive comments and feedback. The detailed explanations and the example always came with whichever questions I asked. Both of you never put the anger on me, although I made any mistake, making me feel more comfortable speaking out and learning more lessons while making the corrections. They always propose distinct points of view that truly improve this work. Their distinguished expertise in the field of LCA has been invaluable to me. Overall, this research could not have been nicely structured and captured the great attention of the public without two involved advisors. They have not only driven and motivated me but also enriched my research; thank my advisors for this.

I am also very grateful to Associate Professor Dr. Aras Ahmadi for providing immense help in conducting the biomass gasification modeling. Without his favor, this thesis would not have been completed.

Many thanks go to the members of the jury members: Professor Catherine Azzaro-Pantel as the president of the jury, Professor Robert Malina, Professor Benoît Gabrielle, Professor Florian Simatos, and Sandra Beauchet for your interest and for accepting to spend their consideration and time evaluating this piece of work.

I thank all the members we met during these three years at INSA Toulouse and elsewhere. I have to apologize for my bad memories of their names, but your birthday and all activities we made are consistently embedded in my heart. Albeit we had a little time spent together, it was such a wonderful moment with Patrick, David, Concetta, Shivesh, Dominika, Ariane, Angle (and their lovely huge but little heart Pitbull), Julia and Megan. My life would not be that lively without my friends in Cambioscop (I cannot imagine staying without them). All of my memories here always came with their pictures.

Xièxiè to Dr. Zhou, who always encourages me and provides a positive vibe, drove me to travel (though my French has not improved, I can confirm that you can use French fluently at the restaurant). The word “Gamsahabnida” to Seughey Lee, my warm friend from South Korea, who always helps, talks, and listens to me. Thank you for your recommendations to live in Europe and always take good care of others (You are a professional). I cannot be missed “Merci” to the icebreaking couple Ugo and Nia, who gave me their enthusiasm and encouragement to continue with my work and often cooked and drove me elsewhere. The term “Gracias” expresses all my Spanish friends: Christhel, Carlos, Camillo, Ernesto, and Marco, who always invite me to their dancing parties to broaden my experiences (with the talented dancers). I can say more for Christel for sharing time and many moments in Barcelona, doing shopping. I hope all your Pugs and cats are doing well and making you in comfortable mode (with a peaceful sleeping time). “Salamat” to you, Gleeza as our newcomer, for sharing the living and working experiences, eating out, and consistently doing me a favor.

Thank you also to all my friends in office 228: Dr. Ryma (I hope you have a brilliant way from now on and in the upcoming future), Phal (whom I always called her father’s name and who did shop with me), Jeremy (always shares his life and works), Solomon (gives me a welcoming greeting), Laura and Fred (such a friendly and hardworking

interns). Thanks to others from the neighbor team for smiling at me while we are passing by and having small talks always: Meike, Vincent, and many more

It does not matter where we are from and who speaks different languages. I can proudly mention that this place provides me with excellent educational sections and a wonderful and forever friendship, which is equally important. Thank you for the memorable experiences.

This incredible journey in windy Toulouse has not have been achieved without the generous funding from Mimistere Affaires Etrangeres (French government) and great care from Ms. Wanpan Sirapan (Thai coordinator from the French embassy in Thailand) for being the support in my home country. Special thanks to another financial aid source, the Cambioscop project, for providing a great opportunity as a member of this great project. Thank you for giving me this chance to come to France and do this research.

I will not be here and be mine as today without my beloved family. Always thanks for being trusted and making me explore the new journey on my way. My first memories as I have born come from this warming family. My granddad, grandmom, daddy, mommy, aunty, uncle, sister, and clingy pets are the most precious and always and forever be the top priority in my life. Thanks for their love and unconditional and inexhaustible support despite being 10,000 km away.

Without all support, I would not have come to finish this work.

Pimchanok Su-ungkavatin



LIST OF PAPERS

1. Su-ungkavatin, Pimchanok; Tiruta-Barna, Ligia; Hamelin, Lorie. “Biofuels, Electrofuels, Electric, Hydrogen?: A review of current and emerging Sustainable Aviation Systems”
(Preprint: <https://doi.org/10.31224/osf.io/8sqpy>, Submitted to “Progress in Energy and Combustion Science”. The first submission was on 29 June 2021, the second on 29 July 2022, and the third on 1 November 2022. Currently under review).
2. Su-ungkavatin, Pimchanok; Tiruta-Barna, Ligia; Hamelin, Lorie. “Framework for Life Cycle Assessment (LCA) of Sustainable Aviation (SA) system”
(Preprint: <https://dx.doi.org/10.2139/ssrn.4267918>, Under review in Science of the Total Environment, Submitted on 2 November 2022).
3. Su-ungkavatin, Pimchanok; Tiruta-Barna, Ligia; Hamelin, Lorie. “Uncovering the environmental performances of emerging candidates for sustainable aviation” (Under preparation and will be submitted to a scientific journal in December 2022).

CONFERENCE PAPER

Su-ungkavatin, Pimchanok; Tiruta-Barna, Ligia; Hamelin, Lorie (2022) Insight from the first Life Cycle Assessment comparing biofuels, electrofuels, electric & hydrogen systems for future aviation. *Proceedings of the Towards Sustainable Aviation Summit (TSAS 2022)*, 18-20 October 2022, Toulouse, France. (Presented as an oral presentation on October 18th, 2022). Available in Chapter 4 (section 4.6, Appendix).

CONFERENCE ABSTRACT

Su-ungkavatin, Pimchanok; Tiruta-Barna, Ligia; Hamelin, Lorie (2021) Comparative framework for alternative fuels in the future aviation biofuels, electrofuels, electric batteries and hydrogen. *29th European Biomass Conference & Exhibition (EUBCE 2021)*, 26-29 April 2021. Presented within a plenary session (virtually due to COVID-19) on 27 April 2021.)

Life Cycle Assessments require maximum transparency in the data, hypothesis, and calculations used. Therefore, each paper of this PhD work is accompanied by Supplementary materials, available online in the Callisto repository of the Federal University of Toulouse, as detailed in **Table 0** below. Each chapter ends by providing details about these supplementary files.

Table 0 Details on the supplementary materials associated with this thesis

Paper	Name and description of files	DOI Link
1	<p>SM 2.1 Word file containing additional details for biofuels and electrofuels productions and co-product generations. This includes the assumptions for sustainable biomass potential computations. In addition, different fuel characteristics and potential producers with their current partnerships are summarized. Finally, the methanol synthesis and the Fischer-Tropsh (FT) pathways for electrofuel production have been investigated.</p> <p>SM 2.2 Excel file containing several additional assumptions and calculations for feedstock availability, whether biomass (for biofuels) or electricity (including H₂O demands, H₂ requirement, direct air capture</p>	<p>All are available at: https://doi.org/10.48531/JBRU.CALMIP/MIGWAL. SM 2.1 is also available within this PhD manuscript</p>

(DAC) plant needed) (for electrofuels). The available LCA electrofuel studies are investigated. The amount of co-product(s) generations for each system is computed. Additionally, the background data for the semi-quantitative ranking tool can be found herein.

- 2 **SM 3.1** Word file containing domestic and international segment definitions applied in this work, the selected representative aircraft of each segment and the additional information on non-CO₂ tailpipe emissions and impacts. This includes the existing GWP and GTP characteristics. Additionally, the tailpipe emission calculations with the results of each fuel system are demonstrated.

All are available at:
<https://doi.org/10.48531/JBRU.CALMIP/N4TNMA>.
SM 3.1 is also available within this PhD manuscript

SM 3.2 Excel file containing several modelling assumptions, including aircraft characteristics, the calculation procedure for mass penalty and blending quota. The required numbers of aircraft have been revealed for each considered system.

SM 3.3 Excel file containing the calculation procedures for aviation tailpipe emissions, including the applied characterization factors. Climate change Characterization factors (CFs) and Emission factors (EFs) are documented.

- 3 **SM 4.1.** Word file detailing several modelling assumptions, along with the impact assessment results. It also supplies the process flow diagrams for all individual biofuel pathways analyzed.

No link for **SM 4.1**, which is directly included in this PhD manuscript

SM 4.2 Dataset Folder. “Dataset for uncovering the environmental performance of emerging candidates for sustainable aviation”. This consists of a folder containing 101 files detailing the impact assessment results, for each of the 16 impacts of the Environmental Footprint method separately, for the long-term (L) and near-term (N) scenarios for international (I) and domestic (D) segments. It also contains all the Life Cycle Inventories (LCIs) used and information on the counterfactual (CF) uses of constrained resources. It also contains the Global Sensitivity Analyses (GSA) calculation files and Sensitivity Analyses (SA) details, as well as details on the calculation of the different Reference Flows (RF).

The complete dataset of **SM 4.2** is available at
<https://doi.org/10.48531/JBRU.CALMIP/D0PWA8>.



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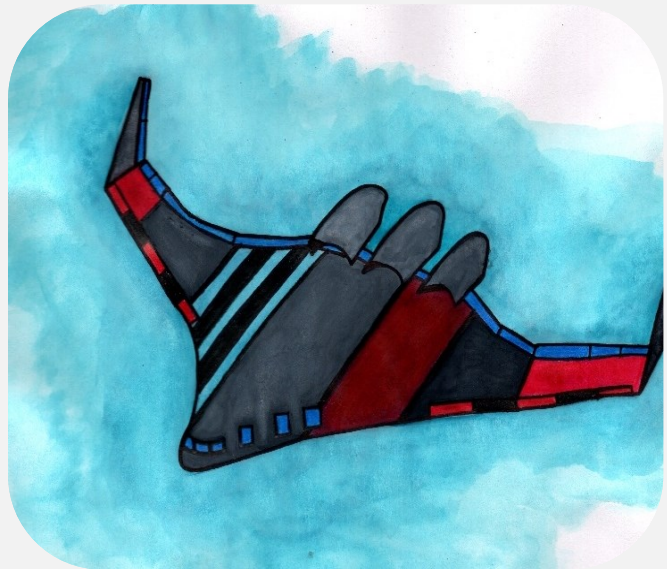
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1

General introduction



1. General introduction

With ca. 920 Mt carbon dioxide (CO₂) emissions per year (year 2019; [1]), the global aviation industry (commercial, private and military) represented approximately 2.5% of all-human induced CO₂ emission (37 Gt in 2019; [2]) and accounts for ca. 12% of emissions from all transport sources [3]. Despite growing public concerns on the contribution of the flying industry to climate change [4–7], the aviation traffic was, prior to the COVID-19 outbreak, forecasted to grow 4.3% per annum and the number of passengers to increase by as much as 20 trillion revenue passenger kilometers (RPK) by 2038 [8,9], compensating most gains obtained from years of fuel consumption efficiency improvements (the global amount of fuel burned per passenger dropped by 23% between 2005 and 2017, from 4.4 L per 100 km to 3.4 L per 100 km; [10]). Although the outbreak of coronavirus has lowered the revenue passenger kilometer (RPK¹) growth to 3.6% [11], strong recovery trends are gradually demonstrated, rising to 71% of the 2019 (the pre-pandemic) level in 2022 [12]. This is striking, in particular considering that less than 15% of the world population is traveling by air [13]. Moreover, it should be highlighted that high altitude emissions (at subsonic aircraft cruise altitudes of 8-12 km; [7]), including CO₂, and non-CO₂ species such as NO_x, soot, water vapor, and contrails, are of considerable concern as they affect the radiative balance of the atmosphere differently and presumably more intensively than emissions at the ground level (including fuel consumption in the taxi phase, varying from 3-40% upon the distance travelled estimated on the CO₂ emissions [14]), and thus the resulting impact on climate change [15–17].

The aviation sector itself acknowledges the need of finding sustainable alternatives to fossil fuels. A variety of mitigation measures have been proposed by the original equipment manufacturers (OEMs) in recent years, whether spurred by regulatory frameworks (national, regional, and international scale of implementations) or innovation projects towards cleaner aviation. For instance, the International Civil Aviation Organization (ICAO) launched the CORSIA initiative (Carbon Offsetting and Reduction Scheme for International Aviation) in 2016, with the vision to achieve CO₂ emission mitigation for the aviation sector corresponding to a carbon (C) neutral growth by the year 2020 (CNG2020 target). It thereby became the first economic sector to adopt a global, universal, and binding system to control its GHG emissions. In addition, the International Air Transport Association (IATA) and the Air Transport Action Group (ATAG) have set CO₂ emission reduction goals of 50% for 2050 (relative to 2005 levels). Additional examples are the development of new aircraft configurations, the development of advanced generations of engines, the implementation of improved air traffic management (ATM), and the use of alternative energy sources (fossil-fuel independence). While the three formers are directly related to the objective of minimizing fuel consumption, the latter focus on the fuel (or rather energy source) itself. Besides the supply side, there are also solutions focusing on reducing the demand side, though these measures will be outside the scope of the present work.

This PhD study assesses the environmental performance of alternative energy sources for aviation, this being seen as promising by the industry, and hence where large investment are likely to happen in a near future. The main objective is to answer the following overarching research question: which energy source is the most promising alternative for future aviation, in terms of environmental performance, and under which framework conditions? As the question is generic, several sub-questions are required to provide a complete assessment:

I. What are the alternative energy options likely to be available for the medium- to long-term future, for aviation?

II: For all options of (I), what are the different existing and emerging sub-systems, and which ones are likely to be the most promising, in terms of environmental performance?

III: How should the environmental assessment of future aviation systems be conducted to fairly and quantitatively compare the benefits and trade-offs of the different systems captured in (II)?

¹ Revenue Passenger Kilometer is defined as the multiplying the number of revenue passengers (which the airline receives remuneration) carried by the travelled distance.

IV: What are the environmental performances of those alternative aviation systems, and what are the key parameters shaping the overall impacts?

These research questions are addressed in different chapters of this PhD thesis, as detailed in Table 1.

Table 1. Overview of the thesis chapters with the addressed research questions

Chapter	Topic	Research question			
		I	II	III	IV
2	Biofuels, Electrofuels, Electric or Hydrogen?: A review of current and emerging Sustainable Aviation systems	X	X		
3	Framework for Life Cycle Assessment of Sustainable Aviation systems			X	
4	Uncovering the environmental performances of emerging candidates for Sustainable Aviation systems				X

Chapter 2 presents an in-depth review of the emerging alternative technologies for sustainable aviation. At the light of the European sustainability regulations (e.g., ReFuelEU [18], Renewable Energy Directive [19]) and the developing trends from the OMEs, four large families of sustainable approaches have been studied: Biofuels, Electrofuels, Electric and Hydrogen, from here onwards referred to as Sustainable Aviation (SA) systems. Each approach comprises a variety of pathways that are thoroughly detailed. In total, nine biofuel and nine electrofuel pathways were reviewed, for which we supply the detailed process flow picturing all input, output, and co-products generated. The market uptake and use of these co-products was also investigated, along with the overall international regulations and targets for future aviation. As most of the inventoried pathways require hydrogen, we further reviewed six existing and emerging carbon-free hydrogen production technologies. Our review also details the five key battery technologies available (lithium-ion, advanced lithium-ion, solid-state battery, lithium-sulfur, lithium-air) for aviation. The possible configuration schemes for electric propulsion systems are documented and classified as: i) battery-dependent and ii) other electric systems including fuel cell and turboelectric configurations. To the best of current knowledge, a semi-quantitative ranking tool for ex-ante prioritization for in-depth environmental assessments has been established covering three criteria: technology status, economic aspects, and environmental performance. This tool has been applied to 33 pathways, for both near- and long-term scope. The prioritized technologies are subsequently undergoing a full environmental assessment in the third stage of this study (Chapter 4).

A framework for Life Cycle Assessment (LCA) of SA systems has been developed in **Chapter 3**. First, the globally projected RPK, usually expressed in air traffic capacity, is proposed as the functional unit best describing the service supplied for all SA systems. Two time scope are proposed (medium- and long-term), as well as two generic segments, namely domestic and international. The framework proposes, for each of the studied SA systems, a methodology to translate projected RPK into energy requirements. Generic system boundaries are defined with their key activities for all SA systems, with the biofuel system being sub-divided into two categories: (i) biofuel from residual biomass and (ii) biofuel from land-dependent biomass. The activities are grouped in seven categories: (i) conventional (fossil-based) kerosene activities, (ii) conversion processes from feedstock supply to fuel or energy production for aircraft operation, (iii) counterfactual uses of the feedstock and displacement effects associated to co-products, (iv) aircraft manufacture, (v) aircraft operation, (vi) additional infrastructure needed, and (vii) end-of-life management (applied to aircraft and batteries). The model also includes a methodology to handle: (i) hybridization (the use of more than one source of energy to power an aircraft), (ii) the mass penalty affecting the number of carried passengers, and (iii) impacts stemming from non-CO₂ tailpipe emissions - aspects that are currently neglected in most LCA studies.

Environmental performances of the prioritized technologies (obtained from Chapter 2) are quantified in **Chapter 4**, using the comparative LCA framework for SA systems developed in (Chapter 3), applied to the two-time scopes and segments it proposes. Besides the difference of total RPK to be supplied, specific scenarios are applied to the medium- and long-term time scopes. In contrast to the medium-term, the long-term scope considers that no blending with fossil kerosene is required for biofuels and electrofuels due to technological advancements. It also considers electrified heat, while the medium-term considers heat based on natural gas. Differences in overall propulsion efficiencies are also considered, as well as in the efficiencies of batteries. The impacts on 16

environmental impact categories are quantified, but six are interpreted in detail, namely climate change, photochemical ozone formation, particulate matter, freshwater & marine eutrophication, and water scarcity. The detailed Life Cycle Inventories (LCI) of the 12 assessed systems are transparently presented for reproducibility. All studied scenarios are compared to fossil kerosene commonly used for commercial aviation [20]. The key activities contributing to the studied environmental impact categories have been uncovered through a detailed contribution analysis. The key parameters to which results are particularly sensitive, as well as those defining the uncertainty of the results, have been uncovered through a global sensitivity analysis (GSA) approach. Scenario-based sensitivity analyses have been performed to assess the sensitivity of the results to specific scenario changes, for instance, the location of the fuel production (United States and China instead of France), which in turn define the type of electricity mix being used.

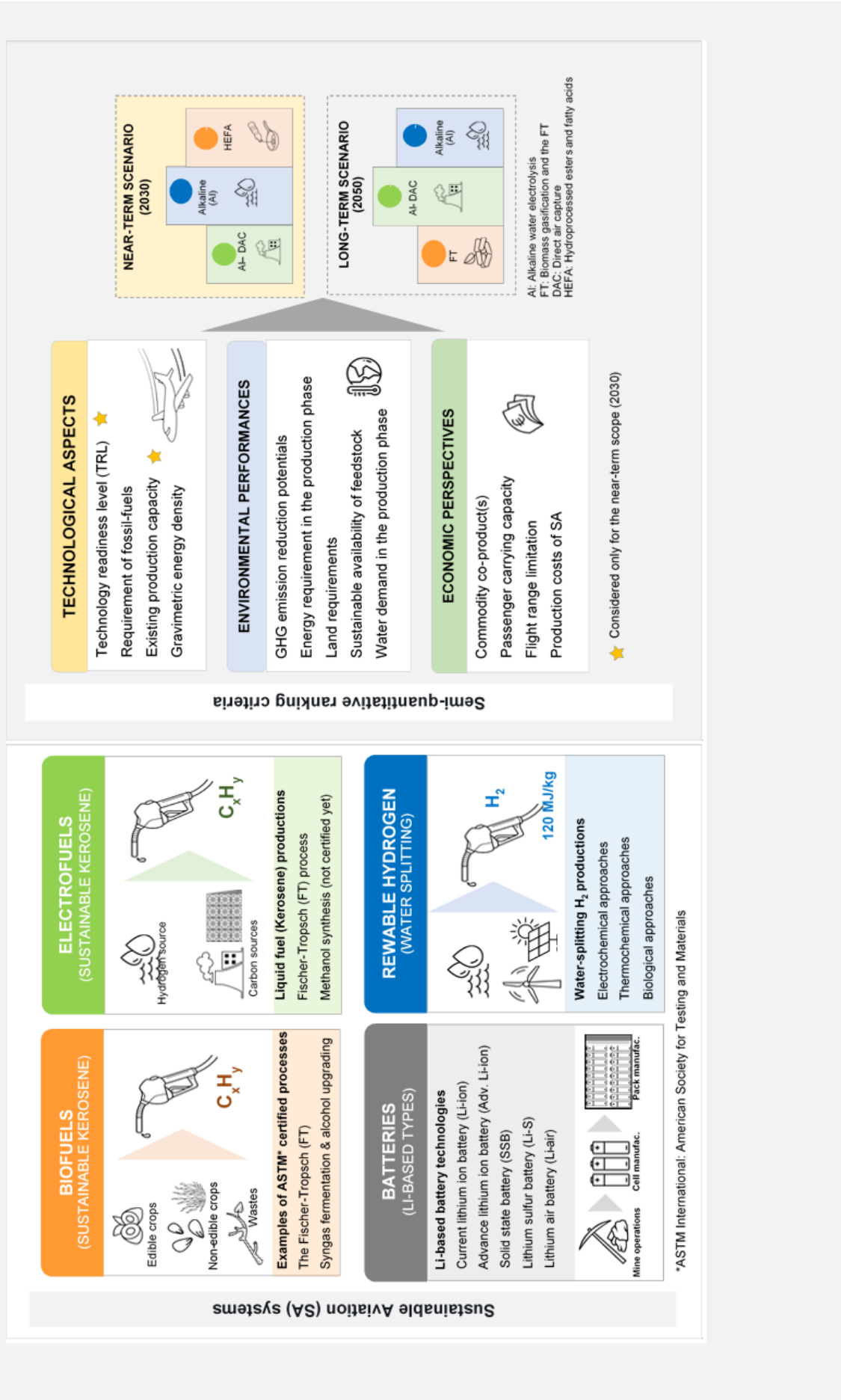
Finally, in **Chapter 5**, concrete answers to the research questions are provided. This chapter also includes a perspective for further research and a critical discussion of the scientific short-comings of this PhD work.

2

Biofuels, Electrofuels, Electric, Hydrogen?:

A review of current and emerging Sustainable Aviation systems





ABSTRACT

Climate neutrality is becoming a core long-term competitiveness asset within the aviation industry, as demonstrated by the several innovations and targets set within that sector, prior to and especially after the COVID-19 crisis. Ambitious timelines are set, involving important investment decisions to be taken in a 5-years horizon time. Here, in-depth review of alternative technologies for sustainable aviation revealed to date are provided, classified into four main categories, namely i) biofuels, ii) electrofuels, iii) electric (battery-based), and iv) hydrogen aviation. Nine biofuel and nine electrofuel pathways were reviewed, for supplying the detailed process flow picturing all input, output, and co-products generated. The market uptake and use of these co-products was also investigated, along with the overall international regulations and targets for future aviation. As most of the inventoried pathways require hydrogen, six existing and emerging carbon-free hydrogen production technologies are further reviewed. This review also details the five key battery technologies available (lithium-ion, advanced lithium-ion, solid-state battery, lithium-sulfur, lithium-air) for aviation. A semi-quantitative ranking covering environmental-, economic-, and technological performance indicators has been established to guide the selection of promising routes. The possible configuration schemes for electric propulsion systems are documented and classified as: i) battery-based, ii) fuel cell-based and iii) turboelectric configurations. Our review studied these four categories of sustainable aviation systems as modular technologies, yet these still have to be used in a hybridized fashion with conventional fossil-based kerosene. This is among others due to an aromatics content below the standardized requirements for biofuels and electrofuels, to a too low energy storage capacity in the case of batteries, or a sub-optimal gas turbine engine in the case of cryogenic hydrogen. Yet, the latter was found as the only available option, based on the current and emerging technologies reviewed, for long-range aviation completely decoupled of fossil-based hydrocarbon fuels. The various challenges and opportunities associated with all these technologies are summarized in this study.

Keywords : Batteries; Environmental performance; Kerosene; Regulatory frameworks; Sustainable Aviation Fuels (SAF); Fuel cells

HIGHLIGHTS

- Review with all sustainable aviation (SA) systems reported to date
- The full process flow diagrams of SA technologies are documented & represented
- The market uptake for the co-products generated with liquid fuels is documented
- Water-splitting H₂ production, batteries & H₂-fuel cell technologies are reviewed
- A review of current regulations and targets is presented

2.1 Introduction

With ca. 920 Mt carbon dioxide (CO₂) emissions per year (year 2019; [1]), the global aviation industry (commercial, private and military) represented approximately 2.5% of all-human induced CO₂ emission (37 Gt in 2019; [2]) and accounts for ca. 12% of emissions from all transport sources [3]. Despite growing public concerns on the contribution of the flying industry to climate change [4–7], the aviation traffic was, prior to the COVID-19 outbreak, forecasted to grow 4.3% per annum and the number of passengers to increase by as much as 20 trillion revenue passenger kilometers (RPK) by 2038 [8,9], compensating most gains obtained from years of fuel consumption efficiency improvements (the global amount of fuel burned per passenger dropped by 23% between 2005 and 2017, from 4.4 L per 100 km to 3.4 L per 100 km; [10]). The aviation sector itself acknowledges the need of finding sustainable alternatives to fossil fuels. For instance, the International Civil Aviation Organization (ICAO) launched the CORSIA initiative (Carbon Offsetting and Reduction Scheme for International Aviation) in 2016, with the vision to achieve CO₂ emission mitigation for the aviation sector corresponding to a carbon (C) neutral growth by the year 2020 (CNG2020 target). It thereby became the first economic sector to adopt a global, universal, and binding system to control its GHG emissions. In addition, the International Air Transport Association (IATA) and the Air Transport Action Group (ATAG) have set CO₂ emission reduction goals of 50% for 2050 (relative to 2005 levels).

The mitigation of the climate impact of aviation is thus the main driver of the present work. Here, the focus is on commercial aviation (passengers and cargo) as this represents 88% of the CO₂ emissions from global aviation ([13]; military, private, and other flights, e.g. emergency, represent the remaining 12%). Commercial aviation relies essentially on airplanes covered by the European Certification Specification 25 (CS-25) [21] and excludes air taxis [22]. From here onwards, the term “aviation” will thus specifically refer to commercial aviation. Reducing CO₂ (and overall GHG) from aviation may be achieved either by a decreased demand (itself spurred by e.g., shifts in transportation habits), or by technological means (e.g., enhancing fuel consumption efficiency, developing alternative energy sourcing). This study focuses on the latter strategy, i.e. the potential of alternative energy sources to enhance the environmental performance of aviation in comparison to flying on fossil-based kerosene. Four large families of emerging alternative energy sources for fueling future aviation can be highlighted: biofuels, electrofuels (liquid hydrocarbons produced through an electricity input), electricity (battery-based), and hydrogen. These all involve several variants and are here referred to as “sustainable aviation” (SA) systems, though the term sustainability remains to be assessed as later detailed. One commonly used denomination is “sustainable aviation fuels” (SAF), but it will not be used through this PhD work for two reasons. First, this term is typically used to represent biofuels (e.g. [23–26]), although the recent ReFuelEU aviation initiative and its regulation proposal have explicitly expanded it to electrofuels (also designated as synthetic fuels) [27–29]. Second, some of the emerging technologies (e.g., batteries) do not fit within the concept of fuel. Here, the more inclusive “sustainable aviation” terminology is instead proposed and used.

In the literature, several terminologies are used to designate aviation fuels, such as jet fuels or kerosene. In industry, it is referred to as Jet A or Jet A-1 (among all differences between these, the most notable one relates to their freezing point; Jet A -40°C (233K), Jet A-1 47°C (226K); [30,31]). Through this study, the term kerosene (C₈-C₁₆ hydrocarbons) is used to refer to liquid aviation fuels in general, whether these are fossil-based or not. Fossil-free aviation fuels deriving from bio-based feedstock (denoted as bio-kerosene or biofuels; the latter term is used herein) are drawing great interest in achieving GHG emission reduction targets for the aviation industry [32]. Today, biofuels generated from different technology pathways must be certified by the American Society for Testing and Materials International (ASTM) (ASTM D7566 – Standard Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons) or equivalent standards (e.g., Standard 90-091 of United Kingdom’s Ministry of Defense; [33]) before it can be used in commercial aircraft. So far, there are only six certified pathways for biofuels, namely the Fischer-Tropsch (FT) process, hydroprocessed esters and fatty acids (HEFA), direct sugar to hydrocarbon (DSHC), alcohol-to-jet (ATJ; with isobutanol or ethanol intermediates), and catalytic hydrothermolysis jet (CHJ). Some of these pathways involve variants (e.g. FT with added aromatics). Here, sugar and syngas fermentation (followed by upgrading of the produced alcohol) are considered separately instead of

being aggregated under the umbrella term “ATJ”, as often found in the literature (e.g. [18,25,34]). This is done to reflect the drastically different technologies and overall process flow involved in both cases, among others.

Besides biofuels, additional alternative kerosene for fossil-free aviation include electrofuels (sometimes known as synthetic fuels or powerfuels or power-to-liquid). Aviation electrofuels require a source of carbon and hydrogen (H_2) to generate hydrocarbon liquid fuels having properties similar to those of fossil-based kerosene. Hydrogen may be produced via water-splitting technologies including approaches such as water electrolysis [35], thermochemistry [36], or bio-photolysis [37]. Carbon may stem from biomass-free options such as direct capture of carbon dioxide (CO_2) from the atmosphere (typically termed Direct Air Capture, DAC) [38,39]. The carbon source may also arise from biogenic carbon through the use of syngas stemming from biomass gasification. The syngas may also stem from high-temperature co-electrolysis (using water and CO_2 as input, the latter being biomass-derived or not) [40]. Carbon may also stem from CO_2 captured from a point source (industrial process) [41–43]. Liquid fuels are then produced through the FT process [40] or methanol (CH_3OH) synthesis [44,45], although only the former has been certified by ASTM [44,45]. At present, both electrofuels and biofuels can be used as drop-in fuels, i.e. they are, up to a certain blending limit, interchangeable with conventional kerosene, and do not require adaptation of the fuel distribution network or the engine.

So far, there are four main categories of alternative kerosene. They include i) Synthetic paraffinic kerosene (SPK) largely composed of normal- and iso-paraffins (e.g., obtained with the FT, HEFA, SuF, SF pathways), ii) Synthetic aromatic kerosene (SAK), primarily consisting of aromatics designed as blend components (e.g. produced in the APR pathway), iii) Synthetic iso-paraffin (SIP) consisting essentially of farnesane ($C_{15}H_{32}$), and iv) Synthetic kerosene (SK) consisting of a composition similar to fossil-based kerosene (e.g. produced in the CHJ pathway; a new SK fuel from this pathway (CHJ-SK) has just been certified in 2020) [25,46]). SPK is however the predominant type of alternative kerosene generated from the currently certified pathways [34].

These four types of alternative kerosene are reported to provide cleaner combustion, with reductions of soot; [47,48], particulate matter (PM); [49], and sulfur emissions [50], among others because of the lower aromatic content in the fuel (when not zero). On the other hand, a low aromatic content has the disadvantage to cause shrinkage of some elastomers in the engine seal [51,52]. Reflecting this risk, ASTM D7566 requires a minimum aromatics content of 8% by volume, and as a result alternative fuels have been used as blends with conventional kerosene, up to a certain blending limit varying between 10% (DSHC) and 50% (all other certified processes) of the total fuel volume [26,34,51]. For longer-term solutions, state-of-the-art engines (with novel sealing materials) are being developed to be compatible with unblended aviation biofuels and electrofuels, as tested and announced by aircraft and engine original equipment manufacturers (OEM), namely Airbus [53], Boeing [54], Rolls-Royce [55], Deutsche Aircraft [56].

Through this review, electric aviation refers to the use of batteries as energy sourcing to power aircrafts (whether for propulsion, on-board operating systems, or both in a hybridized mode). One challenge this poses is the development of energy-dense batteries as light and compact as possible, which is challenging with today’s lithium-ion (Li-ion) battery technology (around 300-400 Wh kg^{-1} ; [57]), relative to Jet A-1 (approx. 12,000 Wh kg^{-1} ; [30]). Lithium-based batteries (with the introduction of novel electrodes/electrolytes such as advanced lithium-ion batteries (Adv. Li-ion), solid-state lithium-ion (SSB), or lithium-sulfur (Li-S)), are foreseen as the most promising approaches for mass sensitive applications like aviation, owing to their higher specific energy density [58,59]. However, these advanced Li-based batteries are still in the early stages of research, and many challenges need to be tackled before their mass production. Current Li-ion batteries have nevertheless been applied as a sole energy source for small aircraft capable of carrying less than 20 passengers per flight missions (e.g. Eviation’s Alice aircraft; [60], Bye Aerospace’s eFlyers aircraft; [61], Pipistrel’s Velis Electro; [62], Heart Aerospace’s ES-19; [63]). For larger aircraft, electric aviation requires to be combined with another energy source such as conventional (or alternative) kerosene, an approach commonly known as hybridization [64].

Additionally, hydrogen (both gaseous and cryogenic forms) [65,66] is currently researched as an alternative option for use in commercial flights. In the perspective this hydrogen is produced through water-splitting approaches, most of the associated environmental impacts are reported to be related to the type of electricity used [67–69].

Because of the low volumetric energy density of H₂, the heavy on-board system infrastructure required to accommodate H₂ weakens its benefits, as in the case of batteries [70,71]. Moreover, additional external infrastructures are required in both cases, including a charging station for the case of batteries, a H₂ refueling station for hydrogen, while redesigned airframes making the plane lighter or improving its aerodynamic performances are optional. Unlike electric aviation, H₂ systems require a refueling time comparable to conventional (and alternative) kerosene [72].

These two approaches (electric and hydrogen) are not associated with CO₂ emissions during the flight. Although the principle of zero tailpipe emissions applies to 100% electric (battery-based) aviation, the pollution occurring during batteries manufacturing (and recycling) is not zero and needs, as for all upstream activities of all other SA approaches, to be addressed as well [73]. Similarly, the emissions generated during the production of H₂ may be important, especially if stemming from conventional steam reforming of natural gas instead of water electrolysis or other carbon-free approaches [69]. Water vapor and nitrogen oxides (NO_x) are tailpipe pollutants from H₂ aviation and are considered as predominant climate forcers [65,74,75]. They are potential precursors, along with soot (emitted with liquid kerosene), for contrail and cirrus cloud formations, depending upon the ambient atmospheric conditions, which in turns affects the amount of heat trapped within the technosphere [71,73,76,77]. The formation of NO_x (also responsible for tropospheric ozone formation) from H₂ combustion is reported to be lower compared to the NO_x emissions from kerosene combustion [65,71].

There is, thus, a variety of technical possibilities towards a more sustainable aviation sector, and each involve a variety of options in terms of feedstock. While some options can act as drop-in fuels, others require additional infrastructure, and all options affect the environment (not only climate) in different ways. It thus remains unclear, in the perspective of long-term investment decisions towards tomorrow's aviation, which option leads to the highest overall environmental performance, and even whether some of the options are truly sustainable and environmentally superior to fossil-based kerosene. Clear requirements defining sustainability for aviation do exist, among others through the sustainability criteria elaborated in CORSIA by ICAO [78] and to some extent in the Recast Renewable Energy Directive (RED II [19]) for biofuels, electrofuels as well as (renewable) hydrogen feedstock, although these are not aligned with one another [18]. It should be noted that the former criteria go well beyond the sole GHG reductions, also including criteria on enhancing water quality and availability, or soil health, for example.

Nevertheless, to quantify sustainability, Life Cycle Assessment (LCA) is acknowledged as a central tool for environmental management and decision support, in the European Union in particular [79]. Because it can address impacts in a full system perspective, LCA has grown to become one of the key tools for assisting the direction of the so-called "green transition". Yet, to perform such analysis, vital and timely for the case of aviation, the very first step is to have the full overview of the process flow of the alternatives under assessment, including the overview of the types of co-products being generated. It is our claim that such overview is not yet in place for all alternative SA options simultaneously, being one possible reason why no LCA comparing all four-alternative exist at the moment. Although reviews have been published to document the production process, and, to some extent, the sustainability aspects of alternatives to fossil kerosene, these reviews focused mainly on only one of the SA categories distinguished herein. Aviation biofuels have been the most widely reviewed. Notable reviews are the ones of [80,81], where the conversion processes are extensively described, with key technological advances and challenges. In addition to that, economic and environmental aspects of biofuel pathways are comprehensively discussed by [82] and [52]. Similarly, an overview of the state-of-the-art implementation of biofuels within the aviation sector was presented by [83]. Although not as extensively reviewed, the main synthesis pathways for a variety of electrofuels were qualitatively discussed in [84], with regards to the required physical and chemical properties of these fuels when used in airplanes. The studies of [85] as well as [86], albeit not focusing on the aviation sector per se, carried out an economic analysis for a variety of electrofuels documenting several technologies and variations in plant size. However, the electrofuels investigated in these studies can be considered only as intermediates for aviation fuel production. The recent work of [87], on the other hand, represents a notable advance where a general overview of both carbon-free and biofuels options is described. Albeit valuable, the study

of Bauen [87] remains largely qualitative and does not detail the technical conversion pathways and processes involved, and completely excludes electrofuels. Moreover, all of the above-mentioned studies, except [52,82], completely overlook the co-products generated along the production process. Yet, these do generate market interactions that in turn are part of the overall economic and environmental performance of these new alternatives, and accordingly must be understood.

In the perspective of bridging these gaps, and in the vision of supplying a harmonized comparative background to assess the environmental consequences of current and emerging options for fueling the aviation sector, the present study presents a comprehensive review intending to supply a holistic understanding in the field of sustainable aviation. Concretely, this review intends to gather and discuss information and data relevant and necessary for comparative environmental assessments (in particular LCA) of emerging candidate options for sustainable aviation.

The review is organized into thirteen sections. The underlying methodological approach used for the review is first described (section 2.2). The review starts with detailing the biofuels, electrofuels, electric (battery-based) and hydrogen families and options within each (sections 2.3, 2.4, 2.6, and 2.7, respectively) as well as the co-products obtained in the liquid fuel pathways (biofuel and electrofuel families) and their potential uses as alternatives to fossil-based products (section 2.5). A semi-quantitative ranking is proposed (section 8), covering environmental, economic, and technological performance indicators, in order to provide a preliminary screening of the environmental performance potential associated with each approach in the near- (2030) and long-term (2050) timescales. In addition to the four dominant SA approaches that are the object of this study, other marginal alternative energy sourcing are reported in section 2.9. The electric propulsion systems (i.e., those involving electric motors; either battery- or fuel-based) are discussed in section 2.10. Section 2.11 discusses the development of regulatory frameworks and legislations related to clean aviation. Finally, sections 2.12 and 2.13 address the challenges and prospects for the deployment of SA, with emphasis on the availability and sustainability of raw materials and the scientific and technological advances needed.

2.2 Methodological approach

Overall, approximately 600 records, including scientific literature, patents, (company) reports, conference proceedings, and company websites, were extensively screened and reviewed. Efforts were made to ensure that the most recent data from announcements and literature were used. However, in the very process of writing this article, some of these announcements have changed (e.g., the cancellation of the Airbus E-Fan X project in April 2020), and although we strived to keep all the information presented herein up-to-date, it can happen that some will no longer apply following the publication of this article.

The scientific literature search was performed through two key search engines, namely Google Scholar and Web of Sciences, while the Google Search engine was used for screening the grey literature. A variety of generic keywords such as “aviation decarbonization,” “alternative aviation fuels,” “sustainable aviation regulation” have first been used, while snowballing strategies [88] were applied to capture additional content. A few variations of the abovementioned keywords have also been used to capture additional records. This procedure was repeated for each specific topic addressed in this review.

Moreover, although all key terminology used within the manuscript is strived to explain (e.g., what the notion of electrofuels exactly encompasses), a glossary is provided (supplementary material 2.2 ; SM 2.2) to clarify all terms and acronyms used. Throughout the manuscript, we report the units as supplied in the original references but provide the conversion in units of the International System of Units (SI).

2.3 Aviation biofuels

Because of their maturity and compatibility with the existing fueling infrastructure, biofuels is the most dominant SA family.

Three large biofuel categories are here distinguished according to the feedstock used: carbohydrate-rich, lignocellulosic and oil-based biomass. These will be used within this section to organize the description of each biofuel.

Fig. 2.1 presents, in relation with these three categories, an overview of nine different biofuels pathways for which known investments in terms of capacity have been made.

Among the nine pathways covered in Fig. 2.1, six are already certified by the ASTM D7566. The remaining three are either under the process of certification (APR, IH²; integrated hydropyrolysis and hydroconversion) or under development (HDCJ pathway). Some pathways are well developed, documented, and applied in large-scale production (pilot/demonstration plants), while some, such as the CHJ and IH² pathways, are less extensively documented. These are briefly described herein, and additional insights on, e.g., the biofuels properties, blending ratios, or the leading industrial producers to date are available in supplementary material 2.1 (SM 2.1) (Tables S2.1-S2.2).

Low readiness level emerging pathways are disregarded from this section because they are scarcely documented, including the one described by e.g. [89], where volatile fatty acids (VFAs) from anaerobic digestion of residual biomass are processed for catalytic upgrading to kerosene-ranged paraffins [89]. It also includes the emerging methanol-based pathway to produce kerosene described in e.g. [90].

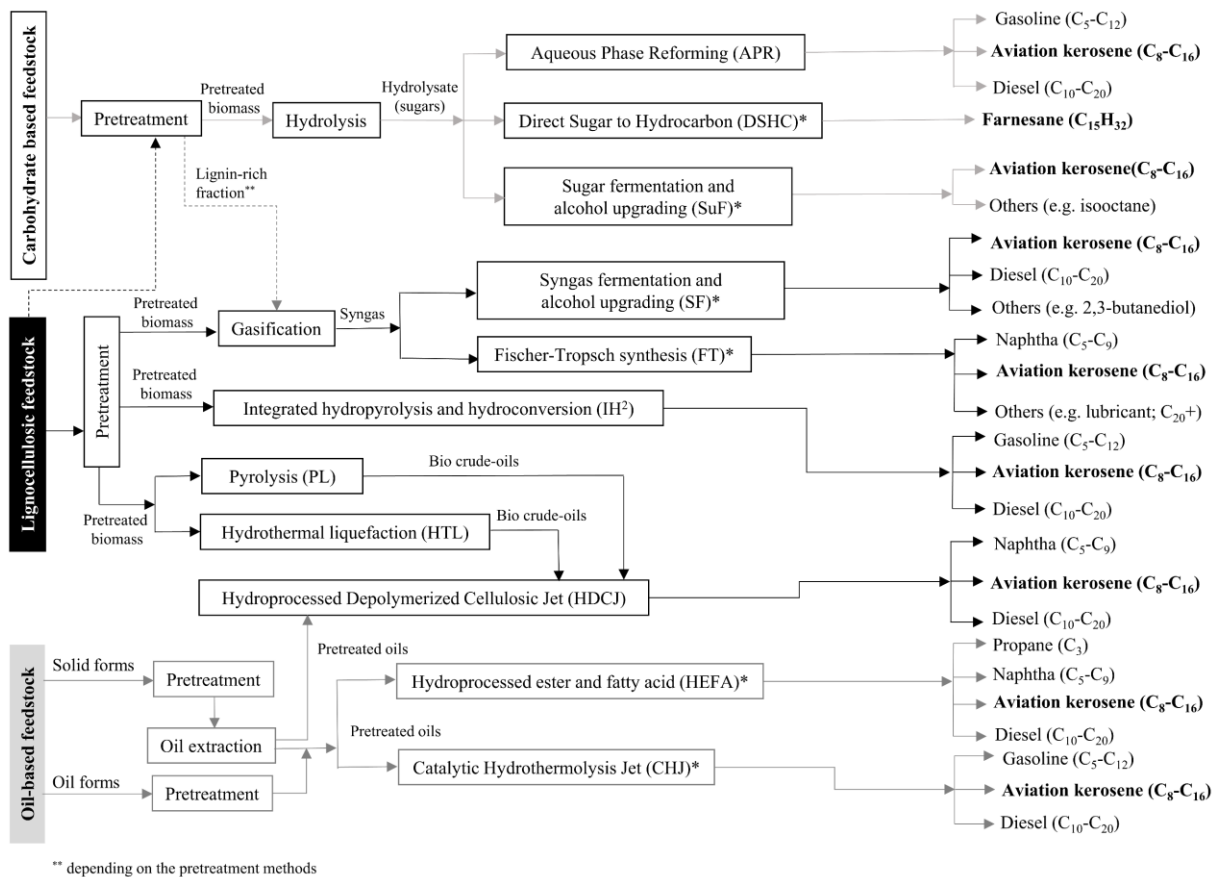


Fig. 2.1 Main conversion pathways in the production of aviation biofuels. (*) Indicates that the pathway is certified by ASTM. ** It is considered that the pretreatment methods are varying depending upon the characteristics of feedstock applied.

2.3.1 Biofuel pathways involving carbohydrate-rich feedstock

This category comprises three pathways (Fig. 2.1). They greatly rely upon carbohydrate-rich feedstock such as sugarcane, sorghum, maize dextrose, maize, etc., but can also be used with less dense carbohydrate sources such as molasses. Simple mechanical pretreatment for particle size reduction (milling, chopping, grinding, etc.) may be performed for sugar-rich feedstock (e.g., sugarcane, maize, fodder beet). For lignocellulosic-rich feedstock (e.g., straw, woody crops, and/or residues), mechanical pretreatment is followed by delignification. In this step, the lignin fraction is typically separated from cellulose and hemicellulose by alkaline deacetylation, followed by vacuum filtration [82,91]. The remaining lignin may be utilized in various applications, such as the generation of heat and electricity or the production of syngas (through gasification) for liquid fuel production [92,93]. The cellulose and hemicellulose fractions are further processed with enzymatic or acid hydrolysis approaches to recover C₅ and C₆ sugars. As a result, a hydrolysate is produced and further used as input for the pathways described in this section, namely the aqueous phase reforming (APR), DSHC, and SuF pathways.

2.3.1.1 Aqueous phase reforming (APR)

In this pathway, the generated hydrolysate (Fig. 2.2) first undergoes a purification and concentration process. In this step, numerous techniques may be applied, for instance, alkaline solvents for ash and residual lignin removal and filtration for insoluble solid residues removal [81,92]. Depending on the initial feedstock characteristics, the sugar-rich hydrolysate produced in the concentration step undergoes an hydrotreating process to convert sugars and organic acids through hydrogenation (forming polyhydric alcohols) and/or hydrogenolysis (forming shorter-chain compounds) [93,94]. Oxygen is then removed from the obtained molecules through two successive steps: the APR followed by a condensation process.

In the APR process, the aqueous phase is reacted in the presence of a catalyst under a large variety of operating conditions. A temperature range of 175–300°C (448–573K) and pressure range of 10–90 bar (1–9 MPa) are necessary [93] when catalysts such as Cu, Re, Ni, Fe, Co, Ru, Pd, Rh, or Pt are used [92]. Examples of specific operating conditions reported in the literature are summarized in SM 2.1. The reactions happening within this process strongly depend upon the specific configuration and typically include dehydrogenation of alcohols, hydrogenation of carbonyls, deoxygenation, hydrogenolysis and cyclization. As a result of this step, the water-soluble oxygenated compounds are converted into a liquid mixture (APR liquid), which is a complex mixture of hydrocarbons and undesired oxygenated hydrocarbons (e.g. alcohols, aldehydes, ketones). These may be separated at this stage or fed directly to the subsequent condensation step [94] as illustrated in Fig. 2.2. A gas phase rich in H₂, CO₂, CO and light alkanes is also produced (Fig. 2.2), which can be directly used for heat and power production [91], among other uses. Alternatively, the H₂ produced in the gas stream could be separated and recirculated to the process [91,95], prior to burning the light alkanes (C₁–C₄) for heat and electricity [91,92,95]. The exact mixture of both gas and liquid output is rather difficult to predict given the complex mixture of hydrocarbons and oxygenated hydrocarbons involved [96].

Through condensation reactions, the liquid mixture from the APR process is upgraded to longer-chain hydrocarbons. For example, base condensation is applied for the production of gasoline and kerosene. The liquid condensate may, prior to distillation, undergo hydrotreating according to the desired hydrocarbon fuels output. The resulting products are polyhydric alcohols or shorter-chain compounds depending on the hydrotreating approaches used. Dehydration of alcohols into alkanes and oligomerization (using solid phosphoric acid or zeolite as catalyst) is used for kerosene production [93]. Hydrogenation and/or isomerization might also be required to ensure conformity with the specific market requirements (e.g. the mandatory ASTM D1655 for aviation fuel blends to be used in commercial aviation) [92]. As illustrated in Fig. 2.2, these processes can be combined in different configurations and with different operating conditions to fit with the desired final product. Finally, the generated products are subsequently condensed and distilled to produce the desired aviation fuels, here as hydrodeoxygenation synthetic aromatic kerosene (HDO-SAK) or hydrodeoxygenation synthetic kerosene (cycloparaffin-rich fuel) (HDO-SK), along with hydrocarbons co-products including naphtha, and diesel [91,93]. Currently, both HDO-SK and HDO-SAK are under consideration for ASTM certification [97].

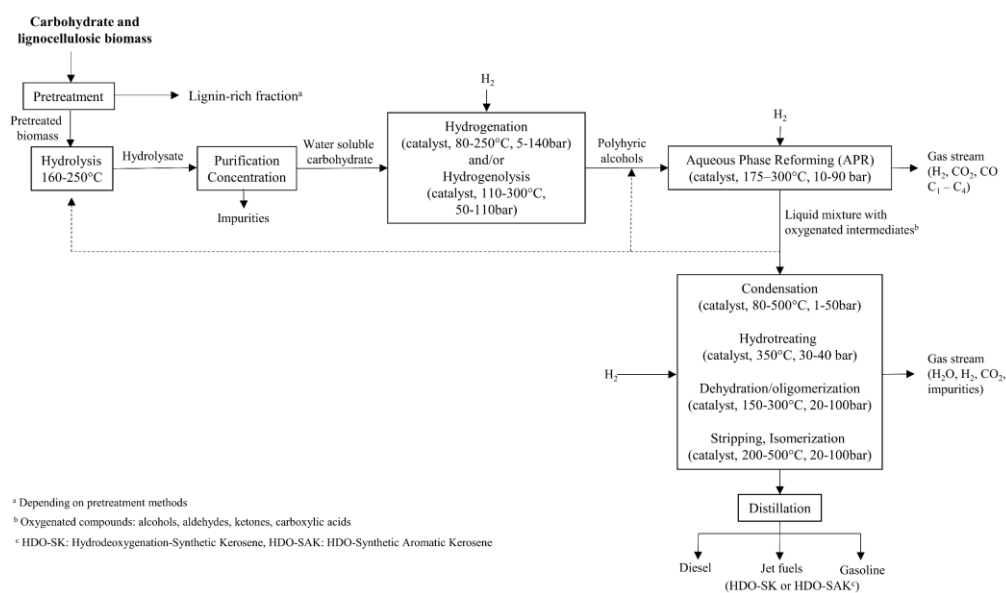


Fig. 2.2 Process flow diagram for the aqueous phase reforming (APR) pathway

2.3.1.2 Direct sugar to hydrocarbon (DSHC)

The DSHC pathway allows to produce aviation biofuels without an alcohol intermediate (Fig. 2.3). The sugars derived from the biomass feedstock input are converted to $C_{15}H_{24}$ (denoted as isoprenoid farnesene) through fermentation, subsequently hydrogenated to farnesane ($C_{15}H_{32}$), which can be used as aviation fuel [98,99]. The joint venture between Amyris and Total is the main global developer of the DSHC pathway with carbohydrate-rich feedstock such as maize, sugar beet, sugarcane [100]. These companies engineered microorganisms capable of fermenting both C_5 and C_6 sugars [101,102]. Accordingly, lignocellulosic-rich substrates can also be used as a feedstock in this pathway. Additional examples of industrial partnerships developed to produce aviation biofuels via the DSHC pathway are described in SM 2.1.

The fermentation process with the engineered yeasts takes place at operating temperatures of 30–34°C (303–304K) [101]. A liquid/solid centrifugation process separates the yeast cells and fermentation broth. The supernatant, consisting of farnesene oil, farnesene emulsion and fermentation broth, is collected for further purification. Within the purification process, the collected supernatant is heated in the de-emulsification unit (65–70°C; 338–343K) with the addition of surfactant and is transferred to liquid/liquid centrifugation in order to separate the oil and aqueous phases [101]. The distillation stage separates the contaminants into a heavy fraction containing triglyceride, monoglyceride and salts, and a light fraction of the distilled farnesene. Distilled farnesene then undergoes hydrogenation in the presence of catalysts such as Ni, Pd, Ru, Pt, Mo, Zn, etc. [103]. The purification step may be combined with hydroprocessing in downstream operations for achieving high recovery efficiency (97% reported) [101] (not shown in Fig. 2.3). The farnesane produced can be used as diesel fuel for terrestrial transport or as aviation kerosene, although the former tends to be preferred due to the low blending ratio allowed for the kerosene obtained from this pathway (10% by volume; Table S2.1). Alternatively, the farnesene can be chemically converted to produce a variety of products including fragrances, flavors, cosmetics, lubricants, etc. The co-products derived from the separation and purification step (Fig. 2.3) are reported to be used in anaerobic digestion for biogas production [102], where the biogas is subsequently led to a steam methane reforming (SMR) process in order to produce part of the hydrogen needed for the hydrogenation step.

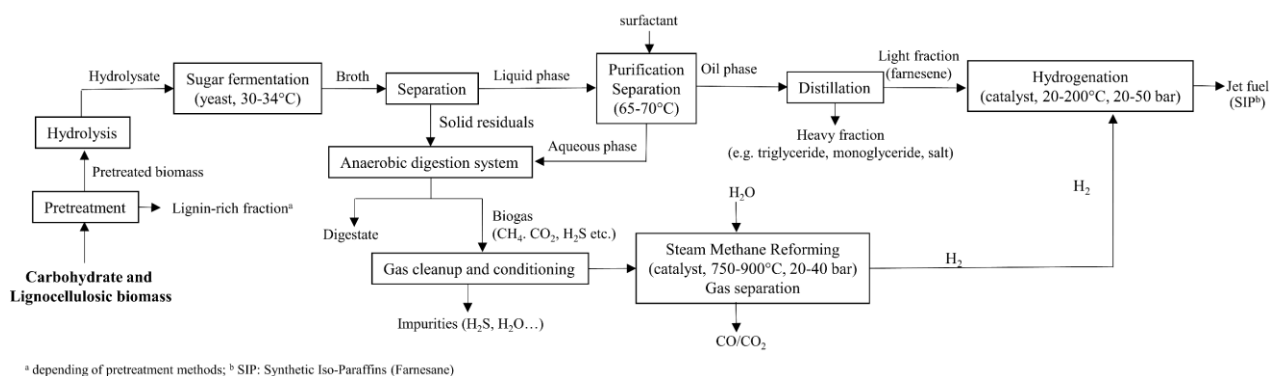


Fig. 2.3 Process flow diagram for direct sugar to hydrocarbon (DSHC) pathway

2.3.1.3 Sugar fermentation with alcohol upgrading (SuF)

This pathway is based upon the fermentation of the hydrolysate derived from carbohydrate-rich biomass (e.g. molasses, sugarcane, sweet sorghum, sugar beets, food waste, inedible fodder maize) or lignocellulosic-based biomass (e.g. cereal or rice straw) to produce alcohols [104–106]. The generated alcohol, typically ethanol or isobutanol [107,108], is then further upgraded to aviation biofuel through a series of four key processes (Fig. 2.4) described below (fermentation generating an ethanol or isobutanol intermediate, dehydration, oligomerization, hydrogenation). Both alcohol intermediates are certified by ASTM [25]. The solid residue (often referred to as distiller grains) not converted to alcohol is generally dried and sold as a protein-rich ingredient for animal feed [109–111]. This pathway is often aggregated with the SF pathway (2.2.1.1) under the umbrella of “alcohol-to-jet (ATJ)”, and the biofuels production with those pathways are referred to as ATJ-SPK.

In the fermentation step of SuF, bacteria, in particular Clostridia and a modified strain of *E. coli*, are commonly used for isobutanol production through the acetone-butanol-ethanol (ABE) fermentation process [112], albeit other microorganisms are also possible in the presence of yeast *S. cerevisiae* [113] or engineered yeast (details in SM 2.1). For ethanol, *S. cerevisiae* yeasts are typically used [114]. Fermentation temperatures from 20°C (293K) to 95°C (368K) are reported, depending upon the microorganisms used [109,113,115,116]. After the fermentation, the broth containing the desired alcohols, microorganisms and other organic compounds is separated into an alcoholic fraction and distiller grains (by e.g. membrane separations, distillation, solid/liquid separation, etc.) [109]. The alcohol obtained from the fermentation stage will typically not be pure but consists of a mixture of C₂-C₆ alcohols including ethanol, propanol, butanol, isobutanol and pentanol [109].

In the case of the isobutanol intermediate pathway, the produced isobutanol is typically converted into isobutenes in the presence of dehydration catalysts such as inorganic strong acids, metal oxides, zeolites, acidic resins, etc. at operating temperatures ranging from 250-350°C (523-623K) [105,117] (dehydration stage; Fig. 2.4). Isobutene monomers are oligomerized in the presence of acid- or metal-based catalysts, which results in a liquid mixture of longer chains alkenes (C₁₀-C₁₆) and shorter chains (C₄-C₈) ones (oligomerization stage; Fig. 2.4). Shorter chains alkenes are separated and recycled to the oligomerization unit [105]. The heavier olefin fractions (C₁₀-C₁₆) are then fed to the hydrogenation process (Fig. 2.4) [118]. The hydrogenated hydrocarbons are distilled into distinct fractions, namely the ATJ-SPK along with an isooctane co-product [52]. A variation has been proposed where the heavier olefin fractions are, prior to hydrogenation and fractionation, enriched in aromatics (C₈-C₁₆; content of ca. 20 vol.% [46]) in order to get a fuel without blending limits, leading to the production of so-called synthetic kerosene with aromatics [34]. This is promoted by among others Byogy and Swedish Biofuels and is under ASTM certification process [97,119]. However, at the light of the available information [120,121], it remains unclear whether the upstream part of this process involve direct biomass fermentation as described herein, or the fermentation of gasified biomass (i.e. syngas), which is further described in section 2.3.2.1.1. Additional details on the SuF process are presented in SM 2.1. The process with the ethanol intermediate is similar; oxygen is removed via a catalytic dehydration process, producing ethylene, then turned into linear or non-linear (branched)

α -olefins through a catalytic oligomerization process, in turn hydrogenated to produce paraffins (C_9 - C_{16} alkanes) [122].

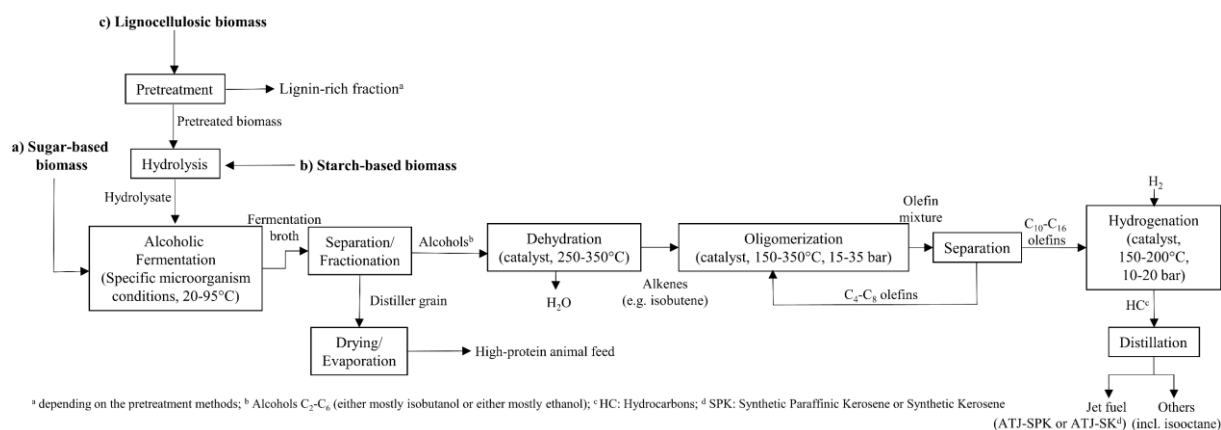


Fig. 2.4 Process flow diagram for the (conventional) sugar fermentation and alcohol upgrading (SuF) from different types of feedstocks (a, b and c)

2.3.2 Pathways handling residual and lignocellulosic biomass feedstock

Some pathways can be considered as specifically targeting residual (often lignocellulosic) biomasses such as primary forestry residues, crop residues, municipal solid waste (MSW), etc., although these can also technically be used in the previously described biofuels pathways if subjected to pre-treatments. These low-value residues have attracted tremendous attention due to their potential to avoid the competition with food production [123], and their potential important bio-physical availability [124–126]. The pathways described herein use thermochemical conversion processes to convert lignocellulosic biomasses into kerosene. The vision is whether to first convert residual biomasses to gas, and then convert this gas into liquid fuels through so-called Gas-to-Liquid (GtL) processes, or to convert the biomass into a bio-oil to be further processed to kerosene.

2.3.2.1 Biomass-to-gas via gasification: a prerequisite to several biofuels and electrofuels pathways

Gasification and anaerobic digestion are the two most known technologies to convert biomasses into gas. While the former targets biomasses with dry matter content of at least 65%, the latter is typically considered for wet biomasses (dry matter content below 30%) [127]. The exact amount of carbon from the biomass that will convert to gas, as well as the gas composition itself, will heavily depend upon the technology, process conditions and biomass composition. Anaerobic digestion can be expected to convert ca. 60% of the biomass carbon into biogas [128] while gasification is expected to convert at least 75% of the carbon into syngas [129]. The present review will, based on the reviewed pathways, only focus on gasification, as none consider anaerobic digestion (for kerosene production).

Prior to gasification, biomass must be pretreated into fine particles (80-100 mm) by mechanical techniques (including chopping, grinding) in order to enhance the efficiency of moisture removal, which in turns facilitates the biomass conversion to syngas [130–132]. Gasification typically occurs at temperatures of 600-1,000°C (873-1,273K) or even higher with controlled amount of oxidizing agent such as air, steam, oxygen, their mixture or supercritical water [130–132]. Supplying the appropriate amount of oxidizer is an important parameter for a high syngas production and for limiting the amount of by-products generation (e.g. char) [131]. During the gasification process, carbonaceous materials are transformed through several reactions including drying, pyrolysis (PL), combustion and reduction of feedstock to produce syngas, water vapor, tar, and a solid co-product denoted as char [133].

Syngas, based on the experimental data compiled by [129] for fixed bed gasifiers, is a gaseous mixture of H₂ (10-20%), CO (15-23%), CO₂ (8-18%), CH₄ (1-4%) and N₂ (42-60%). Syngas impurities are composed of tar particles, nitrogenous compounds (NH₃, HCN), sulfur compounds (H₂S, COS, CS₂), hydrogen halides (HCl, HF), and trace

metals (Na, K) [134]. Hence, syngas needs to be further conditioned to reform tar contaminants, and remove particulate matters and acid gases prior to utilization in downstream gas-to-liquid processes (Figs. 2.5 and 2.6). Depending on the gas-to-liquid process to be used, additional steps to adjust for the H₂/CO ratio of the cleaned syngas may be required. While it could be avoided entirely for the SF pathway, the FT typically requires adjusting the H₂/CO ratio to ~2.0 to avoid methane formation. In addition, syngas must be strictly purified from acid gas and ash to avoid catalyst deactivation during the FT step as well as downstream corrosion [131]. Details on gasification and syngas conditioning and cleanup processes are presented in SM 2.1.

2.3.2.1.1 Gas-to-liquid: Syngas fermentation and alcohol upgrading (SF)

The syngas deriving from waste gases from industrial processes and/or gasified biomass can be converted into various intermediate products (e.g. alcohols, organic acids) through fermentation process (Fig. 2.5) after cleanup/conditioning as above described. Different microorganisms can be used to obtain a panel of co-products [135]. Typically, the objective is to convert syngas into ethanol, which is subsequently upgraded into kerosene.

Microorganisms such as acetogenic *Clostridium* spp. convert syngas into several intermediates including ethanol, 2,3-butanediol (2,3-BDO), and acetic acid [116,136,137]. Optimum fermentation conditions intensively depend upon the microorganisms used [138], however, pressures higher than ambient pressure are preferred for enhancing the syngas transfer between the gas and the liquid phase [139]. After the fermentation, the broth including co-products and microbial biomass is fractionated through several processes depending on the co-products formed. For example, distillation is typically used for ethanol recovery [137], while simulated moving bed chromatography may be used for 2,3-BDO recovery [140].

The fermentation residue, comprising microbial biomass and other organic fractions (also known as distillation grains), is filtered [141]. The filtered liquid stream, consisting of soluble nutrient mixtures, can be further recycled back to the fermentation reactor while the filtrated insoluble sludge is typically sent to anaerobic digestion. The resulting biogas can be used for internal steam and power generation [137,140].

Ethanol may be upgraded to kerosene through a variety of processes. First, ethanol is converted to ethylene in the presence of catalysts such as γ -alumina (Al₂O₃), transition metal oxides, or zeolites at operating temperatures of 320-500°C (593-773K) [142]. Oligomerization then converts the produced ethylene to linear long-chain olefins at operating temperatures of 100-300°C (373-573K), also in the presence of catalysts [143]. Nickel complexes are commonly used as catalysts for industrial ethylene oligomerization (e.g. used in the Shell Higher Olefin Process; SHOP) [143,144]. Aluminum-based catalysts (tri-ethyl-aluminum) generate, through the Gulf and Ethyl process, linear α -olefins and by-products (alkanes and branched α -olefins) [144].

The longer-chain olefins generated are afterwards hydrogenated into alkanes. Copper, zinc chromite or sulfide are utilized as catalysts for high-pressure hydrogenation with temperature ranges of 150 and 200°C (423 and 473K) and under a pressure of 200-350 bar (20-35 MPa) [144]. Hydrogenated hydrocarbons are further distilled to recover the C₈-C₁₆ fraction known as ATJ-SPK. In addition, naphtha and diesel can be obtained as co-products [140].

The SF pathway, when deriving from lignocellulosic biomass, has an overall reported energy efficiency of 57%, while the FT pathway has an overall reported energy efficiency of 45% [145].

The fermentation pathway provides numerous advantages such as operating conditions near the ambient temperature and pressure [146]. However, the main challenge with the SF pathway is the low solubility of syngas in the fermentation medium, which limits the mass transfer to the liquid phase, in turns resulting in the generation of untargeted (or less desired) products [147,148].

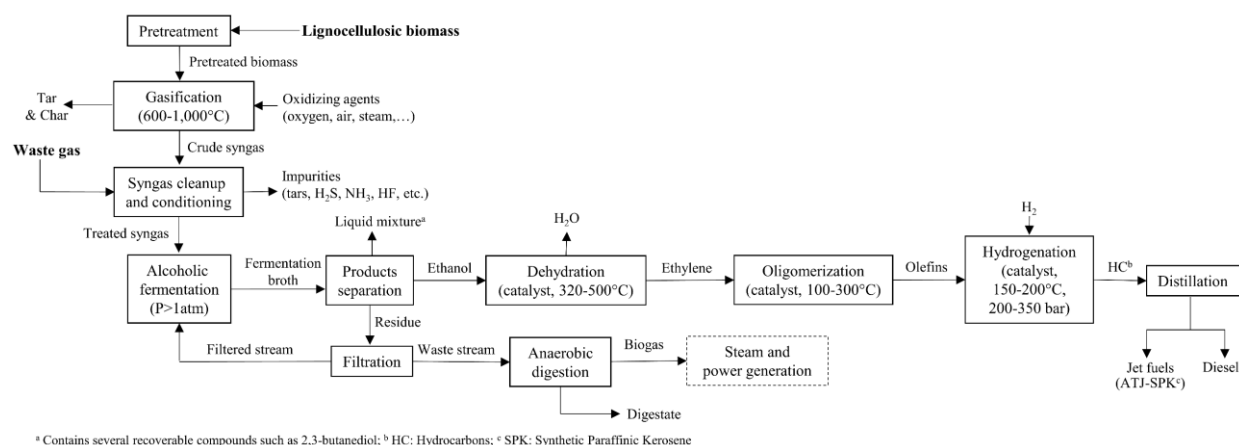
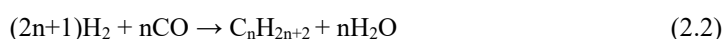


Fig. 2.5 Process flow diagram for biomass gasification, syngas fermentation and alcohol upgrading (SF) pathway

2.3.2.1.2 Gas-to-Liquid: Fischer-Tropsch (FT) process

The FT technology has been extensively used for the production of synthetic liquid fuels and chemicals (e.g. diesel; [30]; kerosene; [149,150]; naphtha; [151]). FT consists of a series of catalytic processes (Fig. 2.6) which convert purified syngas (mostly composed of H₂ and CO) into liquid fuels. During the FT synthesis, the purified syngas is passed over catalysts in specific process conditions to form a variety of hydrocarbons (ranging from gases to waxes) following three main reactions [152]:



The hydrocarbon product composition is strongly influenced by the operating temperature, pressure, syngas composition, and used catalyst [52,154–157]. The FT process can be categorized into high temperature (HTFT) and low temperature (LTFT). Gasoline, solvent oil and olefins as shorter-hydrocarbon compounds can be generated through HTFT process with operating temperatures of 310-340°C (583-613K). LTFT will typically involve operating temperature of 210-260°C (483-533K) and generate an hydrocarbon mixture consisting of ca. 50% solid wax, the remaining consisting of a liquid phase containing aromatics and cycloparaffins [150]. The wax can later be processed to produce naphtha, kerosene and diesel, among others [131,157]. It should be noted that the wax is sometimes defined as C₂₀ [158], C₂₁ [159], C₂₂ [160] or C₂₃ [150] and heavier fractions. Common catalysts used are transition metals like Fe, Co, Ni and Ru. Fe and Co are widely used catalysts, with distinct selectivity. For example, Fe-based LTFT generates higher olefins concentration as Co-based LTFT, but with lower hydrocarbon conversion and more CO₂ production. Cobalt-based catalyst is often preferred for GtL FT due to its high activity and selectivity to linear paraffins [52,161–163].

There are three fractions generated from the FT process: gaseous, liquid and wax phases. The gaseous phase represents unconverted syngas and contains CO, H₂, CO₂, and potentially N₂. It can either be fractionated for H₂ recovery or be recycled back to the FT unit in order to maximize kerosene yield [161], while a fraction (ca. 10% of the syngas) will end as off-gas (Fig. 2.6). The liquid hydrocarbons from FT undergo an hydrotreating process including deoxygenation, decarboxylation and decarbonylation in the presence of supported base metal- or supported noble metal- catalysts [149]. Additional hydrogenation may be applied for transforming olefins and residual oxygenated molecules into saturated hydrocarbons. Wax (C₂₀₋₂₃₊) produced in the FT unit are transformed to smaller molecules by hydrocracking followed by isomerization into branched hydrocarbons. Obtained hydrocarbons with different lengths are distilled to produce naphtha, kerosene, diesel and lubricants [115,150,164].

This technology allows the use of lignin deriving from lignocellulosic biomass as primary feedstock for bio-based kerosene production (SPK). The SPK derived from the FT process, denoted as FT-SPK, consists of a high

proportion of n- and iso-paraffins with a maximum of 15% by weight of cycloparaffins resulting in a high cetane number, high specific energy, and high thermal stability. FT-SPK provides a high quality kerosene in the absence of sulfur, nitrogen, and other impurities [51,94]. FT-SPK with the addition of aromatics (denoted as SPK/A) is another FT-SPK variation, certified in 2015 [34]. This variant is here considered within the overall umbrella of FT-SPK.

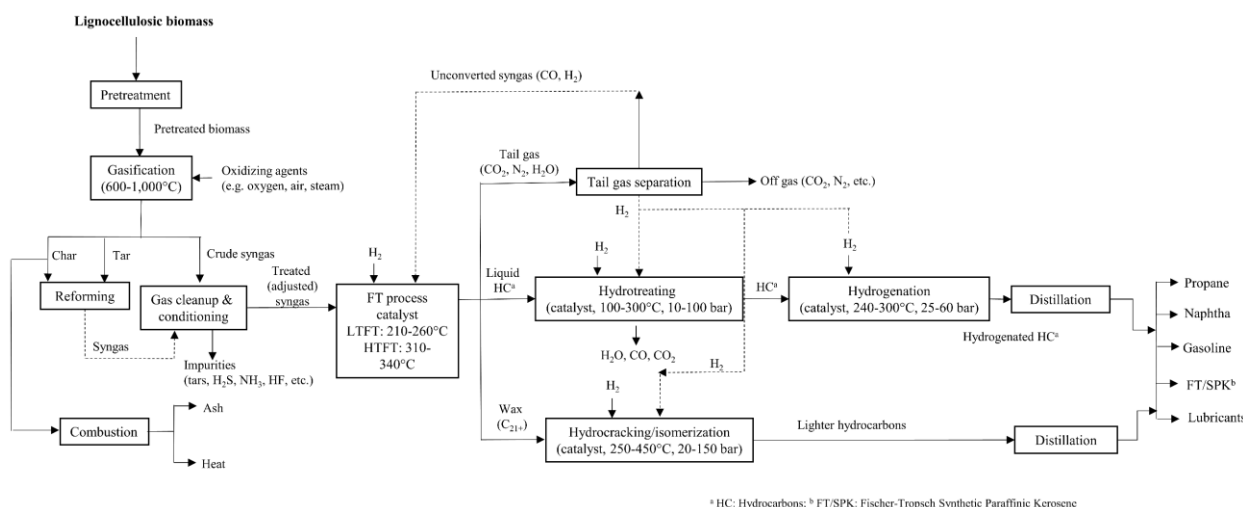


Fig. 2.6 Process flow diagram for biomass gasification and Fischer-Tropsch (FT) pathway

2.3.2.2 Hydrotreated depolymerized cellulosic jet (HDCJ)

Residual biomass can be converted into liquid fuels via a pyrolysis (PL) process, denoted as HDCJ-PL, or via hydrothermal liquefaction (HTL) for wet substrates, denoted as HDCJ-HTL (Figs. 2.1 and 2.7). Oily feedstock (e.g. waste cooking oil) can also be used directly (i.e. straight to the separation/upgrading process of Fig. 2.7).

The PL process converts dry biomass into bio-oil, gases, and biochar, the proportion and composition depending on the process conditions and the nature of the feedstock [165]. Biomass feedstock, finely ground (< 5 mm), is dried to achieve less than 10% moisture content by weight, often seen as mandatory for the PL process, especially in the perspective of quality bio-oil production intended for use as a transport fuel [166–168]. Fast PL is conducted at relatively high temperatures (450–550°C; 723–823K) and ambient pressure with short residence time of the gas phase (typically less than 2s) [169]. Fast PL is proposed for maximizing the production of liquid hydrocarbons (bio-oil) while lower temperatures PL mainly produce a solid product known as biochar [170]. In the HTL process, residual biomass reacts with water at temperature ranging from 200–450°C (473–723K) and pressures of 50–280 bar (5–28 MPa) [171] with or without a catalyst. This process is suitable for the conversion of relatively wet biomass (5–35% dry matter content) into bio-crude oil; drying pretreatment processes are therefore not necessary [169,171–174]. During the HTL process, bio-oil is produced through multiple reactions such as hydrolysis, dehydration, decarboxylation, condensation, cyclisation or, polymerization. The produced bio-oil contains lower oxygen (in oxygenated compounds) and moisture content with higher heating value in comparison to the PL bio-oil [99,175,176]. Moreover, PL bio-oil has higher acidity and weaker thermal stability relative to the HTL bio-oil [176]; therefore it requires more extensive upgrading processes. More details about the HDCJ processes and examples of industrial developments can be retrieved in SM 2.1. During the upgrading process of the bio-oil to kerosene (Fig. 2.7), distillation, centrifugation and extraction are preliminary processes for the fractionation of the bio-oil into a gaseous phase, a liquid bio-crude oil phase (the main output), an aqueous phase and solid residue (e.g. tar). Subsequently, other upgrading processes are performed, for example, emulsification, catalytic cracking and/or, steam reforming [177]. The liquid bio-crude oil phase is further refined by hydrotreating to increase its alkane composition, by reduction of heteroatom-containing molecules and by hydrogenation of unsaturated molecules. Hydrotreated hydrocarbons are distilled into liquid fuels including naphtha, kerosene and diesel.

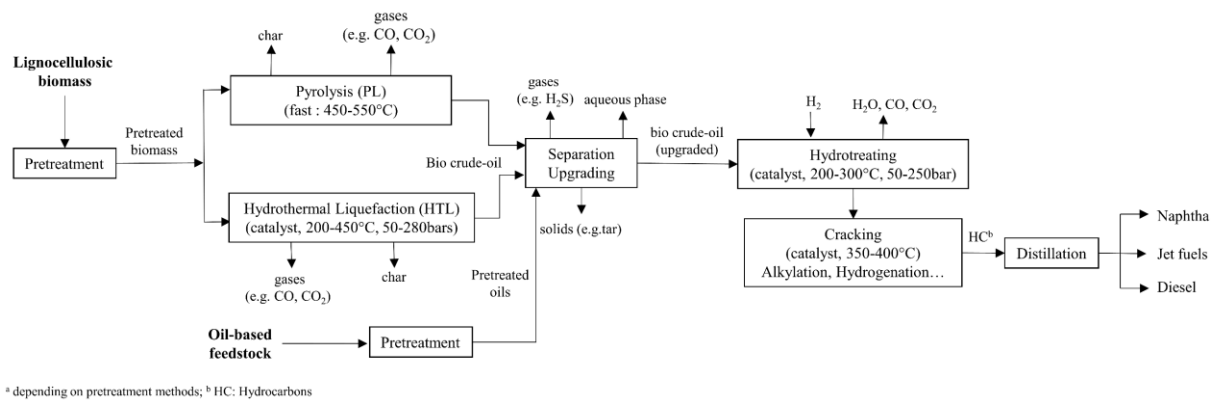


Fig. 2.7 Process flow diagram for hydrotreated depolymerized cellulosic jet (HDCJ) pathway

2.3.2.3 Integrated hydrolysis and hydroconversion (IH²)

The integrated hydrolysis and hydroconversion (IH²) pathway is characterized by a series of thermochemical processes, enabling the conversion of lignocellulosic biomass into hydrocarbon fuels, namely gasoline, kerosene, and diesel ranged hydrocarbons [178]. Four key processes are involved: pretreatment, hydrolysis, hydroconversion, and steam reforming (also known as hydrogen manufacturing unit) [178] (Fig. 2.8).

Lignocellulosic biomass is first passed to the pretreatment unit (including size reduction and drying). Pretreated biomass is sent to the catalytic hydrolysis, operated at temperatures of 350–450°C (623–723K), where it is reacted with hydrogen at an incoming pressure of 20–35 bar (2–3.5 MPa) in the presence of a catalyst. As a result, it is converted to deoxygenated vapors along with light gases vapors (C₁–C₃ hydrocarbons, and CO), and char [179,180]. This process minimizes the undesirable properties of standard pyrolysis bio-oil, namely a high acid number, low heating value, high oxygen content, low liquid fuels yields, etc., by adding hydrogen to the pyrolysis process [179]. Char is continuously removed by cyclones, followed by a hot filter [179]. Light gases are further converted to hydrogen (to be reused in the process) through a steam reformer [34,181]. Char, on the other hand, is passed to the hydroconversion reactor. It operates at temperatures 340–400°C (613–673K), at essentially the same pressure as the hydrolysis, with a catalyst that induces hydrodeoxygenation and hydrogenation to take place [181,182]. Within this unit, deoxygenated vapors are converted to hydrocarbon vapors (of gasoline, diesel, kerosene) through a hydrotreating processes (e.g. hydrodeoxygenation, hydrogenation). They are subsequently recovered through condensation (e.g. via a distillation column) to liquid hydrocarbon fuels [179,182].

Currently, this pathway is going through the ASTM certification process [34,97]. IH² could be a blending component owing to its high aromatic content (up to 92 vol.% when from woody biomass; [181]), which is above the maximum limit for aviation kerosene (25 vol.%) [46]. They can be additionally added to SPK (low/lacking aromatics) [181].

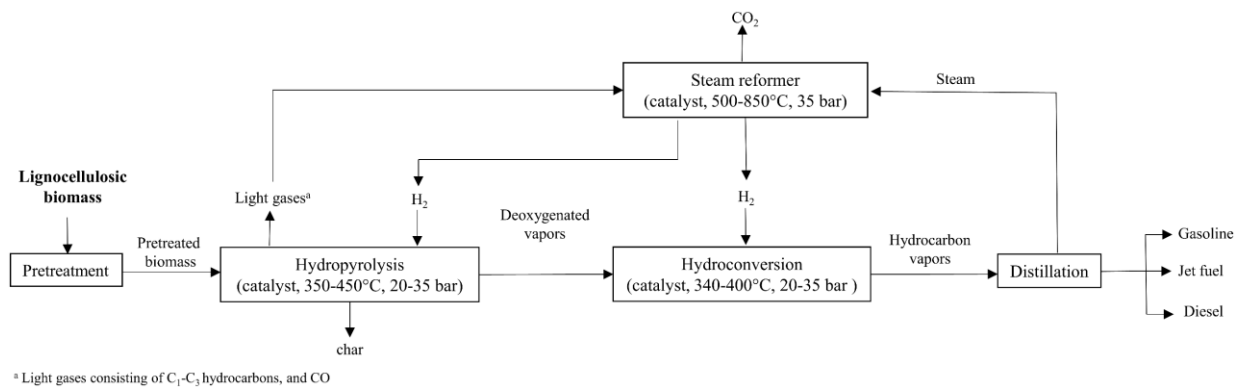


Fig. 2.8 Process flow diagram for integrated hydrolysis and hydroconversion (IH²) pathway

2.3.3 Pathways involving oil feedstock

Oil feedstock may be derived from many sources, for example, non-edible oil crops (e.g. camelina, jatropha, carinata, pongamia, pennycress) or oleochemical wastes (e.g. waste cooking oils; WCO, waste animal fats, greases stemming from municipal waste facilities). Crops are converted to oil through several processes such as, mechanical processes (e.g. chopping, pressing, chipping), chemical extraction with solvent and/or enzymatic methods [183].

2.3.3.1 Hydroprocessed esters and fatty acids (HEFA)

Triglycerides containing saturated and/or unsaturated fatty acids can be converted to liquid hydrocarbons (naphtha, kerosene, diesel) by hydroprocessing under various conditions [168,184,185], as illustrated in Fig. 2.9. In the literature, this is typically referred to as hydroprocessed esters and fatty acids (HEFA) when related to terrestrial biofuels production, and as hydroprocessed renewable jet (HRJ) when related to aviation fuels. In term of process pathway, these terminologies are here considered as equivalent.

Waste fats and oils with different degrees of unsaturation are firstly hydrogenated to saturate the double bonds leading to the production of propane along with free fatty acids. The hydrogenated fatty acids are subsequently converted into straight chain hydrocarbons through hydrotreating processes including deoxygenation, decarboxylation and decarbonylation with the formation of H₂O, CO₂ and CO, respectively [80,82,186]. Subsequently, the hydrocarbons produced are transformed by isomerization and hydrocracking reactions. Isomerization converts straight chain hydrocarbons into highly branched alkanes exhibiting a low freezing point, a desired property as a blending component. Long chain hydrocarbons are broken through an hydrocracking process to desirable carbon length compounds (e.g. in the range of C₈ to C₁₆ aviation kerosene) [187]. The product is distilled into naphtha, kerosene and diesel [188,189].

Several parameters have an impact on product generation during the HEFA process, for instance, the type of catalyst used, the fatty acids profile of the feedstock used and the operating conditions [188,190,191]. A variety of research and industrial experiments resulting in the production of aviation biofuels with the HEFA pathway under various conditions are summarized in SM 2.1.

The HEFA pathway is considered as a relatively mature technology at commercial scale. However, the availability and the cost of the sustainable oleochemical feedstock, in particular if waste-based (as in e.g., [192,193]) or relying on limited marginal lands (e.g., [194–197]) to grow the feedstock, may become a limiting factor in the perspective of increased biofuels demand in the future. The HEFA pathway with the variant of using third-generation feedstock (e.g. oils stemming from microalgae *Botryococcus braunii*, denoted as Bb oil) has been recently certified (ASTM approved for 10% maximum blend in 2020) [198]. This pathway produces biofuels known as hydroprocessed hydrocarbons HEFA-SPK (HH HEFA-SPK).

High freeze point HEFA-SK (HFP HEFA-SK, also known as HEFA+) is another variation of already certified HEFA, nearing final ASTM approval [97,119]. The production cost is expected to be reduced as involving lower requirements for the upgrading process (e.g. isomerization) relative to HEFA-SPK [34]. This is among others due to the longer length of the molecule chain, varying from C₁₅ to C₁₈ [34,199,200].

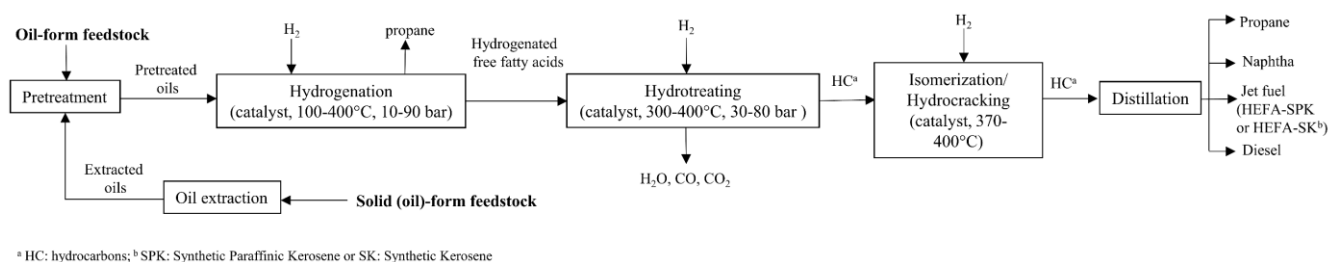


Fig. 2.9 Process flow diagram for hydroprocessed esters and fatty acids (HEFA) pathway

2.3.3.2 Catalytic hydrothermolysis jet (CHJ)

The CHJ pathway, similarly to the HTL process, is based on high temperature water chemistry (hydrothermal processes), converting oil-based feedstock into a mixture of straight, branched and cyclic hydrocarbons as shown in Fig. 2.10. The process is composed of four steps including hydrothermal pre-conditioning, catalytic hydrothermolysis (CH), upgrading through hydrotreatment and products fractionation.

During the pre-conditioning stage, the oil-based material is cracked resulting in the production of free fatty acids with the removal of heteroatoms (S, N, metals, etc.) in the presence of steam and catalyst under operating temperatures of 150-300°C (423-573K) and pressures of 5-50 bar (0.5-5 MPa) [201]. These generated fatty acids are converted in a CH unit at elevated temperature (240-450°C; 513-723K) and pressure (15-250 bar; 1.5-25 MPa) [201]. Within the CH unit, numerous reactions take place including cracking, hydrolysis, decarboxylation, isomerization, and cyclization to produce a mixture of paraffin and cyclic hydrocarbons. In a nutshell, the outputs of the CH unit consist of an organic phase and an aqueous phase. The aqueous phase is composed mostly of low molecular weight carboxylic acids (C₂-C₅), glycerol, and some of small polar molecules [201]. They are transformed through decarboxylation and dehydration into alkene products. These intermediates could be upgraded to aviation biofuels through alcohol recovery stage (oligomerization, hydrogenation and distillation) as described above. The organic phase, referred to as CHJ bio-crude, is further decarboxylated, hydrogenated, and finally distilled into several product fractions including naphtha, kerosene (denoted as catalytic hydrothermolysis jet-synthesized kerosene; CHJ-SK) and diesel [202].

Aviation biofuels obtained with this process contain high density aromatics, iso-paraffins and cycloparaffins [201,203]. Additional details on the CHJ pathway and its industrial developments are presented in SM 2.1.

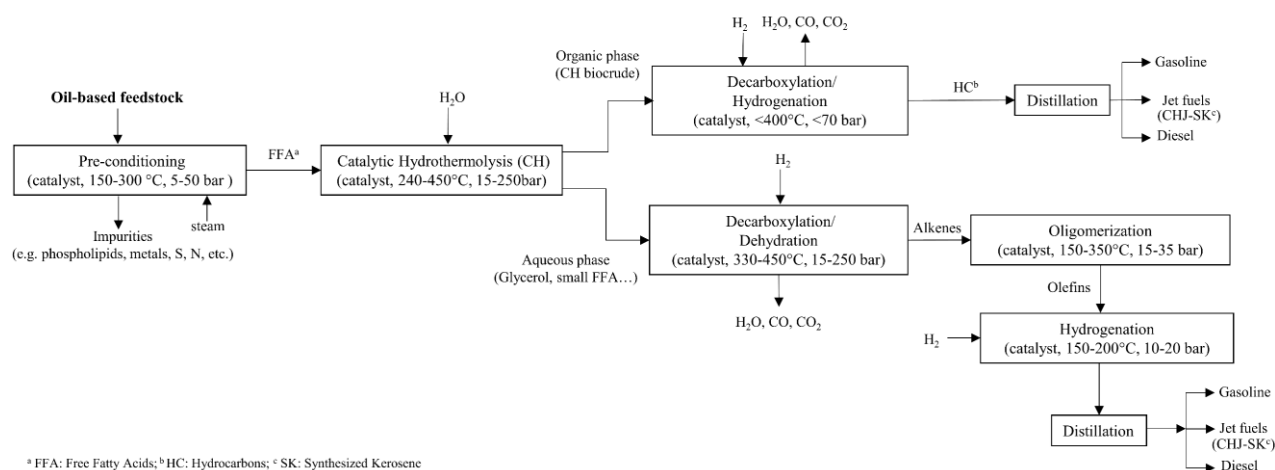


Fig. 2.10 Process flow diagram for catalytic hydrothermolysis jet (CHJ) pathway

2.4 Aviation liquid electrofuels

Electrofuels (power-to-liquid) allow, pushed to its extreme, to decouple the production of kerosene from the demand of biomass, relying on water-based hydrogen (H₂), and atmospheric CO₂ [28,204]. Through hydrogen produced from water electrolysis, electrofuels involve the storage of electrical energy within chemical bonds in the form of liquid fuels, these providing more energy density and lower aircraft mass, compared to emerging electric (battery) aviation and hydrogen aviation.

Clear climate benefits have been documented when renewable sources of energy (whether electricity or heat) are employed to produce the required H₂ [186–188; SM 2.2].

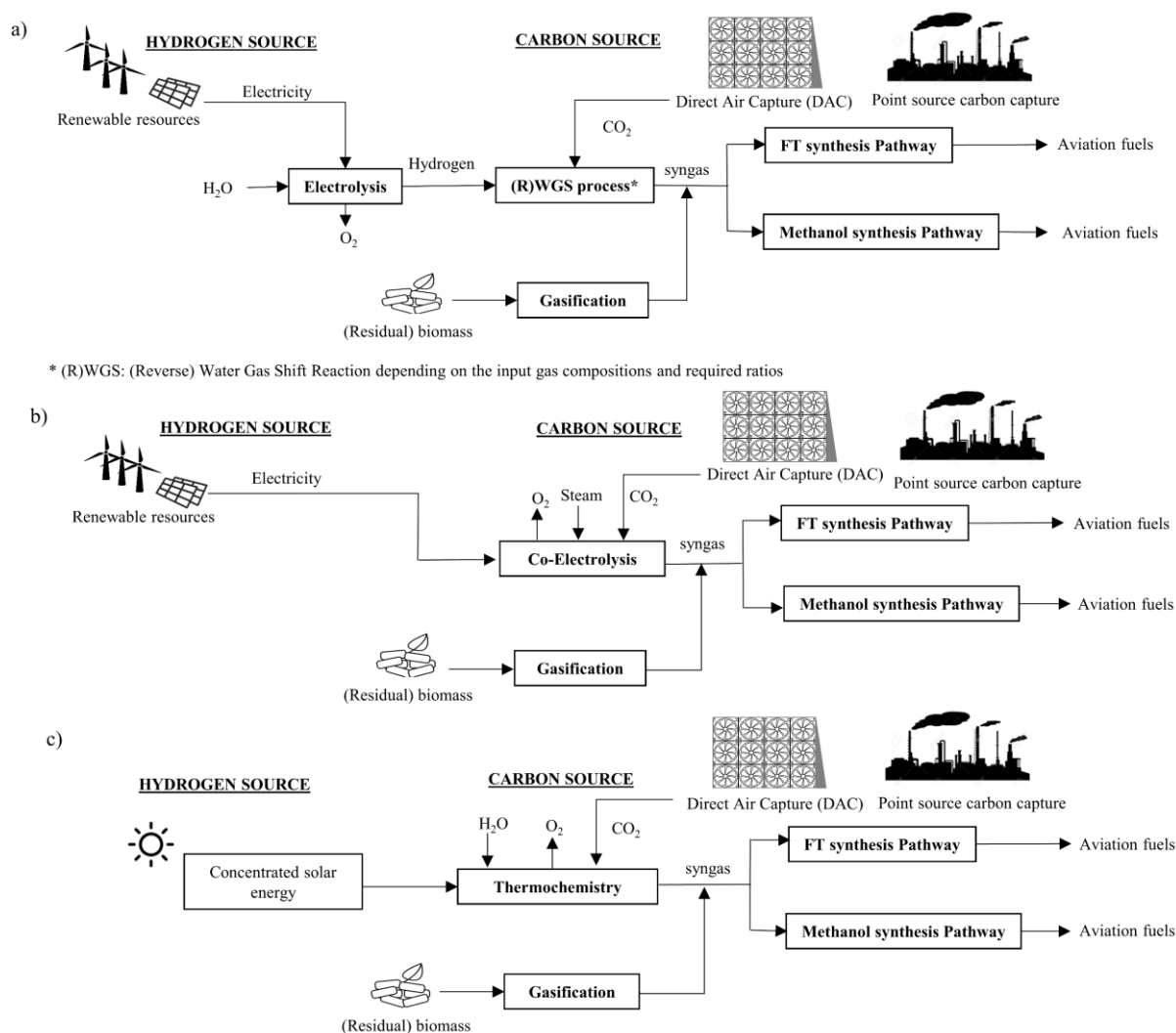


Fig. 2.11 Electrofuels production process by water electrolysis (a), co-electrolysis (b), and solar thermochemical process (c). The FT and methanol synthesis comparisons can be found in Table S2.3 (SM 2.1).

2.4.1 Hydrogen supply

There are several pathways to produce hydrogen with different resources, e.g. from fossil fuel resources through steam reforming and/or partial oxidation, from non-fossil resources through biomass gasification or fermentation, and from water-splitting technologies [208–212]. Today, around one-third of global hydrogen supply is obtained as a by-product from industrial processes, (e.g. chlorine production from electrolysis of brine; [213–215]). Here, the focus is on hydrogen production decoupled from a carbon source, and as the main product driving the production process.

Water is a promising resource generating growing interest for hydrogen production. Several pathways are possible, such as electrochemistry (including water electrolysis and photo electrolysis) [216,217], thermochemistry [218], or biological water-splitting such as bio-photolysis [37,211] as summarized in Fig. 2.12. The latter, along with photo-electrolysis, have however not been considered any further herein, being still in early development stages.

Water electrolysis, in particular if powered with fluctuating power in excess of demand, has attracted growing attention as a process to generate so-called green hydrogen [210,219]. There are different water electrolysis technologies available such as alkaline electrolysis [220], proton/polymer exchange membrane (PEM) electrolysis [221], or solid oxide electrolysis (SOE) [222,223] (details on these technologies are presented in SM 2.1).

However, these technologies remain relatively expensive, and their profitability is bound to low renewable energy prices [66,70]. Alkaline electrolysis, for example, provides two to four times the production cost of the conventional steam reforming of natural gas [70,224,225], as further detailed in SM 2.1.

2.4.2 Carbon sourcing

Carbon sources include (i) biomass (undergoing gasification), (ii) fossil or biogenic carbon stemming from industrial activities captured at a point source (e.g. biofuel/bioethanol production, waste gases from steel production and cement industry, from biogas upgrading process, mine gases, etc.; here denoted as point source CO₂) and (iii) atmospheric carbon captured by DAC (Fig. 2.11) [137,204]. As DAC, point source carbon also requires a capture process, as further described in SM 2.1. It should be noted that biomass here also acts as source of H₂.

There are two major technical approaches for DAC. One is based on the absorption of CO₂ using low-toxicity solvents such as water (through a scrubbing process) and alkaline aqueous solutions (NaOH, Ca (OH)₂ KOH) with a CO₂ strong affinity. In addition to water and alkaline solutions, amino acid salts, ammonia, polyglycol ether and ionic liquids can also be used as solvent for CO₂ extraction [226]. The solvent-based technology is mature and is already applied in large-scale plant, however, the solvent regeneration is a high energy-consuming process. The second approach utilizes an alkaline carbonate bonded to a mesoporous solid support in which the sorbents can be easily regenerated. The most promising technology is the use of supported amine materials; this solid sorbent-based approach revealed higher sorption performance with higher capacities and selectivity, and lower heating requirement compared to the liquid sorbent-based method [39,227]. However, the tradeoff is the high operational expenditure resulting from sorbent degradation [227].

On the other hand, capturing technologies for industrial point sources are already well addressed and deployed (details in SM 2.1). CO₂ concentrations vary greatly according to the origin of the point source, ranging from 15-30 vol.% for the cement industry, to up to 90-100 vol.% for natural gas processing [228,229]. The capture cost is around ten times less than the DAC technology cost, and is mainly associated to the cost of energy needed [38,85,228,230].

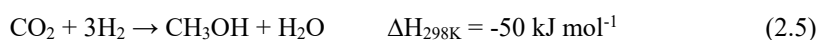
2.4.3 Liquid hydrocarbon synthesis

In this step, hydrogen is combined with CO₂ to produce syngas. This happens with a reverse water gas shift reaction (i.e. reaction (6) below, from right to left) in the direct electrolysis pathway (Fig. 2.11a) or through a co-electrolysis process where water thermal splitting and reverse water gas shift reactions jointly occur, thereby converting steam and CO₂ into syngas [231] (Fig. 2.11b). This is in particular possible with high temperature electrolysis using SOE (600-1,000°C; 873-1,273K) [231]. Co-electrolysis provides high conversion and energy efficiencies utilizing the industrial waste heat derived from other industrial processes such as the FT synthesis [82,223]. The reverse water gas shift reaction implies operating conditions of varying from ca. 300--800°C (573-1,073K) depending on the use of a catalyst (typically copper-based; [232-235]) as well as the operating conditions (e.g., syngas compositions; [235]).

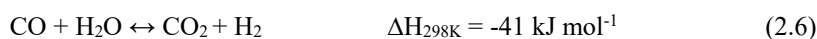
As shown in (Fig. 2.11c), a third option is to thermochemically combine H₂ (from H₂O) and CO₂ for syngas production through the direct use of concentrated solar radiation as energy source. Nuclear and geothermal resources are also possible [236]. Here, the H₂O and CO₂ conversion into syngas is carried out by multi-step thermochemical cycles such as cerium-chlorine, copper-chlorine, sulfur-iodine, iron-chlorine, etc. [209,236-238]. This was demonstrated in the SOLARJET project [209], with a 4 kW solar reactor prototype. The upscaling of this solar thermochemical reactor (50 kW) is being performed within the SUN-to-LIQUID project [212,239], where syngas is to be produced from concentrated solar energy.

To produce liquid fuels, the syngas is further used in either the FT or methanol synthesis process, as depicted in Figs. 2.11a-c (and Table S2.3). For the FT route, the syngas-to-kerosene conversion is exactly as described for biofuels (Fig. 2.6).

In the methanol route, syngas is converted at temperatures of 150-300°C (423-573K) and under pressures in the range of 10-100 bar (1-10 MPa) in the presence of copper-based catalysts (e.g. Cu/ZnO) [240]. The hydrogenation of CO/CO₂ can be described by the following reactions [241]:



The water gas shift reaction occurs simultaneously according to the following reaction [241]:



Subsequently, the methanol is condensed and separated by distillation. It can then be processed to the desired chemicals and fuels [240,241]. This conversion and upgrading of methanol to desired fuels and chemicals comprises several processes depending on the preferred target product. For instance, methanol may be used for olefin synthesis (an alkene intermediate to produce kerosene) via di-methyl ether, oligomerization and hydrotreating [45,240,242]. The methanol generated from syngas could also serve for the production of gasoline (denoted as methanol-to-gasoline), as currently done in commercial plants, for example ExxonMobil [243]. However, no aviation electrofuels have yet been produced via the methanol pathway [45]. On the other hand, FT-SPK has already been tested, and approved by ASTM D7566 as a blending constituent. To the best of our knowledge, the first electrofuel industrial plant (Power-to-Liquid for the production of e-kerosene) was officially opened at the beginning of October 2021 in Werlte (Emsland, Germany) [244]. The Lufthansa Group announced, in October 2021, purchases of at least 25,000 L (ca. 25 m³) annually over the next five years [245].

2.5 Co-products generation in liquid fuels production pathways (biofuels and electrofuels)

The technologies previously described (sections 2.3 and 2.4, Figs. 2.2-2.11) generate, besides the desired fuels, multiple co-products, no matter which route is used. As such, biofuel/electrofuel production pathways are to be seen as refineries rather than mere kerosene suppliers (Table S2.2). Their co-products include liquid fuels (other than kerosene), chemicals, animal feed, etc. and their generation depends on the specific technologies and operating conditions being used within a given conversion route as illustrated in Table 2.1. In some cases, it may also depend upon market conditions, where the production chain can flexibly be adjusted towards enhanced production of the most valuable product. These co-products represent an additional market or value generation opportunity for the production plant. These co-products are here grouped in three major categories: chemicals, liquid fuels, and other products.

2.5.1 Chemicals

Various chemical compounds are generated as co-products during production processes. Those that have been reported by biofuel producers are detailed here.

2.5.1.1 Propane

Propane (C₃H₈) is formed as a co-product in the FT and HEFA pathway (Figs. 2.6 and 2.9, respectively). Propane is used in a variety of applications, for instance as a fuel for commercial boilers, camping stoves, heating animal houses (e.g. piglet nursery) in livestock production, etc. It can also be used as refrigerant [246,247]. Propane is generally pressurized and stored as liquid in storage vessels or tanks. Due to its high energy density and high quality combustion characteristics, propane is also used as alternative vehicle fuel for internal combustion engine [248,249]. Propane is categorized as one of the bulk components of liquefied petroleum gas (LPG) in combination with other gases such as butane, isobutene, isopentane. Currently, propane is typically generated as a co-product of natural gas processing and petroleum refinery [144]. The cost of propane thus corresponds with fossil fuels resources. The global propane market has been estimated to reach \$84 billion (with 200 million tonnes in its production) by 2030 [250].

2.5.1.2 Naphtha

Naphtha is a mixture of liquid hydrocarbons comprising carbon compounds ranging from C₅-C₉ [251]. Naphtha is the main combustible component of both gasoline and kerosene. It has a great potential for diverse industrial purposes including plastic production or its use as a cleaning extraction or dilution agent [252,253]. Naphtha is traditionally generated as a co-product in fractional distillation processes from the petrochemical industry, including the production of (fossil-based) kerosene for aviation fuel. The market price of naphtha is thus closely tight to the price of crude oil [254].

Biofuel pathways involve the production of naphtha as a co-product (including FT, HDCJ, and HEFA; Figs. 2.6, 2.7, and 2.9, respectively). It can be recirculated within the process, for instance in the FT pathway it can be fed into the partial oxidation unit and reformed as syngas feedstock to produce a greater amount of aviation fuel [255]. Additional examples of such bio-based naphtha use are described in SM 2.1.

2.5.1.3 2,3-Butanediol (optional)

2,3-BDO (C₄H₁₀O₂) is a bulk commodity chemical. It is seen as a promising fuel additive or gasoline blendstock for enhancing the octane number [256]. 2,3-BDO is readily convertible to butadiene, butane, methyl-ethyl ketone (MEK) which could be used as intermediates in a variety of product manufactures. In particular, MEK is used in several applications such as solvents in surface coating, printing inks, dewaxing agent, liquid fuel additive, indirect food additive for adhesives and polymers [257]. According to [256,258,259], 2,3-BDO will reach a global market around \$220 million by the year 2027.

2,3-BDO is usually produced on the industrial scale by conventional chemical (or synthetic) methods [260,261]. In the production of aviation biofuel, 2,3-BDO is involved in the SF pathway (Fig. 2.5). It is not directly generated (hence the optional label above), but can be recovered providing adjustments to the product separation step prior to ethanol production, if favorable market conditions makes it desirable [256]. For recovery, the fermentation broth including liquid mixture or a mixed alcohol stream containing 2,3-BDO would be processed with separation techniques such as fractional distillation, evaporation, pervaporation, adsorption [256]. For instance, LanzaTech has patented the production of 2,3-BDO from CO-rich industrial waste gases (from the steel industry) by fermentation (Table S2.2). Their commercial ethanol/2,3-BDO production plant has a production capacity of 30-50 million gallons (ca. 0.11-0.19 million m³) and costed \$75-125 million. In partnership with Orochem Technologies (USA), LanzaTech seeks to economically convert its 2,3-BDO into MEK or 1,3-butadiene through thermocatalytic processes [256].

2.5.1.4 Isobutene (optional)

Isobutene (C₄H₈) may be optionally recovered in the SuF pathway. It is produced after dehydration of alcohols, just prior the oligomerization process (Fig. 2.4). If the market conditions are favorable to isobutene, a choice could be made to stop the process after the dehydration process for a certain proportion of the stream, and not continue further to kerosene production. Isobutene production thus implies less bio-based kerosene production; hence its “optional” label.

Isobutene is used as a building block in the manufacturing of several industrial products namely fuel additive, butyl rubber, plastic and lubricants, domestic gas, chemicals and cosmetics, etc. Isobutene can be reacted with methanol leading to methyl tert-butyl ether (MTBE) or with ethanol leading to the production of the gasoline additive ethyl tert-butyl ether (ETBE), used as an anti-knocking agent for the automotive industry [262]. The isobutene polymerization generates butyl rubber that can be used as precursor in several products such as window seals, bottle stoppers, protective gloves, etc. Isobutene is also one of the main constituents of LPG. Moreover, isooctane (a gasoline blendstock) could be generated by dimerization of isobutene [262].

Currently, isobutene as a key chemical building block, is massively obtained from petrochemical sources. Being a major precursor in various industrial applications with continuous demand, its market is worth \$25 billion with 15 million tonnes produced annually and used as cosmetic ingredients and specialty fuels [263].

2.5.2 Liquid fuels

2.5.2.1 Isooctane

Isooctane is a co-product produced in the SuF pathway (Fig. 2.4), during the oligomerization/hydrogenation steps. Isooctane represents a large share of gasoline composition and has properties (e.g. high energy content, high antiknock quality) that make it suitable as a blending component for the production of premium-grade fuels [264]. Isooctane is typically produced through the dimerization of isobutene and isopentene generated as by-products from steam cracking of naphtha and light gas oil in refineries, dimer separation and hydrogenation in conventional industrial processes [264]. Isooctane is further used as a feedstock to produce gasoline, in a process where it is blended with naphtha [265].

The major market for the isooctane co-product generated in the production of aviation biofuels appears to be its use as drop-in blending component for the automotive industry, with a global market reaching \$99 billion in 2019 [266]. Yet, new markets are also emerging. For instance, high purity solvents or specialty fuels used for racing and classic cars [267].

2.5.2.2 Gasoline

Gasoline is a refined product of petroleum consisting of hydrocarbon mixtures, additives and blending agents. The gasoline composition strongly depends on various parameters such as the crude oil sources, the refinery process available and product specification defined by octane rating [268]. Gasoline may be generated in particular in the SuF (Fig. 2.4) and FT (Figs. 2.6 and 2.11) pathways. In the latter, gasoline is not directly produced as a co-product, but can be produced from the isooctane generated as explained above. Similarly, gasoline (C_5 - C_{12} hydrocarbon ranged; [269]) can also be produced from the APR, FT, and CHJ pathways (Figs. 2.2, 2.6, 2.10, respectively); it is not directly visible in the figures, but is captured within the naphtha fraction. The fraction generated strongly depends upon the operating conditions, which in turn can, to some extent, be adjusted according to the market value of bio-based kerosene, diesel and gasoline. For instance, in the production of aviation biofuel through LTFT process, the proportions of gasoline observed correspond to approximately 10-15% of product distillation output [270]. Additional information about renewable gasoline is described in SM 2.1.

2.5.2.3 Diesel

Diesel is a key fuel powering compression ignition engine. As for gasoline, it is derived from petroleum refining, and its exact composition is influenced by market demands and prices.

Diesel with carbon distribution ranging C_{10} - C_{20} is produced in aviation biofuel pathways such as SF, FT (Figs. 2.2, 2.5, and 2.7-2.10) and in considerable volumes. It is optionally produced in the SF pathway, derived from ethanol upgrading processes. Furthermore, diesel is also generated as the co-product from the FT process where the volume produced is also depended upon the operating conditions [270]. The main market for the diesel co-product appears to be as a renewable fuel for terrestrial transport as reflected by several recent examples of purchasing agreements and collaboration deals detailed in SM 2.1.

2.5.3 Others

2.5.3.1 Waxes

Waxes are generated as a co-product in the FT pathway (Figs. 2.6 and 2.11). They consist primarily of straight chain alkanes (C_{20-23+}) which are typically not used in fuel refinery due to their physical properties with i.e. high melting point, low viscosity and hardness. During the LTFT route, the heavy fraction of the FT syncrude accounts for 20-30% weight of total hydrocarbons. The molecular mass of the wax fraction generated is higher relative to the wax produced in the HTFT process [270]. These wax fractions can be cracked into lower molecular weight compounds appropriate for use as liquid fuels or may be sold as precursor of a variety of products. These heavy alkanes have a high potential commercial value due to their competitive prices and versatility in both industrial and medical applications including petroleum jellies, lithium grease, engine oil, industrial gear oil, industrial cleaners, adhesives, etc. [271]. Examples of wax purchase agreements are listed in SM 2.1.

2.5.3.2 High-protein animal feed

An animal feed co-product is generated in the SuF pathway (Fig. 2.4), where the protein-rich solid residues derived from the fermentation broth can be further processed. Upon drying, these are often referred to as distiller dried grains, and typically have a high concentration of crude protein with an amino acid profile suitable for animal feed [272]. Ten pounds (around 4.5 kg) of animal feed can be produced from one gallon (ca. 0.0038 m³) of aviation biofuel [273]. As in the case of the distiller dried grains co-generated with bio-based alcohol (e.g. ethanol) production, the access to the feed market is real and already in place [274].

Table 2.1 Summary of the co-products generated in the various liquid biofuels production pathways for aviation

Co-product	Conversion pathways	Production status	Market uptake and Displacement	Co-product ratio ^a (kg MJ ⁻¹ kerosene) (% mass) ^b
Chemicals				
Propane	FT HEFA	Generated from triglyceride hydrogenation	<ul style="list-style-type: none"> • One of the main LPG constituents • Used as fuel in numerous applications (e.g. commercial boiler, burner, etc.) • Displaces fossil-based propane from petrochemical sources (natural gas processing, crude oil refinery) 	0.0003 ^{1,12} (1.1%) 0.004 ^{2,3} (9.7%)
Naphtha	FT HDCJ HEFA	Generated along with aviation biofuel (final production step)	<ul style="list-style-type: none"> • Gasoline blending component • Precursors for plastics manufacturing • Can be recycled in the FT unit to produce additional aviation fuel • Displaces fossil-based naphtha from petrochemical sources 	0.0004 ^{1,12} (1.3%) 0.019 ⁴ (27.0%) 0.005 ^{2,3} (12.5%)
2,3-butanediol (2,3-BDO)	SF	Generated along with ethanol, may be recovered through a separation process before the ethanol production (optional)	<ul style="list-style-type: none"> • Conversion to various precursors namely MEK, 1,3-butadiene, etc. • Displaces 2,3-BDO from chemical engineering (or synthetic) methods 	0.013 ⁵ (if they are recovered from the fermentation process) (33.0%)
Isobutene	SuF	Derived from isobutanol, which can be further processed the dehydration (optional)	<ul style="list-style-type: none"> • Precursor for numerous products such as butyl rubber, plastics, isooctane, etc. • One of the main LPG constituents • Dimerization for isooctane production • Polymerization in butyl rubber production • Displaces isobutene from petrochemical sources 	Unclear, because isobutene is an intermediate that can either be processed (fully or partly) to kerosene or not depending on the market context (flexible production)
Liquid fuels				
Isooctane	SuF	• Generated along with aviation biofuel (final production step)	<ul style="list-style-type: none"> • (Premium-grade) gasoline production • Displaces fossil-based isooctane from petrochemical sources 	0.002 ^{6,7} (7.5%)
Gasoline	APR FT IH ² CHJ	<ul style="list-style-type: none"> • Derived from isobutanol in the SuF process, which can be further upgraded to isooctane (optional) • Generated along with aviation fuel (final production step) 	<ul style="list-style-type: none"> • Transportation fuel • Displaces fossil-based gasoline derived from petrochemical source 	0.003 ⁸ (8.0%) 0.004 ^{a,1,12} (14.7%) 0.086 ⁹ (72.2%) 0.016 ¹⁰ (28.1%)

Diesel	APR	<ul style="list-style-type: none"> • Generated along with aviation fuel from APR, FT and HEFA processes • Derived from isobutanol in the SuF process, which can be further upgraded to diesel (optional) 	<ul style="list-style-type: none"> • Transportation fuel • Displaces fossil-based diesel derived from petrochemical sources 	0.012 ⁸ (32.0%)
	SF			0.003 ⁵ (8.7%)
	HDCJ			0.028 ⁴ (40.1%)
	HEFA			0.009 ^{2,3} (21.1%)
	IH ²			0.010 ⁹ (8.3%)
	CHJ			0.018 ¹⁰ (31.0%)
Others				
Waxes	FT	<ul style="list-style-type: none"> • Generate along with aviation biofuel (final production step) • Derived from fermentation residues and may require further processing such as evaporation/drying 	<ul style="list-style-type: none"> • Raw materials for various products such as petroleum jellies, adhesive, etc. • Displaces petrochemical-based waxes • High protein and nutrient concentrations derived from dried distiller grains • Displaces marginal carbohydrate, protein and lipid sources (maize, soybean meals and palm oil) in animal feed 	0.001 ^{1,12} (2.9%)
High-protein animal feed	SuF			0.037 ¹¹ (59.4%)

Notes. ^a Co-product ratios presented are extracted from the available literature in which the operating conditions intend to maximize kerosene production. This could not be done for the advanced IH² process, which is currently essentially used for gasoline production as demonstrated in the study of [181].

^b The mass (%) of the co-products are provided in parenthesis. This includes the % (mass) out of all products (including kerosene); therefore the total is lower than 100%. The calculation procedure can be retrieved in SM 2.2. The considered lower heating value (LHV) of kerosene is 43.0 MJ kg⁻¹.

References: ¹ [150]; ² [275]; ³ [276]; ⁴ [277]; ⁵ [140]; ⁶ [278]; ⁷ [279]; ⁸ [280]; ⁹ [181]; ¹⁰ [281]; ¹¹ [273]; ¹² [282]

2.6 Electric (battery) aviation

Batteries can serve as the energy sourcing for either propulsion (as further explained in section 2.10.1) or non-propulsion systems (overall electricity within the aircraft). The latter is often referred to as the “more electric” architecture, and is applied in aircraft to power services such as the flight control system and cabin environmental control system, or the auxiliary power unit (APU) [57,283,284]. “More electric” architectures were implemented in the Airbus A350 and Boeing 787 [59,283].

Albeit battery is one of the most promising energy sourcing (for propulsion) in terms of climate impacts (further discussed in section 2.8), there are several limitations to overcome for a widespread implementation within aviation. First, they cover essentially short-haul flights due to the limited energy storage capacity. Table 2.2 details the emerging lithium-based battery technologies for aviation applications [284]. The present lithium-ion batteries (Li-ion) have a maximum specific energy of 400 Wh kg⁻¹ (1.44 MJ kg⁻¹) [57,285], which is relatively low in comparison with conventional kerosene, having a specific energy density of ca. 12,000 Wh kg⁻¹ (43.2 MJ kg⁻¹). This introduces a crucial mass penalty factor to consider [284,286,287], and affects the final supplied service (e.g. reduction of the number of seats and thus passengers carried, a lower distance travelled; [64,286]).

To overcome this challenge, different innovations are in place. The main focus has been on the use of different materials for the cathode/anode, and on the use of different electrolytes (Table 2.2). This has led to the development of high performance batteries including advanced lithium metal/silicon anode (Adv. Li-ion) [57], solid-state electrolyte battery (SSB) [285,288], lithium-sulfur (Li-S) [289,290] and lithium-air (Li-air) batteries [291,292]. Moreover, nickel-rich NCM (Nickel-Cobalt-Manganese)-811 cathodes [57,293], alternative anode material to graphite (e.g. silicon, lithium metal) [294], approximate solid-state electrolytes in SSB [57], prevention of polysulfide shuttle effects in Li-S batteries [295,296] and improvement of moisture sensitivity in Li-air batteries [292,297] are additional avenues being investigated.

Other advances for batteries have been introduced, for instance with systems based on sodium, magnesium, zinc, and aluminum [298], albeit, still in the early stage of research and development. These can be potential candidates to substitute the lithium, cobalt, natural graphite, silicon metals used as the major materials for the electrodes (defined as EU critical raw materials; CRM [299]) [300]

Another concern applying to battery electric aviation relates to safety, among other associated with overheating of the battery, which can cause failure of thermal runaway, known to be a key cause of undesired incidents [301,302]. For example, the fire incident of the Boeing 787 Dreamliner in 2013 was reported to be due to the failure of the Li-ion batteries, powering the aircraft APU [303]. Therefore, the development of high-performance, long-lived batteries with thermal stability is one of the numerous technological challenges to be solved before broad deployment [293].

One other important issue relates to the charging time of batteries and the possibility to recycle them after their limited lifetime (>1,000 cycles for current Li-ion batteries; [57]). The battery swapping station model, where batteries are not charged but replaced by charged batteries during the turnaround phase of the plane, is one option that has been considered to overcome the charging time issue [304,305], however, this option implies high investment costs because of the great number of batteries involved.

Although battery recycling has advantages over the use of virgin metals (e.g., need for less energy for extraction operations, avoid emissions from batteries disposal) [306], several challenges remain to be alleviated, related to a variety of factors. The efficiencies of the collection and dismantling methods (e.g., difficulties in the dissociating used graphite from others) and the appropriate recycling technologies (e.g., for the developing sustainable methods, for high purity requirements such as 99.9% carbon purity for the graphite; [307]) are some examples [306,308,309].

Table 2.2 Battery technology outlook for aviation

Battery cell chemistry		Lithium-ion (Li-ion)	Advanced Li-ion	Solid-state battery (SSB)	Lithium-sulfur (Li-S)	Lithium-air (Li-air)
Cathode (+)	Lithium metal oxide such as LFP, LMO, Li-NMC, Li-NCA ³					
Anode (-)	Graphite (with silicon)	Lithium metal oxide with Ni-rich fraction (e.g. Li-NMC811) ^{4,5,6}	Lithium metal or Silicon ^{5,11}	Lithium metal oxide with Ni-rich fraction (e.g. Li-NMC811) ^{4,5,6}	Sulfur Graphene Acetylene black ^{6,7,8}	Porous carbon (e.g. carbon nanotube) ¹⁰
Electrolyte	Organic liquid (e.g. lithium salt-LiPF ₆) ³	Organic liquid (e.g. lithium salt-LiPF ₆) ³	Organic liquid (e.g. lithium salt-LiPF ₆) ³	Inorganic solid (e.g. Li ₁₀ SnP ₂ S ₁₂) ^{3,5} Organic solid (e.g. polycarbonate) ⁵	Organic liquid (e.g. LiPF ₆ , LiCO ₄) Aqueous solution (e.g. H ₂ SO ₄) ¹⁰	Organic liquid (e.g. LiPF ₆ , LiCO ₄) Aqueous solution (e.g. H ₂ SO ₄) ¹⁰
Binder	PAA PVDF ^{6,8}	PVDF ^{6,8}	PVDF ^{6,8}	PVDF ⁶	PEI PVP ⁸	PAA ⁸
Conductive additive	Carbon black ^{3,6}	Carbon black ^{3,6}	Carbon black ^{3,6}	Not specified	Not specified	Not specified
Gravimetric (Wh kg ⁻¹) ¹	300 ¹⁴ (1.08)	450 ¹⁴ (1.62)	450 ¹⁴ (1.62)	400-500 ¹⁵ (1.44-1.80)	300-400 ¹⁴ (1.08-1.44)	1,350 ⁹ (4.86)
Volumetric (Wh L ⁻¹) ¹	700 ¹⁴ (2.52)	1,200 ¹⁴ (4.32)	1,200 ¹⁴ (4.32)	Not specified	400 ¹⁴ (1.44)	Not specified
Life-time (cycle) ²	1,000-2,000 ¹⁶⁻¹⁷	1,000 ¹⁸	1,000 ¹⁸	500 ¹⁵ -1,000 ¹⁴	100 ¹⁴	Not specified
Nominal cell voltage (V)	3.7 ¹⁴	3.8 (Li-metal anode) ¹⁴	3.8 (Li-metal anode) ¹⁴	3.8 ¹⁵	2.1 ¹⁴	2.9 ¹⁴
Development status	Commercial scale (TRL 9) ^{14,16}	Commercial scale (TRL 9) ^{14,16}	Demonstration scale (TRL 7) ^{14,16}	Technology validation Small-scale prototype (TRL 3-4) ^{14,16}	Small-scale prototype (TRL 4) ^{14,16}	Technology concept (TRL 1-2) ^{14,16}

¹ Energy density is reported at the cell level derived from published papers and reports which were available at the time of writing. The SI unit of energy (MJ) is presented in parenthesis. ² Lifetime of battery is represented for 100% Depth of Discharge (DoD). TRL displayed has been retrieved from the references as indicated in the table.

Sources: ¹[306]; ²[293]; ³[45]; ⁴[310]; ⁵[955]; ⁶[313]; ⁷[311]; ⁸[955]; ⁹[313]; ¹⁰[314]; ¹¹[315]; ¹²[316]; ¹³[17]; ¹⁴[57]; ¹⁵[285]; ¹⁶[64]; ¹⁷[64]; ¹⁸[319] LFP: Lithium Ferro Phosphate; LMO: Lithium Manganese Oxide; NCA: Nickel-Cobalt-Aluminum; NMC: Nickel-Manganese-Cobalt; PAA: Polyacrylic acid; PEI: Polyethyleneimine; PVDF: Polyvinylidene fluoride; PVP: Polyvinyl pyrrolidone; TRL: Technology Readiness Level

2.7 Hydrogen aviation

The energy density of hydrogen, in terms of energy-to-weight ratio (MJ kg^{-1}) is three-fold that of conventional kerosene, rendering it suitable for longer flights in large planes supporting high payload capacity. Despite being lighter, hydrogen, in its cryogenic liquid form, has an energy-to-volume ratio (MJ L^{-1}) four-fold lower than fossil kerosene, which implies obvious storage challenges [320]. The different pathways for hydrogen production through water-splitting technologies are presented in Fig. 2.12.

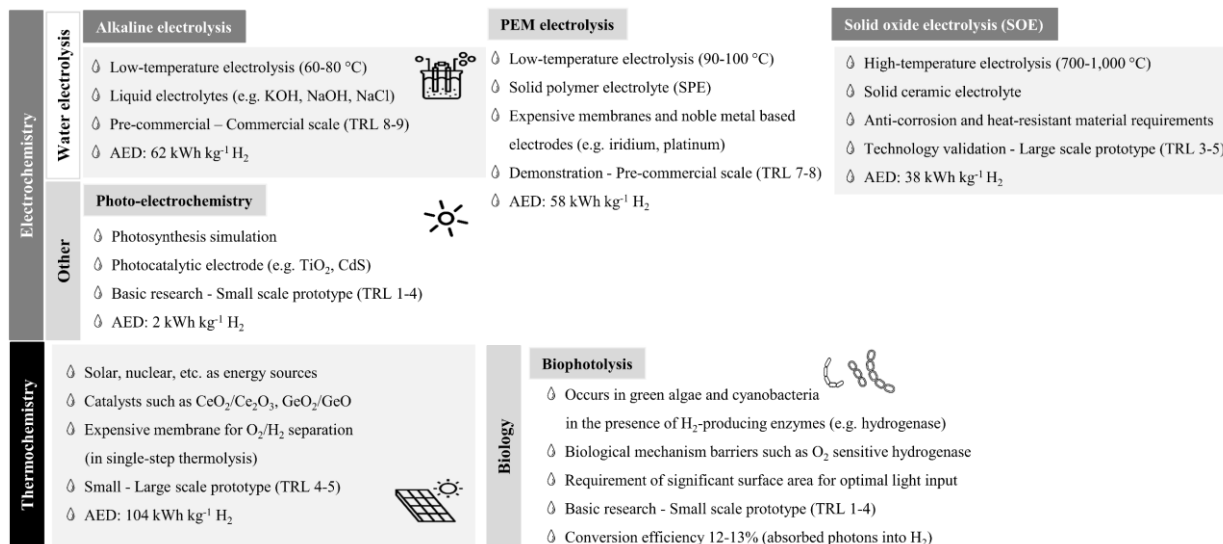


Fig. 2.12 Water splitting hydrogen production technologies. AED: Average Energy Demand, calculated from a compilation of several references (see Table S2.4 in SM 2.1).

Cryogenic hydrogen (referred as liquid hydrogen; LH_2) requires cryogenic storage (-253°C ; 20K) to maintain hydrogen in a liquid form [321]. This is due to hydrogen's high specific volume at standard atmospheric pressure and temperature.

Hydrogen propulsion system have been demonstrated whether in combustion mode or fuel cell mode (the latter is detailed in section 2.10.2.1). The Russian manufacturer Tupolev manufactured, in 1989, the first hydrogen aircraft using both gaseous H_2 (from an LH_2 tank), and liquefied natural gas (LNG) fuel in a gas turbine engine to propel the Tupolev 155 (Tu-155) [322]. The direct use of H_2 in gas turbines and piston engines generally involve that LH_2 is pumped from the tank to a heat exchanger, where LH_2 is heated to gaseous form prior to being injected into the combustion chamber of the engine [323]. The A380 MSN1 is an additional undertaking demonstrator to be powered by the H_2 combustion mode, which is expected to fly by 2026 [324]. Those require, besides the gas turbine with modified components (such as combustion chamber, fuel injector), a cryogenic tank with insulation system, additional on-board infrastructure such as high-pressure pumps, and a heat exchanger suitable to H_2 combustion characteristics (e.g., a tendency to flashback, a high flame temperature) [70,320,323,325], although scarcely detailed. Hydrogen turbine engines with low- NO_x emissions are already expected as the next improvement of this technology [66,70,71]. Boeing Phantom Eye is another example of an unmanned drone powered by hydrogen combustion in piston engines [326]. Other hydrogen aircraft, and projects can be retrieved in SM 2.1.

Cryogenic LH_2 has a propensity to leak due to hydrogen's high boil-off rate and small size molecule. Because of this, the use of H_2 raises important concerns about safety, and involves stringent procedures and requirements with regards to safety regulation certification, at airports, production and storage sites, transportation, distribution as well as for the aircraft operation, to avoid and control these leakages in case of occurrence [66,320,327]. It is even suggested to build airports where only H_2 would be used for all airport vehicles used for ground operations [328]. Despite this, H_2 has some advantages safety-wise, over conventional kerosene, such as lower flammability (more H_2 leak than kerosene leak is required prior to fire hazards, among others due H_2 rapid dispersion in air), and a higher auto-ignition temperature (550°C ; 823K for H_2 versus 300°C ; 573K for conventional kerosene), leading to a lower risk of spontaneous ignition of the fuel [327–329].

The key challenge of hydrogen as aviation fuel relates to the mass penalty induced by the onboard storage system. The mass penalty derived from the H₂ storage system is, at current technological state, reported to be twice as much as the conventional aviation fuel-based APU, when the compressed H₂ system is applied [66,71].

A light cryogenic storage tank with cooling system advancement is necessary for tackling this challenge [70]. On top of this, the fuselage may need a further redesign to accommodate the cryogenic hydrogen tank. The Airbus ZEROe project for instance announced the use of a blended wing body (BWB), as one type of aircraft allowing to efficiently accommodate hydrogen [330].

2.8 Semi-quantitative comparison and prioritization in the perspective of environmental mitigation

The strengths, challenges and prospects of the four SA families studied herein are summarized in Fig. 2.13. At the light of Fig. 2.13, it however remains unclear which pathways are the most promising from a technical, economic and environmental point of view.

Approaches	Strengths	Challenges and prospects
Biofuels 	<ul style="list-style-type: none"> • Suitable with numerous biomass feedstock (carbohydrate-, lignocellulosic- and oil-based biomass) • Six certified conversion technologies including FT, HRJ/HEFA, DSHC, SuF, SF, and CHJ • Several commercial plants are available • Suitable energy density ($\geq 42.8 \text{ MJ kg}^{-1}$)* • No maximum range limitation 	<ul style="list-style-type: none"> • Induced competition for arable land demands (1st generation feedstock) • High water demand and land requirement • Wastes/residues (2nd generation feedstock) and Algae-based (3rd generation feedstock) can be used as feedstock with lower interaction with land albeit with bounded availability.
Electrofuels 	<ul style="list-style-type: none"> • Abundant feedstock (water, industrial waste gases, CO₂ from air) • Foreseen lower environmental impacts relative to biofuels • Low land requirement • Suitable energy density ($\geq 42.8 \text{ MJ kg}^{-1}$)* • No maximum range limitation 	<ul style="list-style-type: none"> • Limited commercial production • Ongoing projects: KEROGREEN, Westküste 100, etc. • Large energy amount required for CO₂ captured from atmosphere • Improved production processes are required for cost reduction • Methanol synthesis as another promising alternative to liquid FT
Batteries 	<ul style="list-style-type: none"> • Foreseen lower environmental impacts relative to electrofuels: No tailpipe emissions (in case of all electric propulsion scheme) • Low-to-non dependence on carbon-based fuels 	<ul style="list-style-type: none"> • Battery overheating (Proper thermal management system) • New infrastructure needed (charging stations, or battery swapping stations) • Requirements of proper End-of-Life disposal/treatment • Maximum range limitation
Hydrogen (H₂) 	<ul style="list-style-type: none"> • Superior gravimetric energy density (120 MJ kg^{-1}) • Low-to-non dependence on carbon-based fuels • Several production technologies (available and being developed) • Tailpipe with non-CO₂ emissions • No maximum range limitation 	<ul style="list-style-type: none"> • New infrastructure needed (storage, refueling stations) • Modification of engines and/or fuselages • High production cost of renewable H₂ (mainly focused on electrolysis)

Note. * The energy density requires according to ASTM D1655 and ASTM D7566.

Fig. 2.13 Strengths and challenges/prospects of four emerging aviation approaches for low fossil carbon aviation

To this end, a semi-quantitative multi-criteria decision matrix has been established to enable a relative prioritization of the various types of SA approaches elaborated to this point (Table 2.3), inspired by the approach used in [331]. It is meant as a tool to pre-screen the global performance, and is by no means intended to replace state-of-the art quantitative assessment. It proposes three performance criteria (Table 2.3) seen as key for sustainable aviation: technology status, market prospects, and environmental performance, reflecting that short- and longer-term environmental mitigation are deeply intertwined with broader market considerations. For each of these critical criteria, sub-criteria were elaborated, to which a score (from 0 to 3) is given, on the basis of quantitative or qualitative descriptions (Table 2.3). The tool is distinctively applied on two timescales: near-term future (~2030) and long-term (~2050). These 10-20 years' time scopes are used as judged representative to reflect the time elapsed between two generations of technologies [332]. Several supporting references, including literature, scientific papers, patents, industrial/research organization reports, announcements, were accessed to assign scores for all criteria, and all pathways. This is thoroughly documented in SM 2.2.

Table 2.3 Semi-quantitative criteria for prioritizing sustainable aviation approaches^a

Overall criteria	Weight	Sub-criteria			Score	Comments			
		2030	2050	0			1	2	3
Technology current status	0.19	0.25	Requirement of fossil fuels	100% fossil fuel required	> 50% fossil fuel required	> 50% fossil fuel required	≤ 50% fossil fuel required	Not required OR Required for takeoff only	Based on known standards for aviation (e.g. ASTM D7566, etc.)
	0.12	n/c	Technology readiness level (TRL)	0-2	3-4	5-7	8-9	The general principles used for TRL assessment can be retrieved in SM 2.2.	
	0.12	n/c	Existing capacity ($\times 10^9$ MJ y ⁻¹)	<1	1.00-4.99	5.00-9.99	>10	Current energy sourcing production capacity	
	0.01	0.02	Energy density (MJ kg ⁻¹)	<20	20-30	31-40	>40	43 MJ kg ⁻¹ is considered as a default value for conventional (fossil-based) kerosene [30,149]. The ranges proposed herein are based on this.	
	0.03	0.04	Commodity co-products (with offsetting production costs) (€ kg ⁻¹)	<0.10	0.10-0.49	0.50-1.0	>1.0	The average jet fuel price in 2022 was around 0.60 € kg ⁻¹ [333]. We also consider that aviation kerosene has a fuel density of 0.785 kg L ⁻¹ [149].	
Market prospects	0.08	0.06	Passenger carrying capacity (seat)	Not for carrying passenger	1-50	51-100	>100	Electric battery aviation is considered based on [64,332]. Hydrogen aircraft are evaluated based on [71].	
	0.08	0.06	Flight range (km)	<500	500-2,000	2,001-5,000	>5,000	Electric battery aviation is considered based on [64,332]. Hydrogen aircraft are evaluated based on [71].	
	0.04	0.03	Cost competitiveness in low-fossil carbons future (¢cent MJ ⁻¹)	>5.00	3.01-5.00	1.31-3.00	<1.30	Conventional jet fuel price 1.30 ¢cent MJ ⁻¹ [333].	
	0.12	0.17	GHG emission reduction in comparison to fossil kerosene, as reported by studied	<40%	40-60%	60-80%	>80%	The Well-to-Wake GHG emission of conventional jet fuel is considered to be 87.5 gCO ₂ -eq. MJ ⁻¹ [334].	
Environmental performance	0.02	0.08	Energy demand (MJ MJ ⁻¹ fuel produced or battery)	>10.0	5.01-10.0	2.0-5.0	<1.99		
	0.12	0.17	Land requirement	Growing crops with a high impact on the food/feed competition	High share of residual biomass (waste), but crops may be involved	Biomass share overall low, and from residual resources only	No biomass needed	Relates to feedstock sourcing only	
	0.05	0.12	Sustainable availability of feedstock	Highly limited availability of feedstock for food and feed	Limited availability of feedstock otherwise used for food/feed - edible crops)	Limited availability but independent from land (e.g., residual, waste)	Abundant availability (e.g., solar energy, CO ₂ from the air) including EU critical raw materials [299]		
0.02	0.01	Water demand (L H ₂ O MJ ⁻¹ fuel produced or battery)	>100	50.01-99.99	10.01-50	<10	Considering the overall water requirement during their production stage		

^a n/c: not considered. The reference data and rationale used for the scores attributed herein are further detailed in SM 2.2; ^b The weight of each sub-criteria has been calculated through the Analytical Hierarchy Process (AHP) as described in [335].

Fig. 2.14 summarizes, for all pathways considered herein, the score obtained for some of the key quantitative performance indicators of Table 2.3, namely fossil fuel reduction, GHG reduction and technology readiness level (TRL), distinguished according to the time scope. Accordingly, 11 groups of pathways can be distinguished (Fig. 2.14). Pathways of group (1) are, according to the criteria selected in Fig. 2.14, the most promising, implying zero fossil fuels requirement and high (>60%) GHG reductions expected in comparison to fossil kerosene. It involves hydrogen (produced with alkaline or PEM electrolysis) as well as one biofuel and electrofuel pathway. The former is highlighted as particularly interesting due to its higher TRL. On the other hand, pathways of group (11), involving Li-ion and Advanced Li-ion batteries used in hybridized mode (i.e. used for propulsion) are shown as the least interesting, involving a high fossil fuels share and less than 40% expected GHG reductions.

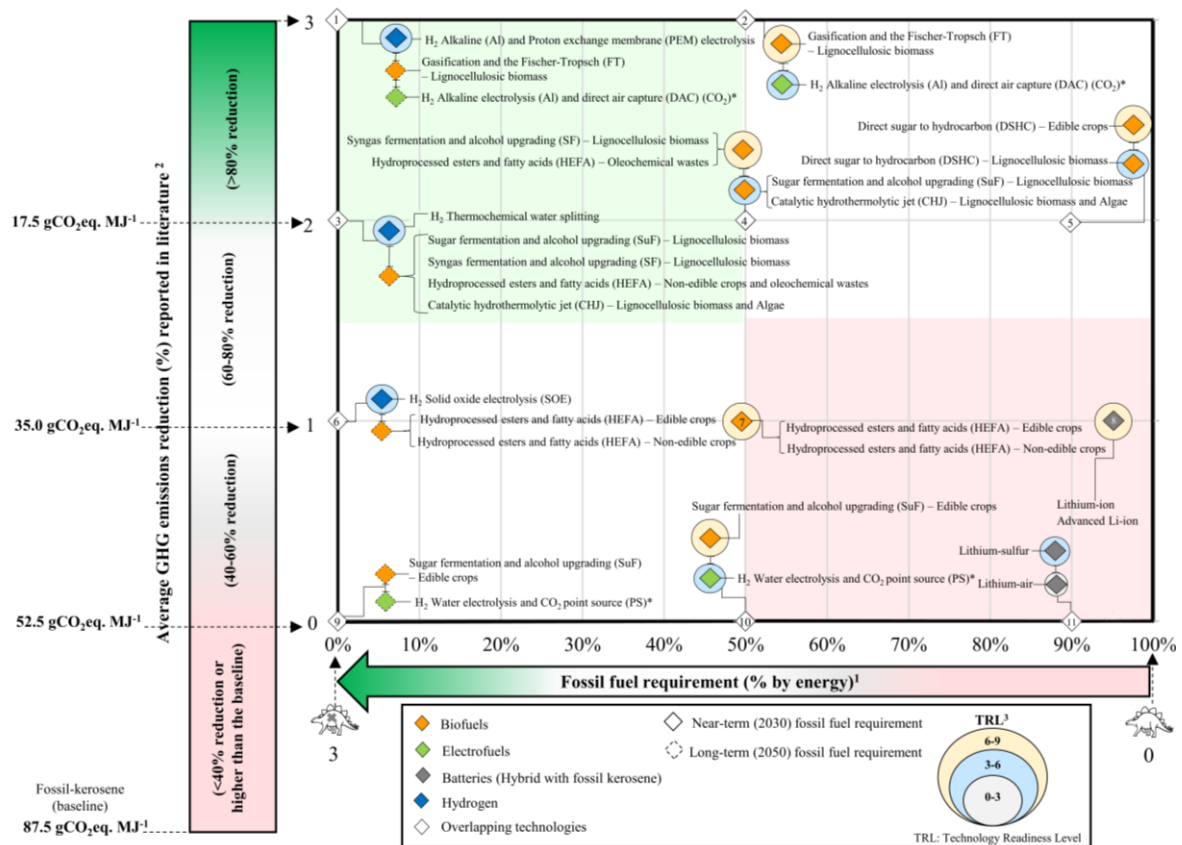


Fig. 2.14 General overview of the reviewed energy sourcing pathways for aviation

Notes. ¹ the requirement of fossil fuel has been estimated based upon: i) maximum blending quota of the certified fuels (whether biofuels or electrofuels) along with their gravimetric energy density (MJ kg^{-1}); ii) the degree of energy hybridization (battery) as reported on the study of [64].

² GHG emissions mitigation have been calculated from existing LCA studies relative to the fossil kerosene (including the combustion phase), considering $87.50 \text{ g CO}_2\text{eq. MJ}^{-1}$ fuel combusted for fossil kerosene [334].

For battery and renewable hydrogen, only the GHG associated to the production phase were considered, due to the lack of data on their use phases.

³ The TRLs of the displayed approaches are assessed based on the general principles as detailed in SM 2.2.

TRL (circle) are depicted only for the near-term time scope.

Water electrolysis covers alkaline, PEM and SOE technologies.

All data including references can be retrieved in SM 2.2.

* For the electrofuel production, the Fischer-Tropsch (FT) conversion is considered, as it is certified.

Despite useful, Fig. 2.14 does not allow to reflect all criteria, especially the qualitative ones, of Table 2.3. In a second stage, the Analytical Hierarchy Process (AHP) protocol proposed by [335] has therefore been used to assign weights to the different sub-criteria through the application of weighting factors between 0 and 1 to each sub-criteria, the total being 1 (Table 2.3). This is of course subjective, but the vision, for the screening exercise to be useful, is to supply a weight choice that is transparently argued (SM 2.2). For instance, here, the sub-criteria “requirement of fossil fuels” is the one with the highest weight for both the short- and long-term, keeping a

maximum of fossil carbon in the ground being seen as a key driver for the development of SA at the first place. Final weighted scores are calculated by multiplying the weighting factors by the sub-criteria assigned scores, as detailed in SM 2.2. The resulting final weighted scores are presented in Figs. 2.15 and 2.16, for near- and long-term, respectively, with a breakdown per sub-criteria.

As a result (Figs. 2.15-2.16), the most promising biofuels technologies uncovered for the near-term (Fig. 2.15) are HEFA (oleochemical wastes) and FT (biomass gasification and the FT process, with residual lignocellulosic biomass), significantly standing out from the other biofuel technologies. This result for (waste-derived) HEFA is explained by two key advantages of this pathway in comparison to the other options addressed: it benefits from existing capacity and it is not directly requiring additional arable land demand. For FT (based on lignocellulosic biomass), this decoupling from additional land demand is also important, along with its expected lower well-to-wake GHG emissions ([336,337]; SM 2.2). Based on available literature, a well-to-wake reduction of GHG emissions of 91% was considered for FT (in comparison to fossil fuels), which is much higher than for all other biofuels (SM 2.2). Yet, this result is to be considered with caution, as essentially reflecting methodological choices attributing GHG credits to energy-dense co-products. For electrofuels, only one technology stands out, namely FT using H₂ from alkaline water electrolysis and carbon from DAC (irrespective of the exact DAC technology), due to its expected lower well-to-wake GHG emissions. For electric (battery-based) systems, current technology for lithium-ion battery is highlighted with a higher weighted score, essentially benefiting from its greater maturity. For H₂ systems, alkaline water electrolysis significantly stands out from the other H₂ production technologies assessed, benefiting from its greater existing capacity (and the weight assigned to this criterion in the near-term).

For the long-term (Fig. 2.16), the results are similar for electrofuels, and biofuels, except that here, the FT lignocellulosic biomass clearly stands out from all other biofuels, essentially because of its expected lower well-to-wake GHG advantage, weighted higher for the long-term (SM 2.2). This explanation also applies for the electrofuels result. The alkaline water electrolysis is again shown as the most interesting technology for H₂ production, but the difference with other technologies is less pronounced than in the short-term. For electric (battery), however, the lithium-air battery is highlighted as the most interesting technology due to its anticipated higher energy density (see Table 2.2) and hence ability to carry more passengers with a longer distance traveled [64] or to the use less fossil kerosene supplement in a hybrid mode. Higher weights are put on these sub-criteria, namely the requirement of fossil fuel, GHG emissions reduction, in comparison to the short-term.

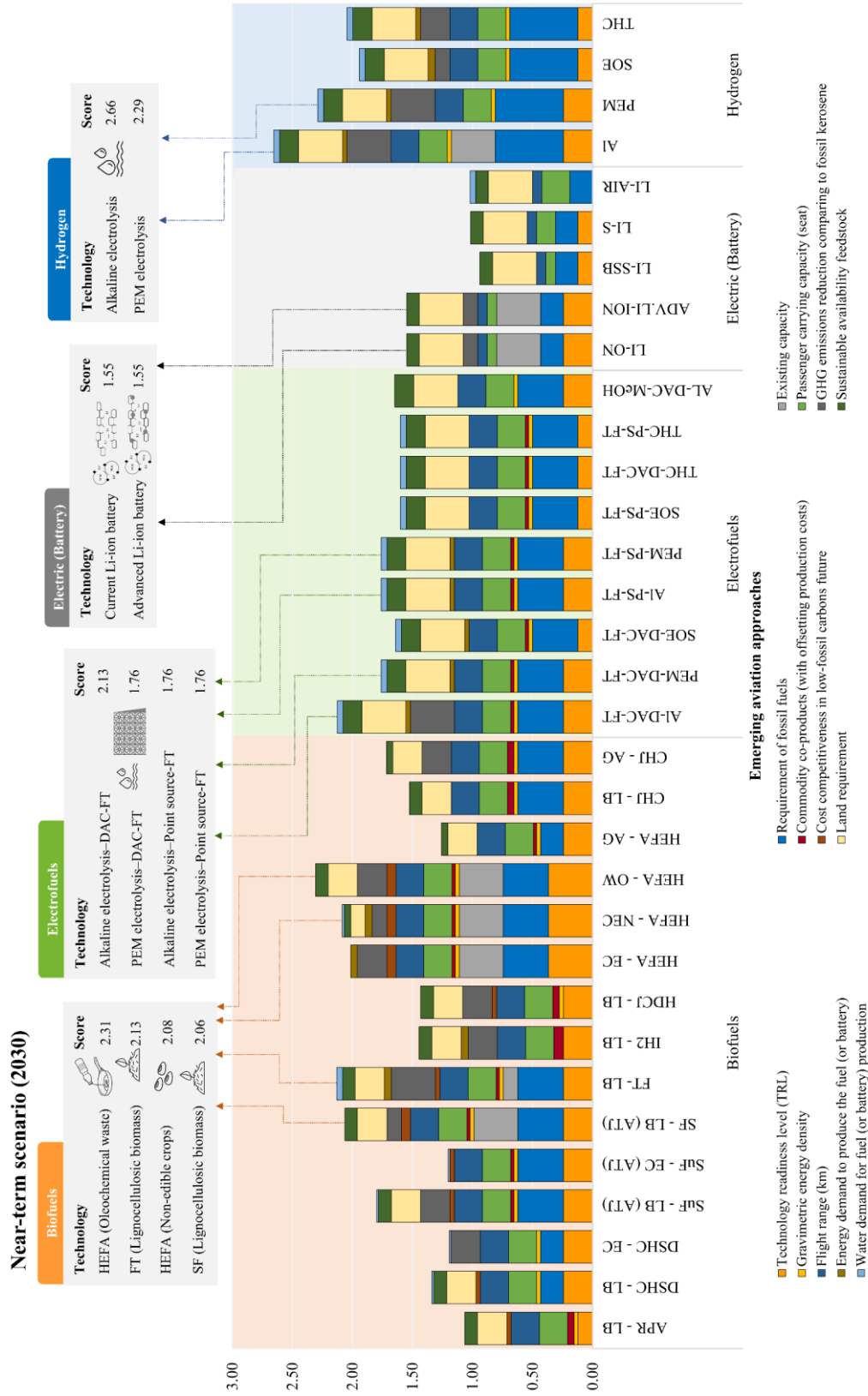


Fig. 2.15 Semi-quantitative ranking for the emerging aviation technology assessments to prioritize, near-term scenario (2030)

Acronyms: ADV: Advanced lithium-ion battery; AG: Algae; AI: Alkaline water electrolysis; APR: Aqueous phase reforming; ATJ: Alcohol-to-Jet; FT: Biomass gasification and Fischer-Tropsch; CHJ: Catalytic hydrothermolytic jet; DAC: Direct air capture; DSHC: Direct sugar to hydrocarbon; EC: Edible crops; FT: the Fischer-Tropsch process; HDCJ: Hydro-treated depolymerized cellulosic jet; HEFA: Hydroprocessed esters and fatty acids; IH²: Integrated hydrolysis and hydroconversion; LI-AIR: Lithium-air battery; LB: Lignocellulosic biomass; LI-ION: Lithium-ion battery; LI-S: Lithium-sulfur battery; LI-SSB: Solid-state battery; LUC: Land use change; MeOH: Methanol synthesis process; NEC: Non-edible crops; OW: Oleochemical waste; PEM: Proton/Polymer exchange membrane water electrolysis; PS: Point source carbon-capturing; SF: Syngas fermentation and alcohol upgrading; SOE: Solid oxide electrolysis (water electrolysis or co-electrolysis); Suf: (conventional) Sugar fermentation and alcohol upgrading; THC: Thermochemical water splitting

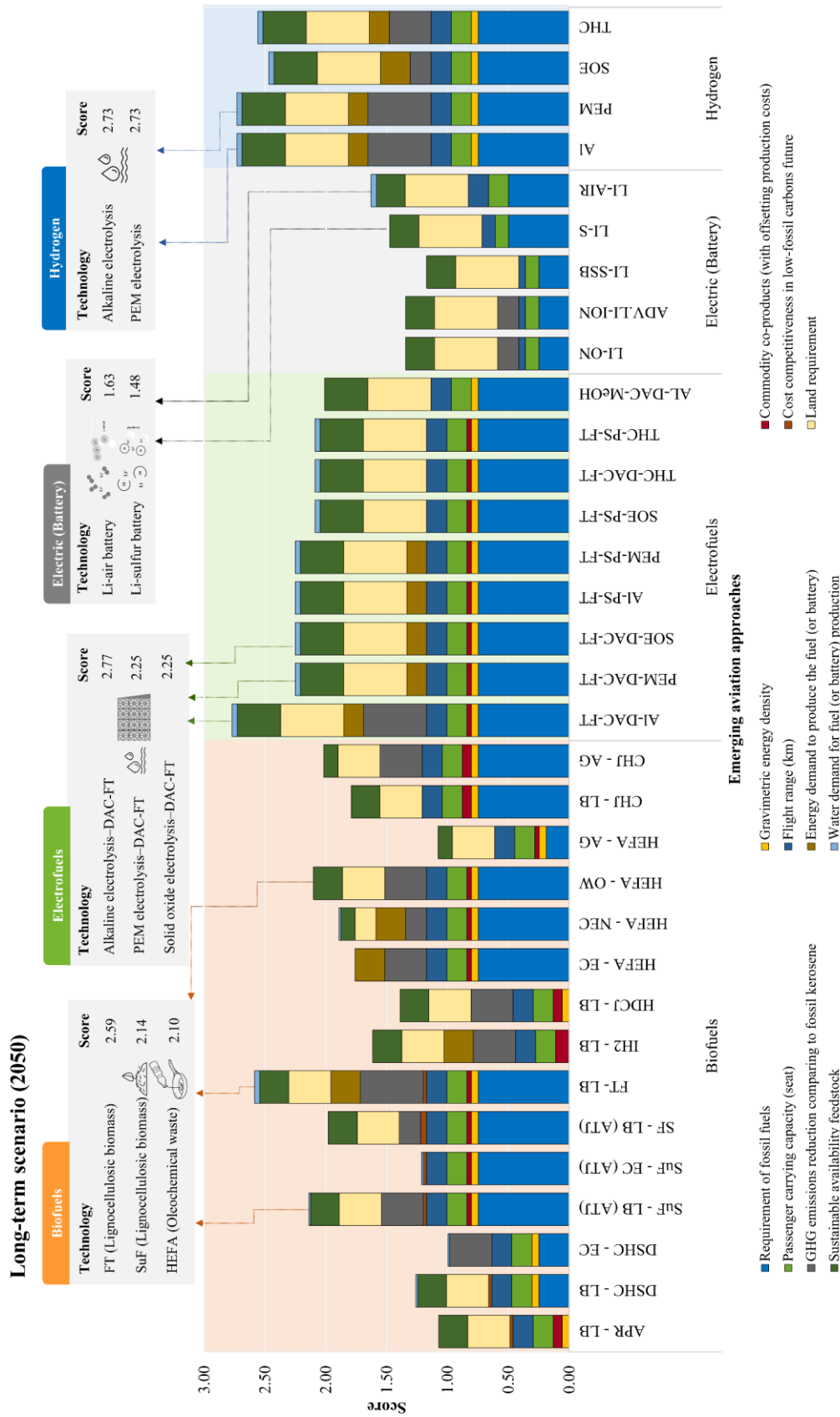


Fig. 2.16 Semi-quantitative ranking for the emerging aviation technology assessments to prioritize, long-term scenario (2050)

Acronyms: ADV: Advanced lithium-ion battery; AG: Algae; AI: Alkaline water electrolysis; APR: Aqueous phase reforming; ATJ: Alcohol-to-Jet; FT: Biomass gasification and Fischer-Tropsch; CHJ: Catalytic hydrothermal jet; DAC: Direct air capture; DSHC: Direct sugar to hydrocarbon; EC: Edible crops; FT: the Fischer-Tropsch process; HDCT: Hydrotreated depolymerized cellulosic jet; HEFA: Hydroprocessed esters and fatty acids; IH²: Integrated hydrolysis and hydroconversion; LI-AIR: Lithium-air battery; LB: Lignocellulosic biomass; LI-ION: Lithium-ion battery; LI-S: Lithium-sulfur battery; LI-SSB: Solid-state battery; LUC: Land use change; MeOH: Methanol synthesis process; NEC: Non-edible crops; OW: Oleochemical waste; PEM: Proton/Polymer exchange membrane water electrolysis; PS: Point source carbon-capturing; SF: Syngas fermentation and alcohol upgrading; SOE: Solid oxide electrolysis (water electrolysis) or co-electrolysis; SuF: (conventional) Sugar fermentation and alcohol upgrading; THC: Thermochemical water splitting

2.9 Other emerging energy sourcing for aviation not considered herein

2.9.1 Liquefied natural gas (LNG) based aviation

The use of LNG (i.e. liquefied methane) as a fuel is highly researched and discussed for the maritime sector ([338,339]), and to some extent the aviation sector (e.g. Savion aerospace; [340]), though it is still very marginal. One driver for the development of this technology is the price of fuels; low natural gas price relative to fossil kerosene may favor the LNG. It is further suggested that LNG aviation fuels could reduce CO₂ tailpipe emissions of approximately 20-25% relative to conventional kerosene, for the same energy content [320,341]. Although LNG is presently derived from natural gas, it could stem from biomethane generated through anaerobic digestion [128], biomass gasification [342], or power-to-methane routes decoupled from biomass [343]. It also has a gravimetric energy density slightly higher than conventional kerosene (around 48-54 MJ kg⁻¹) [341,342].

LNG for aviation, however, still involve a number of challenges. First, it implies, as for LH₂, cryogenic form (-162°C; 111K), and thus a certain mass penalty [320,344,345]. It also implies infrastructure not already in place (e.g. refueling system, LNG storage tanks, liquefaction facilities) [341,344]. Importantly, eventual leakages of LNG is another factor to be considered, as methane has a global warming potential (GWP₁₀₀) around 28 times the one of CO₂ [346].

As LH₂, LNG is compatible with whether combustion mode or fuel cell mode [347]. The former has been showcased in gas turbines (e.g., TU-155 aircraft [322]) as well as within the Advanced Hybrid Engines for Aircraft Development (AHEAD) project [348]. The combustion mode implies that modification and/or change in propulsion systems are required, including engines, injectors and heat exchangers, able to use this fuel [349,350]. The fuel cell mode has been showcased in a solid oxide fuel cell (SOFC) within the Subsonic Ultra Green Aircraft Research (SUGAR) project [347]. To make it viable on long-range aircraft, additional research on advanced materials for fuel cells is however needed [347].

2.9.2 Ammonia based aviation

The use of liquefied ammonia (NH₃) for aviation has been discussed and considered within some research and industrial communities [351,352]. For instance, ammonia-powered aircraft are being developed within the Zero-carbon Ammonia-Powered Turboelectric propulsion project (ZAPturbo) [353]. In comparison to LH₂, it involves lower mass penalties owing to the superior density of liquid ammonia (730 kg m⁻³; [349]). Ammonia requires refrigeration to -33°C (240K) under atmospheric pressure, this implies prior refrigeration when on ground, and is maintained by the outside temperature during cruise altitude (at ca. 8-12 km; [354,355]) through heat exchanger systems [352]. Refrigerated ammonia can be stored in the wings like in the case of conventional kerosene [356].

However, most ammonia is currently produced from hydrogen through steam reforming of natural gas, and N₂ is derived from air separation through the energy-intensive Haber-Bosch process [349,357]. Alternatives using renewable H₂ (derived from water electrolysis rather than natural gas; also referred to as the 2nd generation path) [358,359], or electrochemical ammonia synthesis as an alternative to the Haber-Bosch process (electrochemical N₂ reduction reaction, NRR, known as the 3rd generation path) [357,359,360] are being developed. However, at present, the production cost of renewable ammonia is roughly twice the price of conventional ammonia. Its production cost is essentially shaped by the price of renewable electricity [361]. In addition, ammonia has a low gravimetric energy density (18.6 MJ kg⁻¹; [349,353]), this means that ammonia-powered aircraft would have a shorter flight range relative to (conventional) kerosene and hydrogen [362], considering a similar payload mass. Moreover, an enhanced use of atmospheric N₂ to produce (additional) ammonia implies an enhanced risk for contributing to excess reactive nitrogen in the environment, known to cause a range of negative environmental, socio-economic, and health consequences [359,363], besides being one of the exceeded planetary boundaries [364].

Ammonia per se has a high ignition temperature, and low flow velocity [363,365]. Therefore, a mixture with other reactive molecules (e.g. H₂), has been proposed as one option to improve combustion properties ([359]). In this endeavor, it is proposed to add a cracking unit to the aircraft, where part of the ammonia dissociates into nitrogen and hydrogen, resulting in a mixture of NH₃-H₂-N₂ [353,363]. This feature closely makes it compatible with the current (hydrocarbon-based) gas turbine engines [353,359,363], and is being developed by e.g. Raytheon Technologies Research Center [353] and Reaction Engines Ltd. [351]. Ammonia can also be employed in the fuel

cell mode [366], but no showcasing of this has been found. Water vapor, nitrogen, and nitrogen oxides (NO_x) are considered as the only tailpipe emissions of ammonia [362]. To minimize the effects derived from NO_x formation, mitigation technologies such as a low- NO_x combustors have been proposed [353]. Additionally, new materials for storage tanks (in particular for on-board NH_3) are required to safely deal with the corrosive properties of NH_3 [359]. Ammonia's toxicity (inhalation hazards) is another issue to be tackled and would imply mandatory specific training before handling [359,363].

2.9.3 Solar aviation

Solar energy generates growing attention for aviation [367,368], due to its unlimited availability and envisioned sustainability. Solar-powered aircraft for passenger-carrying purposes however faces many challenges. First, solar panels are limited in their capturing efficiency (around 20%; [369,370]). Even if an increase in efficiency (reaching 100%) has been achieved ([368]), the generated power might not be sufficient to deal with the payload a passenger aircraft implies. In addition, because of low efficiency power devices of solar-powered aircraft (e.g., photovoltaic cells, rechargeable batteries; [370]), the maximum speed would not reach beyond 50 miles hr^{-1} (160 km hr^{-1}) (commercial aircraft traveling at about 600 miles hr^{-1} ; 965 km hr^{-1}) [368]. The high variability of photon capturing angles is also reported to result in lower power generated (relative to the expected maximum power) [368,370]. Other issues are reported, for instance, the vulnerability of solar panel materials to adverse weather conditions, or the need for large wingspans. Nevertheless, solar power is successfully applied and deployed for unmanned aircraft system/unmanned aerial vehicle (UAS/UAV) as a satellite service (additional detail in SM 2.1).

The deployment of solar aviation for carrying passengers therefore appears as an unlikely option till the first half of the century, but it may be considered in hybridization with the other SA systems discussed within the present study.

2.9.4 Others

Finally, additional initiatives, albeit marginal such as methanol [371,372], and ethanol [373,374] direct use, do exist and have not been covered within this review due to a lack of available documentation about these.

2.10 Electric propulsion systems for aviation

Electric propulsion (to be distinguished from battery-electric) represents configuration schemes involving an electric motor to supply mechanical power to the aircraft propulsors (which could be propellers or fans) (Fig. 2.17). These configuration schemes differ with regards to whether they imply or not (i) energy storage from batteries; (ii) a (H_2) gas turbine fueled by H_2 or liquid hydrocarbons and (iii) fuel cells fueled by H_2 or liquid hydrocarbons and supplying electricity to electric motors.

Advancing the propulsion efficiency is, after the energy sourcing itself, one key lever considered to improve the overall environmental performance (including noise reduction) of future aviation. Throughout this section (and in Fig. 2.17), the term propulsor represents devices generating thrust either by a propeller in the turboprop or by fans in the turbofans. It also encompasses the generation of shaft power in the case of turboshaft engines. The term "(H_2) gas turbine" collectively refers to the turboshaft, turboprop, and turbofan engines. Converter refers to the devices converting the voltage of the electrical power source, sometimes denoted as power electronic [283], and considers that one type of converter is an inverter, which converts direct current (DC) to alternating current (AC).

To represent the proportion of electric power in total power, two parameters are used [59,64], respectively degree of energy hybridization (H_E) and degree of power hybridization (H_P). H_E and H_P vary from 0 to 1 depending on the conceptual designs [59,375]. H_E is zero when there are no energy storage devices involved (no batteries), and 1 when the power is solely supplied via batteries. H_P is 1 when only electric motors are supplying the required mechanical power, and 0 if no electric motors are involved in supplying the required power.

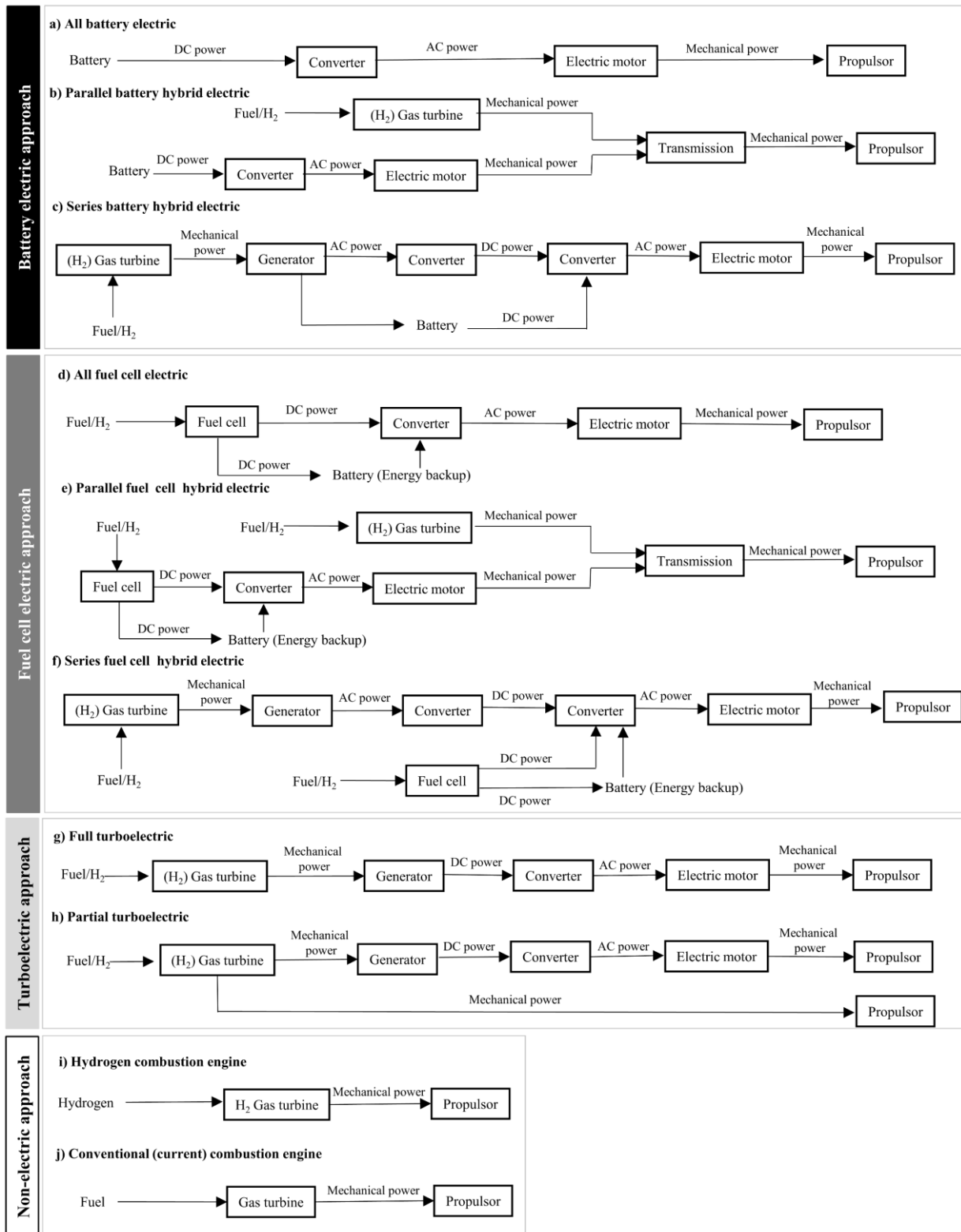


Fig. 2.17 Basic configuration schemes for aviation propulsion systems. DC stands for direct current, AC for alternative current. *(H₂) gas turbine here denotes whether turboshaft, turboprop and turboprop engines. Fuel defined herein represents hydrocarbon-based fuels (conventional fossil kerosene, biofuels, or electrofuels), and hydrogen-based fuels (herein focused on hydrogen (H₂)).

2.10.1 Battery-dependent electric propulsion configurations

Electric aircraft relying on batteries have gained substantial interest in recent years. Batteries can serve as the energy sourcing for propulsion either as standalone (“all electric” concept; Fig. 2.17a) or in combination with other fuels (“hybrid electric” concept; Figs. 2.17b-c).

The all electric concept is also denoted as “full electric” (e.g. in [376–378]). An all electric configuration (Fig. 2.17a) involves that ($H_P=1$) because the propulsor is powered by an electric motor only but also involves that ($H_E=1$) because it relies solely on batteries without any hydrocarbon-based fuels or H_2 [59].

The concept of “hybrid electric” (Figs. 2.17b-c) implies, on top of the electric motor, the use of a (H_2) gas turbine fueled by liquid hydrocarbons or H_2 to generate additional mechanical power. As AC power is required for most of the electric motors that can be used in aviation, converters are required [379]. The parallel and series hybrid electric concepts are the two main configurations that have been tested (Figs. 2.17b-c), however, a series-parallel hybrid scheme has also been demonstrated (not depicted in Fig. 2.17) [379,380]. The parallel hybrid electric configuration (Fig. 2.17b) involves (H_2) gas turbines and electric motors to generate mechanical power from fuels combustion and batteries, respectively, [381]. Hence a mechanical transmission (typically gearbox) is required to integrate and control these two mechanical power sources prior to the propulsor [379,382,383]. In the series hybrid electric configuration, the generator powered by the (H_2) gas turbine produces electricity for both the electric motor(s) (which is directly linked to the propulsor; $H_P = 1$), and to charge the battery onboard ($0 < H_E < 1$) [59,377,384] (Fig. 2.17c).

Several projects have been launched to demonstrate the feasibility of these battery dependent configurations) (Fig. 2.18). For example, the startup Eviation (Israel) launched Alice, a nine-passenger all electric aircraft with an autonomy range of 650 miles (1,046 km), expected to be in service by 2024 [385]. The aircraft relies on a battery that can be fully charged within 70 minutes and is expected to be FAA-certified (FAA: USA Federal Aviation Administration) by 2024 [385]. However, a fire incident has occurred during the Alice ground test in January 2020 caused by a fault with a ground-based battery system [386]. The company magniX (Canada) designed and demonstrated a high-power density electric propulsion system with the world’s first fully electric commercial seaplane, tested on a flight in December 2019 (6-passenger aircraft; flight range of 1,000 km) [387,388]. In May 2020, magniX together with Harbour Air successfully tested an all electric powered system carrying up to 9 passengers for a reported flight range of ca. 160 km (e-Caravan; retrofitted from Ceravan 208) [389,390]. It is announced to be the largest all electric aircraft with a successful test flight (in the middle of 2020). In Europe, EasyJet and Wright Electric are developing since 2017 an all electric aircraft (186 seats) and announced it will start using electric aircraft to cover short-haul routes by 2030 [391,392]. Additional details on these emerging developments along with specifications on these technologies are presented in SM 2.1.

2.10.2 Electric propulsion independent from batteries

Electric propulsion configurations independent from the presence of batteries include: Fuel cell electric and Turboelectric systems.

2.10.2.1 Fuel cell electric propulsion (may involve batteries as backup)

A fuel cell propulsion system could be employed in the mode of all electric (in Fig. 2.17d), or hybrid electric (electric motor and (H_2) gas turbine; Figs. 2.17e-f) [379,393], where hydrocarbon-based fuels or H_2 are converted to electricity that in turns powers an electric motor involving a modification of the propulsion system [70].

Fuel cells serve as energy converters, not as energy storage as in the case of batteries. Fuel cells can continuously produce electricity as long as fuels (whether hydrocarbon-based fuels or H_2) are fed to the fuel cell. The existing fuel cell technologies, for the automobile sector and stationary power applications, include the proton exchange membrane fuel cells (PEMFC) and SOFC, depending on the electrolyte employed, operating conditions, and fuels compatibility [393,394]. Fuel cells can be considered for the propulsion system in aviation, providing an increase in their specific power (targeting 2 kW kg^{-1}) has been achieved [65,71,394]. The electricity produced in excess of what is needed for propelling the aircraft can additionally be stored in batteries as a backup energy source, not directly involved in the propulsion system [70] (Figs. 2.17d-f). Fuel cell propulsion also provide the advantage of short refueling time relative to batteries with fewer risks of reducing the lifetime [66].

Hydrogen fuel cell designs for aircraft are being developed, for instance by Airbus in ZEROe concepts (hybrid hydrogen propulsion system). These aircraft are expected to enter service (with a carrying capacity of 100-200 passengers) by 2035 [330]. Furthermore, the first commercial H₂ fuel cell aircraft (with a carrying capacity of 10-20 passengers, and maximal distance traveled up to 555 km), was announced by ZeroAvia to be ready by the year 2024.

Unlike the H₂ combustion in gas engines and piston engines (Fig. 2.17i) where air is involved in the combustion process (thus involving nitrogen outputs such as nitrogen oxides; NO_x); the only two by-products from H₂ fuel cell systems are water vapor and a small amount of heat. This, however, involves non-negligible cooling requirements [66,71]. Additionally, fuel cell propulsion is unlikely to be competitive for heavy payload and long distances, with four times the mass of current aircraft engines to generate the same power output [66,71].

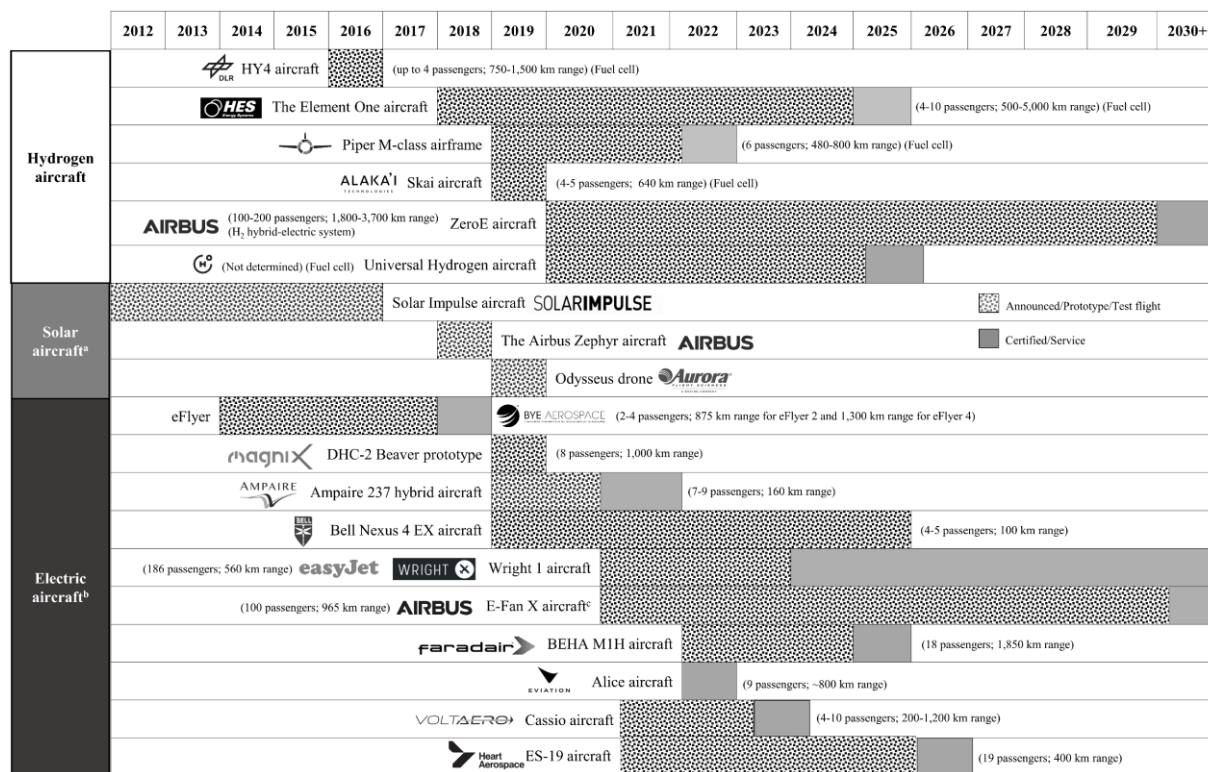
Various projects have been intensively studied in developing and improving hydrogen fuel cell technologies (Fig. 2.17), as detailed in SM 2.1. Hybridization with fuel cell and battery propulsion is another alternative configuration (not depicted herein) [395].

2.10.2.2 Turboelectric propulsion (no batteries)

Turboelectric propulsion (Figs. 2.17g and h) is another configuration for electric powertrain systems, and fully relies on hydrocarbon fuel or H₂ as its energy source. Here, no energy storage (e.g. batteries) is involved [375,376,384]. A (H₂) gas turbine drives the generator that powers electric motors for thrust or shaft power generation. In the full turboelectric system (hence, H_E = 0, H_P = 1; Fig. 2.17g) [59,396], the generic (H₂) gas turbine term denotes a turboshaft engine [397]. In the partial turboelectric concept (Fig. 2.17h), the generated mechanical power from the (H₂) gas turbine is partially delivered to the generator ultimately feeding the electric motor(s), and the remaining power is delivered directly to the other propulsors [59,286,376]. In this case (Fig. 2.17g), H_E would be zero as there are no energy storage devices involved, while H_P would be between 0 and 1 because both a (H₂) gas turbine and an electric motor are used to supply energy to the propulsor. In this particular case, however, a clear standard for attributing the appropriate non-zero and non-one hybridization value is still missing [59,375].

Albeit the propulsive efficiency of electrically-driven propulsors can improve, the integration of the electric system introduces mass penalties (although lighter than the all electric configuration as it does not involve batteries) [286,397–400]. To enhance the overall performance in terms of fuel burnt and mass, this configuration concept has been integrated with optimized aircraft design, for instance in NASA's STARC-ABL aircraft design (Single-aisle Turboelectric AiRCraft with an Aft Boundary - Layer propulsors) [400]. This allowed a 12% reduction of fuel burnt compared to the conventional aircraft concept (conventional kerosene configuration (Fig. 2.17j) and airframe design) [400]. The Wright ECO-150R aircraft capable of carrying up to 150 seats (flight range of ~ 3,000 km) initially demonstrated ca. 44% fuel burn reduction in comparison to the conventional configuration [384]. NASA's N3-X aircraft is another turboelectric concept with a blended wing body in which electric motors are used to drive several distributed electric fans, where the effective bypass ratio (BPR) is increased while reducing the fan pressure ratio [399]. It demonstrated to provide ca. 63% energy and 90% NO_x reductions [401]. This architecture has been proposed as the upcoming technology to meet environmental goals [376,402], where hydrocarbon-based fuels (biofuels/electrofuels) or H₂ can be used instead of fossil kerosene.

Other projects on electric propulsion systems are demonstrated in Fig. 2.18 and can be further retrieved in SM 2.1.



Note. * not for carrying passenger; ^b Electric aircraft are covered all possible electric propulsion; ^c The E-Fan X project was cancelled in April 2020.

Fig. 2.18 Examples of inventoried electric, hydrogen and solar-based projects announced to date (by the end of the year 2021)

2.11 Regulatory frameworks/Sustainability policies

Policy and regulatory frameworks are often pinpointed as essential to encourage the deployment of SA, and to ensure this deployment is sustainable [403–405]. Alternative fuels for aviation have been considered in numerous launched/ongoing regulatory framework and sustainable policy initiatives. These essentially apply to liquid biofuels and to some extent electrofuels, owing to their technological maturity. As of today, the use of biofuels nevertheless remains minimal, with less than 1% of total aviation fuel demand [18,406,407] (electrofuels are not yet widely available for commercial use).

A handful of frameworks/policies have also been paying attention to other emerging alternatives to power aircraft, including electric (battery) aviation and hydrogen (H₂) systems. The regulatory context on alternatives implemented at the point of writing is summarized herein, with a greater focus on schemes affecting the EU countries.

2.11.1 European Union's sustainable & smart mobility strategy

The EU's sustainable & smart mobility strategy (part of the EU Green Deal) has been adopted by the European Commission on December 9th, 2020. Being a strategy, it is not binding, but it aims to ensure that the EU's transport systems are able to achieve the climate targets for 2030, and the 2050 climate neutrality [18], and describes the Commission's current vision to reach these goals. A package of milestones for all transport modes are proposed, covering also the aviation sector [408]. For instance, the production and deployment of biofuels and electrofuels (labelled as SAF in the strategy) are highly encouraged at Union airports to reduce aircraft's emissions in line with the ReFuelEU Aviation proposal (section 2.11.5). Alternative propulsion technologies powered by electricity or hydrogen are also required to achieve zero (carbon-) emissions. Other measures, such as improving the air traffic management (ATM) efficiency, developing an environmental label program, and revising the EU Emission Trading Scheme (EU ETS) with respect to aviation (section 2.11.4) are also mentioned [409].

2.11.2 'Fit for 55' package

The European Commission has proposed, as announced in the European Green Deal communication [409], to increase the 2030 GHG emission reduction target (at overall EU level) from 40% to 55%, relative to 1990 levels. To this end, the European climate-, energy- and transport-related legislation is being revised under the so-called Fit for 55 package [410], being a set of proposals to align the EU legislation with the new target. The most relevant points of this package for aviation include: i) the amendment to the Renewable Energy Directive II (RED II) (section 2.11.3); ii) the revision of the EU ETS (section 2.11.4), ii) the ReFuel EU Aviation proposal (section 2.11.5), and iii) the revision of the Energy Taxation Directive (section 2.11.6).

2.11.3 EU Renewable Energy Directive (RED)

The EU Renewable Energy Directive (RED) adopted in 2009 established an overall policy framework for the production and promotion of energy from renewable sources. It is a binding regulation for EU Member States. The RED requires all EU countries to ensure a share of at least 10% of final energy consumed in transportation stems from renewable sources by 2020 [411]. The RED (or RED I) target, however, does not fully include the aviation sector, by limiting, in the calculation of the gross final energy consumed by a Member State, the aviation share to maximum of 6.18% (4.12% in the specific case of Malta and Cyprus).

The RED was further amended with the Directive 2015/1513 to, among others, recognize the opportunity offered by biofuels/electrofuels to enhance the consumption of fuels not derived from fossil resources within the aviation sector. This translated in the so-called ‘voluntary opt-in’ [412]. The Member States could implement this opt-in differently: in form of a certificate system for fuel suppliers, or as a tax exemption for reaching the 10% of final energy consumption from renewable sources by 2020 [413].

The revised RED for the period 2021-2030, denoted as RED II, requires a minimum share of 14% of final energy consumption in transport sector to be derived from renewable energy by 2030, and is set as an obligation for fuel suppliers [19]. It also sets additional sustainability criteria, namely requirements associated to specific GHG emission savings, specific shares of advanced fuels to incorporate (in 2022, 2025, 2030), criteria for feedstock sourced from forest biomass (e.g., harvesting with legal permits, maintaining soil quality and biodiversity during the harvesting process), and the consideration of indirect land use changes (ILUC) to limit the use of high ILUC-risk feedstock from land with high carbon stocks [19,414,415], among others. The new directive further introduces a slight incentive for using non-food biomass for aviation and maritime fuels production through a multiplication factor of 1.2 (of their energy content) in the calculation of renewable energy not stemming from feedstock intended for food and feed consumption. As the original RED, RED II has no specific target for the aviation sector.

Key provisions affecting the aviation sector have been suggested in an amendment to RED II proposed by the Commission in July 2021 [416]. This includes a reduction of the minimum share of advanced fuels for 2025 and 2030, and the introduction of a new sub-category of renewable fuel, namely renewable fuels of non-biological origin (RFNBOs; including electrofuels, renewable hydrogen, renewable electricity). Besides the minimal share of advanced fuels to be supplied to the overall transport sector, the amendment proposes to also ensure a minimal share of 2.6% of RFNBO by 2030.

2.11.4 EU Emission Trading System (EU ETS)

The EU ETS is one of the EU’s policy instrument to mitigate climate change [417], used to implement the current 40% GHG emission reduction target for 2030. It is a mandatory cap-and-trade system and covers approximately 40% of total EU GHG emissions from industrial activities, including the aviation and maritime sectors. The EU ETS aims at achieving economy-wide emission reduction targets through tradable allowances putting a price on carbon emissions.

Currently, for the aviation sector, the EU ETS covers only CO₂ tailpipe emissions. The flights operated within the European Economic Area (EEA) as intra-EEA flights (arriving at and departing from EU airports) are presently accounted in the EU ETS, while flights to and from non-EEA countries are exempted until the end of 2023 [27,418]. Overall, emissions allowances to airline operators covered by the EU ETS, from 2013-2020, are distributed as follows: 82% are granted as free allowances allocated on the basis of airlines’ efficiency in transporting passengers and cargo while 15% are auctioned, for a price reaching ca. €25 for one tonne of CO₂ at the end of 2019 [419] up to about €85 in May 2021 [420]. The remaining 3% are reserved for new entrants (those starting activities after 2010) and fast-growing airlines (>18% average tonne km annual growth between 2010-

2014) [421]. The cap for free allowances is annually limited to 97% of the average aviation emissions for the years 2004-2006 (approx. 210-220 million tonnes CO₂) [422,423]. It was further reduced to 95% for 2013-2020. From 2021 onwards, the cap is to be decreased by an annual linear reduction factor (LRF) of 2.2% [424,425]. For CO₂ emissions exceeding the cap, the aircraft operators have to purchase EU emission unit allowances (EUAs) at auction, or from other sectors, leading to additional costs for the airlines. CO₂ emissions are significantly dependent upon the carried weight, namely the revenue tonne kilometer (RTK) for cargo flight, the RPK for passenger-carrying flight. The EU allowances are used to fund emission-saving projects in lower-income countries, such as the development of innovative renewable energy technologies or, modernization in power sector and energy system [404,426].

The revision proposed for the EU ETS in the framework of the Fit for 55 package includes the following points relevant for aviation: (i) Free allowance distribution will be phased out progressively from 2024 (by: 25%, 50%, and 75%, in 2024, 2025 and 2026, respectively), for a complete phase-out from 2027 onwards [27]; (ii) Starting 2025, the application of a LRF of 4.2% (instead of 2.2%) is proposed to meet the more stringent 2030 emission target (revision proposed by the Fit for 55 package) [244,407,421]; (iii) The allowances will be capped at current level (instead of an average historical amount); (iv) Flights between the EU's outermost regions and flight to Switzerland and the United Kingdom (UK) will be included in the EU ETS; (v) International flights (involving CORSIA participating states; 11.10) departing from or arriving at an airport inside the EEA (extra-EEA flight) will be also be integrated [427,428].

Currently, the uptake of SAF can be an incentive for airline operators as this system counts biofuels/electrofuels (to the extent it complies with the sustainability criteria defined in the RED) as having zero emissions (no allowances required to be surrendered) [18]. However, this approach is not economically incentivized to encourage the use of SAF as their prices has remained higher than the CO₂'s price (the price of at least €160 per tonne of CO₂ emissions is required). This is required to report, of the EU ETS, based on SAF purchasing records [18].

2.11.5 The ReFuelEU Aviation proposal

The ReFuelEU Aviation proposal is a proposal for a regulation to boost the supply and demand for SAF in the EU, by 2050. This proposal has been launched as a part of the 'Fit for 55' package, and was released in July 2021 after several consultation rounds and an impact assessment of the sector [18]. In the context of ReFuelEU, the term SAF specifically covers RED-compliant (section 2.11.3) biofuels including advanced biofuels (e.g. agricultural and forestry biomass; listed in Annex IX Part A of RED II), biofuels produced from feedstock listed in RED II Annex IX, Part B (waste oils and fats), and electrofuels (equivalent to the term synthetic fuels) [19].

The key highlight of the current proposal version is an obligation for fuel suppliers to ensure that the aviation fuel made available at EU airports contains a minimum share of SAF (from 2 vol.% in 2023 to 63 vol.% in 2050), including a minimum share of electrofuels (0.7 vol.% of overall SAF in 2030 to 28 vol.% in 2050) [18]. The European Parliament has recently endorsed the ReFuel EU proposal, and proposed to raise the SAF share from 63% to 85% by 2050 with the inclusion of electricity and hydrogen in the overall (sustainable) aviation fuel mix [429].

However, until 2035, fuel suppliers will be allowed to supply this minimum share of SAF to airports through the trading of SAF certificates obtained by overachievers (suppliers with an excess of SAF) [430]. To mitigate the effects of tankering (the use, prior to enter the EU, of more fuel than required for the flight in order to reduce the amount of SAF to be used, and thus save on fuel costs), ReFuelEU proposes a requirement that EU and non-EU airlines, for all flights departing from the EU, tank at least the whole required amount for their subsequent flight. The proposal also includes an obligation for EU airports to provide the infrastructure required, including hydrogen refueling, electric recharging, to reach the above-mentioned SAF supply targets. Additionally, a Sustainable Aviation Fund is proposed by the Parliament in order to facilitate the establishment of cleaner aviation, including an investment support in sustainable fuels, and in research on innovative propulsion systems [429].

Non-compliance penalties according to the Commission's criteria will be proposed by the Member State authorities and are to be communicated to the Commission by the end of 2023 [430].

2.11.6 The Energy Taxation Directive (ETD)

The Energy Taxation Directive is a European directive in order to support the EU's climate and energy policy frameworks through a taxation system of energy products used as motor fuels, heating fuels, and electricity [431,432].

A tax exemption for (conventional) aviation fuels granted by the ETD for intra-EEA flights to be abolished in the revision of ETD, as part of the 'Fit for 55' package. The revised ETD will raise the minimum tax rate for fossil kerosene for intra-EEA flights: starting at zero from 2023 onwards and to be increased gradually (annual rate of 10%) over a transition period of ten years, until the rate of €10.75 GJ⁻¹ is reached [431,432].

The revised taxation for aviation fuels proposes to consider energy efficiency and environmental impacts [18]. Therefore, the reduction of tax rates or exemption for SAF as well as renewable hydrogen (i.e., minimum tax rate of zero) contribute to make these fuels more economically interesting to airlines, relative to fossil jet fuels, and foster their uptake [18,433]. This strategy would work coherently with the ReFuelEU Aviation proposal to encourage the necessary investment in SAF production and their deployments. These minimum tax rates would not be applicable for pleasure flights and business flights [433].

2.11.7 EU climate law

In the framework of the European Green Deal, the EU launched its first proposal for a Climate Law [434]. This law makes it legally binding for the EU to achieve a balance between GHG emissions and emissions removals (so-called neutrality) by 2050. The current proposal of the Climate Law covers all GHGs. As it stands now, there are no clear measures specifically applying to the aviation sector. The updated GHG reduction target (details in section 2.11.2) along with the climate neutrality target by 2050 is currently in the process of being enshrined into the EU Climate Law [421,434]. For aviation, one consequence of the EU Climate Law could be the quicker deployment of DAC technologies for electrofuels and carbon-free technologies (e.g. batteries, hydrogen), on the premise that decarbonized renewable energy can be used.

2.11.8 The European Advanced Biofuels Flightpath Initiative (EABFI)

The EABFI was launched in 2011 as a partnership between the European Commission and major European stakeholders including airlines and biofuel producers. The objective is to promote the commercialization of biofuels in terms of production, storage and distribution in an endeavor to support the European Commission's ambition to reach energy security [435]. Concretely, this translates in the objective of reaching 2 million tonnes of biofuel consumption per annum by 2020 through the construction of advanced biofuels production plants in Europe. The EABFI is a shared and voluntary commitment to promote the biofuel deployment through appropriate financial mechanisms [435]. However, its 2020 goal has not been met. The EABFI is working on an updated roadmap towards 2030 [435,436].

2.11.9 The French sustainable aviation targets as an example of national initiative

France was one of the first country to announce the ambition of making its aviation industry "the cleanest in the world".

At the end of 2017, France planned to facilitate the production, distribution and deployment for aviation biofuels, corresponding to a "Commitment to Green Growth" with five industrial partnerships including Air France, Airbus, Safran, Total and Suez Environment [437]. The intention, as stated in the French "National Low Carbon Strategy" of March 2019 is the deployment of 2% and 5% biofuels of the expected gross demand of the aviation fuel in 2025 and 2030, respectively [438]. Accordingly, aviation biofuels should be produced from resources listed in Annex IX of the EU RED II [19]. The HEFA from WCO, being a mature technology, is the pathway that received the most focus. By 2050, it is intended that alternative liquid fuels from other advanced pathways (both aviation biofuels and electrofuels) substitute 50% of conventional kerosene [438].

In addition, in early 2020, French government officials announced a 15 billion euros recovery plan for the aeronautical industry, including 1.5 billion euros aid to support research and development into cleaner aviation technologies, for instance, the improvement of engine efficiency with a 30% reduction in fuel consumption for the early 2030s, relative to the current engine, or the development of carbon-emission free aircraft whether electric or hydrogen powered by 2035 [439–441]. Investments to transit towards electric and hydrogen aviation have been

announced, along with investments in the advancement of biofuel/electrofuel production pathways in order to reduce GHG emissions [439].

2.11.10 Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA)

The Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA) was launched in 2016 by ICAO in the endeavor of meeting international goals in terms of GHG mitigation. The aviation industry organizations including IATA and ATAG have set goals of CO₂ emission reductions by 50% in 2050 (relative to 2005 level). It covers all states that are ICAO members. CORSIA aims to offset the emission from international aviation that is not covered under the Paris Agreement. The aircraft operators with emissions greater than 10,000 tonnes CO₂ from the use of aircraft with a maximum certified take-off mass greater than 5,700 kg need to prepare emission monitoring plans and emission reports for all their international flights on an annual basis, from 1 January 2019.

The total CO₂ emissions of each operator are required to calculate in order to demonstrate the offsetting requirements [442,443]. The aircraft operators will then be required to purchase emission units labelled as “carbon offsets” from the Aviation Carbon Exchange (ACE), in order to offset the CO₂ emissions exceeding the defined baseline [444]. These carbon offsets are credits in certified projects that reduce carbon emissions.

Aircraft technology development, operational improvement and deployment of biofuels can be used to achieve their CO₂ offsetting requirements. The sustainability criteria for alternative aviation fuels has been developed under CORSIA Eligible Fuels, which will support the maximum use of biofuels and long-term investment in their productions [445].

ICAO’s CORSIA is being implemented since 2019. The compensation phase thus begins in 2021. This market-based measure encouraged the airlines and other aircraft operators to use SAF. CORSIA SAF are defined in CORSIA Eligible Fuels [78] (SAF in CORSIA corresponds to biofuels in this review). The objective of CORSIA is to reach carbon neutral growth onwards in the aviation sector, in an endeavor to stabilize the net CO₂ emissions from international aviation [78]. CORSIA is composed of three implementation phases: the pilot phase (2021-2023), a first phase (2024-2026) and a second phase (2027-2035). Year 2019 is considered as the baseline emissions for the pilot phase instead of the first proposed baseline of average 2019-2020 due to the pandemic’s impact on the international aviation emissions. The baseline for the first-phase is still under discussion [427,446]. During the pilot and first phases, the offsetting requirements will be applicable for ICAO member states that have volunteered to participate in the scheme. A total of 81 states have officially participated in the pilot phase, representing approximately 76% of international aviation activities in terms of RTK [404]. The second phase is legally binding for all ICAO member states, with the exception of least developed countries and, states with small share of international traffic (less than 0.5% of air traffic), unless they volunteer to participate.

ICAO has launched a detailed requirement for the monitoring, reporting and verification (MRV) of emissions for the CORSIA scheme [445]. It proposes default life cycle assessment (LCA) emission values for five (biomass-based) certified production pathways, these being backed up by a detailed methodological study [445]. However, the calculated default life cycle emission for what CORSIA defines as lower carbon aviation fuels (here referred as electrofuels) and the latest certified CHJ pathway have not been announced at the time of writing.

2.12 Challenges for sustainable aviation

Some challenges for the use of the SA approaches detailed in this review, in the future low GHG emissions, are summarized in Fig. 2.13 and discussed below.

2.12.1 Availability of sustainable biomass feedstock

In the perspective of a sustainable transition towards GHG neutral economies, the procurement of sustainable feedstock not inducing additional arable land demand is a key concern when it comes to biofuels [447], including for aviation biofuels [404,448]. In this context, residual biomasses generated increased attention as they can be decoupled from the need for additional arable land (e.g. [126,449,450]). Residual biomasses have the potential to feed the future low fossil carbon aviation, and several examples have been documented and even show-cased (Table 2.4). Numerous aviation biofuel producers such as LanzaTech or Neste have adapted their technologies to flexibly incorporate residual biomasses (Table S2.2).

Table 2.4 Documented examples of residual biomasses used in the production of aviation fuels

Feedstock	Residues/wastes	Conversion pathway	Comments	References
Carbohydrate	Molasses	SuF	• Co-product from sugar production, albeit already sold as an ingredient for the feed industry	[104]
	Food waste	SuF	• Organic waste from food processing industries, restaurants, and household	[106,273]
	MSW ¹	FT, IH ²	• Organic portion of household waste	[163,181]
	Anaerobic sludge (digestate)	HDCJ	• Digestate from anaerobic digesters • The digestate is used as an input for bio-crude oil production by HTL ¹ , subsequently upgraded to kerosene	[172]
	Algae biomass	HDCJ	• Grown in wastewater • For bio-crude oil production by HTL, subsequently upgraded to kerosene	[451]
	Swine manure	HDCJ	• For bio-crude oil production by fast pyrolysis, subsequently upgraded to kerosene	[166]
Lignocellulose	Forestry waste	SuF, IH ² FT	• Pretreatment requirement • Gasification and syngas conditioning requirements	[105,164,181,273]
	Wheat/rice straw	SuF DSHC	• Pretreatment requirement • Pretreatment and hydrolysis requirements	[273,452]
	Maize stover	SF, FT DSHC APR	• Gasification and syngas conditioning requirements • Pretreatment and hydrolysis requirements • Pretreatment and hydrolysis requirement	[98,139,453]
	Woody chips	SF, FT DSHC APR	• Gasification and syngas conditioning requirements • Pretreatment and hydrolysis requirement • Pretreatment and hydrolysis requirement	[102,139,454]
	Bagasse	SF, DSHC	• Gasification and syngas conditioning requirements • Pretreatment and hydrolysis requirements	[102,137]
	Eucalyptus tips	FT	• Gasification and syngas conditioning requirements	[154]
	Wood sawdust	HDCJ	• For bio-crude oil production by HTL, subsequently upgraded to kerosene	[175]
	Maize stalk	HDCJ	• Pretreatment requirement • For bio-crude oil production by HTL, subsequently upgraded to kerosene	[173]
	Straw stalk	HDCJ	• For bio-crude oil production by fast pyrolysis, subsequently upgraded to kerosene	[455]
	Oil/Fat	Waste cooking oil (WCO)	HEFA CHJ	• Collected from restaurants, food processing industries
Non-edible sunflower oil		HEFA	• Extracted from sunflower residual wastes	[191]
Tall oil pitch		HEFA	• Residue from the distillation of tall oil	[255]
Animal fats		HEFA	• Slaughterhouse waste	[255]
Palm fatty acid distillate		HEFA	• Co-product of palm oil production	[255]
Brown grease		CHJ	• Derived from grease trap waste	[203]

Notes. ¹ MSW: Municipal Solid Waste; HTL: Hydrothermal liquefaction

A key question remains whether the residual biomass potential is large enough to supply the demand. On the basis of the ICAO projections [458], for 2045, a global aviation fuel demand of 16.73 EJ y⁻¹ (ca. 390 Mt kerosene y⁻¹) was estimated. In comparison, it was 7.62 EJ y⁻¹ in 2019 (details in SM 2.2). In the hypothetical case that this future demand should be fully supplied by a biofuel pathway (i.e. disregarding the ASTM D7566 standard on aromatics), considering the FT-SPK pathway as a technology capable to process most residual biomasses, that at least 46 EJ y⁻¹ of biomass feedstock is required (assuming 0.183 kg biomass (dry matter) MJ⁻¹ FT-SPK and 15 GJ t⁻¹ biomass; details in SM 2.2). This alone represents ca. 23% of the global residual biomass potential (being at maximum ca. 200 EJ y⁻¹ based on the meta-study of [124]). Yet, the transition towards GHG neutral economies implies other demands for this limited potential. One example is the plastic sector; based on a forecasted demand of 1,124 Mt plastics for 2050 from [459], and considering a biomass:bioplastic ratio of 1.26 [460], a rough biomass demand of ca. 20 EJ y⁻¹ can be derived if future plastics are to be bio-based (details in SM 2.1). Similarly, supplying 100% bio-based maritime fuels would, considering the 2050 projected demand of 9.50 EJ y⁻¹ [338,339], also require at least 20 EJ biomass y⁻¹ (estimation based on supplying 9.50 EJ y⁻¹ with 100% bio-based LNG, itself deriving from the anaerobic digestion of straw biomass; details in SM 2.1). This rough yet illustrative back of the envelope estimation of the productions illustrates the eventual pressure on the residual biomass potential, where only 3 demands already mobilizes ca. half of the potential.

Further, while some biofuel pathways (e.g., the FT and IH²) can use most types of residual biomasses, other pathways are less flexible, such as the HEFA pathway requiring oil feedstock. At present, aviation biofuels are mainly obtained from the HEFA pathway [255]. This pathway has the advantage of having a greater energy yield in comparison to other biofuels pathways (an overall energy efficiency of ca. 75% for HEFA in comparison to 40% for FT-SPK; [52,461]). The current production capacity of HEFA is reaching ca. 100,000 tonnes SPK y⁻¹ (0.1 Mt SPK y⁻¹) (in 2019; reported by Neste) derives from dedicated oilseed crops and a variety of oil/fat residues [255]. One question is to which extent this new capacity will be based upon waste feedstock versus dedicated oilseed crops. Moreover, basing new investment strategies upon food waste poses the risk of rebound effects encouraging whether the generation of waste, or inducing unforeseen additional demand for the most competitive oil feedstock (often identified as palm oil, e.g. [450]) if no waste oil can be supplied. Globally, the potential of waste fats, oils, and greases has been estimated to ca. 1 EJ y⁻¹ [462]. The current 100,000 tonnes HEFA-SPK y⁻¹ capacity mobilizes ca. 0.02 EJ waste oil and fat. For illustration purposes, supplying the 2045 aviation demand of 16.73 EJ y⁻¹ by 100% HEFA-SPK would require 77.41 EJ waste oil and fats (details in SM 2.1). Despite being an unrealistic scenario, it illustrates that the current potential could only supply 1% of the future demand. On the other hand, competing bioeconomy sectors (e.g. bio-based polypropylene; [463]) also aspire to use these fat waste resources.

2.12.2 Uncertain deployment of DAC

Liquid fuel pathways (biofuels, electrofuels) have the advantage of not requiring heavy infrastructure changes in comparison to the other options discussed in this review. These imply two sources of carbon: biomass and captured-C, either from the atmosphere through DAC or from industrial point sources. While the former and the latter are limited, the potential of DAC is theoretically very large, to the extent the technology is deployed.

There are currently 15 DAC plants operating worldwide, capturing more than 9,000 tonnes CO₂ y⁻¹ (0.009 Mt CO₂ y⁻¹) [38,230]. To produce 16.73 EJ (2045 demand) of electrofuels (FT pathway), approximately 1,200 Mt CO₂ captured would be needed, based on the stoichiometry described in the FT reaction (details in SM 2.2). Keith et al. [38] provide the design and engineering costs for a plausible advanced DAC plant to be implemented at industrial scale, capturing 1 Mt CO₂ y⁻¹ when operated at full capacity. Taking the plant of Keith et al. as a basis, it implies that ca. 1,200 DAC plants would need to operate to supply the carbon needed for future aviation demand by biomass-free FT electrofuels. Yet, the costs of DAC [464] are often pinpointed as a barrier for massive deployment [465,466], along with uncertainties on the markets for CO₂ to ensure a revenue offsetting the costs of capture. Keith et al. [38] report, for the 1 Mt CO₂ y⁻¹ industrial plant they describe, current levelized costs ranging from US\$ 94-232 t⁻¹ CO₂ (range reflecting different technology choices), while other studies report that levelized costs below €50 t⁻¹ CO₂ are achievable by mid-century [467,468]. For comparison, the first commercial-scale DAC plant built in 2017 (with storage of the captured carbon) costed US\$ 600 t⁻¹ CO₂, foreseen to decrease to US\$ 200 t⁻¹ CO₂ as additional plants are built [469]. It is further argued that DAC costs are minor when reported to a country

gross domestic product (GDP) [470], or to global GDP (an emergency massive DAC deployment would imply an investment of 1.2-1.9% global annual GDP; [471]).

Nevertheless, DAC technologies are improving and maturing, reflecting among others their vital role in stabilizing warming at 1.5°C above pre-industrial levels [472–474]. On-going reported improvements include new contactors and tower designs [464,475], optimized operating conditions (e.g. kinetics stability, process stability; [475]), new materials development (e.g. composites of potassium carbonate and γ -Al₂O₃; [464], amine-oxide hybrid materials; [476]), or alternative regeneration processes (e.g. electrochemistry; [477]).

Assuming a favorable techno-economic environment, the potential of DAC is theoretically unlimited. Potentials up to 40 Gt CO₂ y⁻¹ (40,000 Mt CO₂ y⁻¹) by the end of the century have been reported [478] for global warming mitigation, albeit the meta-study of Fuss et al. [469] suggests a potential limited to 0.5-5 Gt CO₂ y⁻¹ (500-5,000 Mt CO₂ y⁻¹). For comparison, the global annual CO₂ fossil emissions were ca. 36 Gt CO₂ (36,000 Mt CO₂) in 2019 [479].

However, it must be highlighted that the driver for DAC is the perspective of inducing so-called negative emissions, i.e., a net long-term sequestration (or removal) of atmospheric CO₂. The use of the captured CO₂ for fuels, as proposed for aviation electrofuels, is therefore deriving the technology from its original purpose.

2.12.3 Need for sustainable hydrogen

All pathways described herein involve hydrogen, with the exception of electric (battery-based) SA, unless part of a hybridized system involving a share of hydrogen fuel or liquid biofuels or electrofuels. Hydrogen is used whether for hydrogenation of aviation biofuels (Figs. 2.2-2.10), electrofuels (Fig. 2.11), as well as for fossil-based kerosene production, although more H₂ is used for biofuels than fossil kerosene (3 to 75-fold more, depending on the pathway; [480]). Yet, some alternatives will require significantly more H₂, namely electrofuels and LH₂ pathways.

Electrofuels, in particular, require H₂ for the reverse water gas shift reaction, where 12 moles of CO₂ are reacted with 12 moles of H₂ to produce 12 moles of CO (Eq. S2.9 and its adjustment in SM 2.1). This CO is then reacted with another 25 moles of H₂ in order to generate for 1 mole of C₁₂H₂₆ fuel via the FT process. This involves that approximately 169 Mt H₂ is required to produce 16.73 EJ (2045 demand) with this pathway (details in SM 2.2), involving 1,520 Mt of water (equivalent to 1.52 billion m³). This clearly exceeds the current capacity of H₂ produced by water electrolysis (around 2% global H₂ production), which amounts to 1.4 Mt H₂ y⁻¹ [480]. Furthermore, the amount of water needed is not negligible either, representing ca. 10% of Australia's freshwater withdrawals (ca. 15.95 billion m³ in the year 2017; [481]). This also applies for electricity, as detailed in 2.12.4.

Albeit not discussed in this study, hydrogen can also stem from biomass-based hydrocarbons through a gasification process, a process that can also be applied to fossil resources (e.g. coal) [482]. This, however, implies an additional demand for limited biomass and land resources as discussed in 2.12.1. Renewable H₂ can also be produced through biogas/biomethane reformation (instead of natural gas) [71], which again implies increasing the pressure on biomass residues to produce the biogas.

Hydrogen fuels (LH₂), on the other hand, are not dependent upon a carbon intermediate, and therefore require slightly less hydrogen when reported by MJ of fuel (details in SM 2.2).

2.12.4 Need for sustainable electricity

Several of the emerging pathways presented in this review involve important electricity requirements, in particular for electrofuels. Electricity consumption for DAC alone may need between 0.23 and 0.37 kWh kg⁻¹ CO₂ captured (0.83 and 1.33 MJ kg⁻¹ CO₂ captured) [38,39,483]. Water electrolysis, on the other hand, requires 30-80 kWh kg⁻¹ H₂ (around 110-290 MJ kg⁻¹ H₂) (Table S2.4), depending on the technologies. To produce the 16.73 EJ demand in 2045 with current technologies for electrofuels, an estimated range of 5,900-10,000 TWh electricity (ca. 21-36 EJ) is needed (i.e. 0.55-0.74 kWh electricity MJ⁻¹ electrofuel produced; 1.81-2.66 MJ MJ⁻¹ electrofuel produced), depending on the DAC and electrolysis technology considered (detailed calculations in SM 2.2). This illustrates, for electricity alone, that 25%-140% more energy is required compared to what is obtained from the produced electrofuel, which only makes sense in the perspective of harnessing the full potential of fluctuating decarbonized energy sources. Independently of the electrolysis-DAC technological combination selected, water electrolysis

always represents ca. 90% of the consumption; the electricity consumption for DAC thus appears negligible in comparison.

The 0.55-0.74 kWh MJ⁻¹ electrofuel derived herein lies in the wide range of estimates found in the literature (0.59-1.00 kWh MJ⁻¹ electrofuel; 2.12-3.60 MJ MJ⁻¹ electrofuel, details in SM 2.2). It should also be highlighted that 5,900-10,000 TWh electricity y⁻¹ (21-36 EJ electricity y⁻¹), i.e. the electricity requirement to produce 16.73 EJ electrofuels, is not a negligible quantity. To put it into perspective, the global electricity consumption in 2019 was about 23,000 TWh (ca. 82.8 EJ) [484]. In other words, the equivalent of 25%-43% of today's global electricity consumption would be required to supply the electricity needed just for producing the H₂ necessary for a demand of 16.73 EJ of electrofuels per year. Similarly, supplying 16.73 EJ of fuels with LH₂ would require only ca. 5,500-9,000 TWh electricity (20-32 EJ electricity), including the liquefaction requirements for ground storage (details in SM 2.1 and SM 2.2). It should be highlighted that in both cases, the lower end of interval is due to the use of SOE technology, based on high-temperature water splitting rather than electricity. This technology requires, per unit of H₂ produced, ca. 40% less electricity than alkaline electrolysis, but 40% more heat (SM 2.2).

2.12.5 Limits of current quantification methods for environmental impacts

To compare the different emerging technologies covered in this study, it must be ensured that the same service is supplied (the amounts of passengers and freight transported over a given distance and time). These may require different number of aircraft (e.g. smaller electric planes), type of aircraft (e.g. to accommodate onboard hydrogen storage systems [65]); infrastructure (e.g. charging), blending with fossil kerosene, etc. Current comparative studies assessing the environmental impacts of alternative fuels often only compare impacts per MJ fuel (e.g. [485-487]), which cannot be applied for SA that are not purely based upon liquid fuels. Further, the requirements for blending with fossil kerosene are typically completely ignored (e.g. [485,486,488]).

Another key issue is the evaluation of the global warming potential related to the non-CO₂ emissions generated during propulsion. Pollutants such as NO_x and particulate matter (including black carbon) serve as precursors for contrail formation, an important climate forcer [76,354]. These are generally ignored in current life cycle assessment studies (e.g., [122,336,489]). Yet, Lee et al. [354] illustrated that the greatest share of cumulative radiative forcing from global aviation between 2000 and 2018 is due to these non-CO₂ effects, and in particular on the radiative forcing effect of NO_x, and to a smaller extent to the aviation induced cloudiness (including cirrus induced by condensation contrails). In the perspective of life cycle assessments, this implies two issues. First, there is a need to quantify these emissions, and second to translate these into warming effect (and eventual other environmental impacts), often through characterization factors.

To date, the most robust method available for the former is to use emission factors relating to the amount of fuel use (e.g., in g of pollutant per g of fuel burnt), which can be found in the literature for all substances including contrails [354,490-492]. Yet, non-CO₂ emissions are not necessarily due to the fuel itself, and are also highly dependent upon the location where they are emitted. Emissions of NO_x, for instance, can be considered as independent from the fuel chemical composition [493], stemming from the nitrogen in the air. Similarly, aviation induced cloudiness is highly influenced by the water vapor saturation of the air where the emission takes place, and by the aerosols (e.g., sulfate, soot) emitted during combustion.

Moreover, there is no consensus on the characterization factors to use to translate NO_x, induced cloudiness, water vapor, black carbon and sulfate to a warming effect. Although recent studies tend to refer to the factors proposed by Lee et al. [354], the differences in proposed factors are really large. For aircraft NO_x for example, the effect will depend not only on the emission altitude but also on the latitude as discussed by Fuglestvedt et al. [490]. A GWP₁₀₀ between -2.1 to 71 can be obtained following the modeling approach. Köhler et al. [494] proposed a GWP₁₀₀ of 75 at the global scale with important variations according to the region of emission. Other methods have also been proposed to translate these non-CO₂ substances into a warming effect, such as the global temperature change potential (GTP), a measure of the temperature change (rather than heat absorbed) over a given time period due to the emission of a gas, in comparison to CO₂ [490,495,496]. Step-change emission approaches (e.g., GWP*, Combined GTP; CGTP) [346] which are applied to a change in emission rate rather than a change in emission amount (as for GWP and GTP) [497], should also be highlighted as existing alternative approaches.

Accounting for non-CO₂ climate forcers will impact the hydrogen-based SA approaches. The hydrogen used in H₂ internal combustion engines or fuel cells, can generate approximately 2.6 times more water emissions relative to conventional kerosene [66,498]. Lee et al. [354] proposed a GWP₁₀₀ of 0.06 for water vapor. Despite useful, this may however not entirely reflect the exact effect that massively deploying hydrogen aviation would have on the radiative equilibrium of water vapor in the low stratosphere [499].

Finally, reductions of soot and particulate matter (PM) have been reported for alternative liquid fuels, in particular biofuels (e.g., HEFA-SPK, FT-SPK) [47,48,493]. This reduction could be explained by the low levels of aromatic content in biofuels [48,493,500]. Some studies, however, consider these differences as negligible (e.g., [336]), while others shed light on the high level of uncertainty still existing regarding these measurements in test rig [493,501]. It thus remains unclear whether biofuels (and electrofuels) really induce a reduction in particulate matters, and the magnitude such reduction could have.

2.12.6 Other impacts

Noise is another impact of aviation especially for residential developments around airports. Novel propulsion systems including battery-electric and hydrogen aviation are foreseen to mitigate and minimize noise impact [66,502,503], facilitating their use in densely populated areas [448,503]. The electric propulsion system, magniX eBeaver aircraft, for instance, has been reported to reduce the average noise level by about 22% (~66 dBA) relative to standard Beaver with piston engines (~85 dBA) [504].

Electric (battery) and H₂ aviation will induce the need for additional infrastructure, among other to charge batteries or store hydrogen. The recharging time, which is mainly dependent upon the charging point (e.g. power outlet capacity) and the battery capacity, is one key challenge of electric aviation to meet desired flight turnaround times.

Similarly, hydrogen refueling stations should be developed with important flow rates to maintain flight turnaround times and prevent hydrogen boil-off issues [66,71]. According to [393], onsite hydrogen production (through water electrolysis) may be possible in a foreseeable future to produce the needed hydrogen on-demand. Cryogenic storage (whether on ground or onboard), which implies the storage of liquefied hydrogen below -253°C (20K) in a double-walled vessel with vacuum insulation [65], implies the need for reliable components including valves, and pumps allowing to ensure these cryogenic conditions as well as safety requirements [505].

2.13 Prospects for sustainable aviation (SA) systems

Despite the potential of the four large SA approaches described herein, there are a number of issues to be addressed prior to broad adoption. This section provides the prospects of their applications for sustainable aviation in the upcoming future. Other sustainable routes are also discussed.

2.13.1 Future aspects for unblended biofuels/electrofuels

All pathways documented in this study require blending with fossil carbon with exception of hydrogen aviation and 100% electric concepts (either 100% battery as shown in Fig. 2.17a, or hybrid LH₂ or fuel cell with battery, as in Figs. 2.17b to 2.17d). The prospects for alternative hydrocarbon-based fuels (biofuels/electrofuels) is summarized herein.

One of the key limiting factors of liquid fuels free of fossil carbon is their low fuel density (below ASTM's minimum specific requirement of 775 kg m⁻³ [506]) and their low (<8%) aromatics content [52,507], which shrinks engine seals. The latter effect is notably observed with the commonly used nitrile rubber material [506,508]. To overcome this, a certain research focus has been placed on the development of new sealing materials preventing leakages [506,509].

The use of 100% alternative liquid fuels is also being investigated through the possibility of combining SAK with HEFA-SPK [510]. SAK is produced through the APR pathway (Fig. 2.2) by converting oxygenated compounds to aromatics in the presence of heterogeneous catalysts such as the aluminosilicate zeolite ZSM-5 [511], a pathway currently under the ASTM approval process [34].

Besides aromatics, cycloparaffins (e.g. cyclohexane, cyclooctane), at a concentration above 30 vol.%, have been shown to supply suitable volume swelling properties [512,513]. They provide increased fuel density, similar to the function of aromatics. Furthermore, they have high gravimetric heat of combustion with the respect to aromatics,

resulting in reduction of particulate matter emissions from fuels containing aromatics [30,513]. These compounds, that could be blended in the fuel, have been produced through multiple pathways and from numerous renewable feedstock, for instance through hydrodeoxygenation of lignocellulosic biomass [514,515]. This approach can be introduced as near-term solution for current aircraft, before new engines capable of handling unblended SPK are widely available.

Another investigated solution is, as earlier reported, the development of alternative fuels identical to conventional kerosene (synthetic kerosene; SK) that could be used without blending. This includes the recently certified CHJ-SK (in February 2020; Fig. 2.10), as well as some biofuels currently under certification (e.g. ATJ-SK from the SuF pathway, HEFA⁺) [34,46]. It is important to note that there is currently no guideline for blending more than one alternative fuel with conventional kerosene (or several alternative fuels without conventional kerosene) within the same hydrant system [516].

Finally, new engine generations capable of using low aromatic fuels may be another solution. For example, the D328neo aircraft manufactured by Deutsche Aircraft Inc. has been publicized in September 2021, to be compatible with unblended alternative fuels by the use of new sealants, surface protection measures, and materials. It is a sub 50 seater regional commuter expected to start its test flight in 2024 and to enter into service by the end of 2025 [56,517].

2.13.2 Electric propulsion development

Motors and generators are key elements for parallel hybrid electric and turboelectric configurations [394] (Fig. 2.17), with additional converters in the case of electric configurations, whether from battery or fuel cell. Further research for the high power-to-weight ratio of electric components is essential to be able to fit with the aircraft weight and volume constraints [396]. A thermal management system, in particular the removal of the generated waste heat, is another key challenge for further research [394]. Alongside, certification standards must be developed to assure the safety and use of batteries (or fuel cells).

High power density fuel cells need to be developed to attain the power requested in propulsion system, and to improve the weight and volume constraints in commercial aircraft. Current power density of fuel cells is ca. 0.75 kW kg⁻¹, whereas 2 kW kg⁻¹ would be required for commercial aircraft [65,71,393].

Another key development is the optimization of the aircraft configuration, in order to optimally integrate the electrical propulsion system and batteries into the aircraft [284], which in turn is dependent on the electric propulsion configuration (Fig. 2.17). This is also studied in combination with alternative design approaches to improve the overall propulsion efficiency (e.g. boundary layer ingestion, wingtip propulsors, BWB aircraft) [518].

2.13.3 Further improvement of hydrogen aviation

Albeit hydrogen can be used as standalone fuel, the integration of either fuel cells or hydrogen combustion engines (whether gas turbines or piston engines) in airplanes remains an engineering challenge. Among others, novel airframes such as the BWB design may present the advantage of having extra volume to accommodate onboard LH₂ storage systems [66,71,320]. In addition to engine developments, airframe designs are required for accommodating cryogenic hydrogen storage, which is beyond the current aircraft capacities. Hydrogen tanks can be placed either inside or outside the fuselage (referred to as integral or non-integral, respectively) [66,519]. Drag penalty can be reduced with the integral method [66] (hydrogen storage inside the fuselage), which may have an impact on overhead luggage storage for short-to-medium ranged airplanes [505]. Placed outside the fuselage, the passenger-carrying capacity remains unchanged, however, the drag is likely to be increased.

Development in new materials (e.g. polymer matrix composites; [520]) for hydrogen tanks is needed in order to make these as light as possible. With the newly developed materials, the gravimetric energy density is expected to reach 10-21 kWh kg⁻¹ (around 36-76 MJ kg⁻¹) of empty storage system [70,71]. If these values are achieved, the system becomes highly competitive with conventional storage systems (ca. 8.9 kWh kg⁻¹; equivalent to ca. 32 MJ kg⁻¹) [521]. Additionally, developments to improve the insulation system for cryogenic LH₂ allowing to minimize boil-off losses (e.g. vaporization) has been demonstrated [519].

As for electric (battery) aviation, developments are needed to optimize the integration of propulsion system and hydrogen storage system, as well as for certifications and regulations ensuring safety through the overall supply chain.

The optimal hybridization between fuel cells and hydrogen combustion engines at the different phases of the flight (i.e. takeoff and climb phase powered by hydrogen turbines; cruise powered by fuel cells) is also being investigated in order to reduce fuel consumption and NO_x emissions [71].

Similarly, improvements are being performed on hydrogen internal combustion system to reduce NO_x emission. For instance, technological and environmental improvements have been obtained with a micro-mix combustor [71,402] or lean direct injection [522].

2.13.4 Other innovations towards sustainable aviation

One notable innovation is the recent AHEAD project, proposing a Multi-Fuel Blended Wing Body (MFBWB) aircraft with hybrid turbofan engines, capable of using both a cryogenic fuel (LH₂ and LNG are specifically mentioned), and a liquid fuel such as biofuel or conventional kerosene. While the BWB is expected to overcome the mass issues related to the cryogenic system, the multi-fuels approach is proposed in order to significantly reduce the overall emissions from engines [348]. A reduction of 50% CO₂ emission (in LNG/conventional kerosene mode) was shown compared to a traditional Boeing 777-200 LR model using fossil kerosene [320,348]. Emissions of NO_x, soot, and CO were also mitigated by ca. 80% relative to the baseline B777-200 ER aircraft [348].

The Taxibot is another example of innovation to reduce the environmental impacts of the aviation sector. It is a pilot-controlled towing vehicle applied for assisting taxiing-aircraft between the terminals and the runway and vice versa while the aircraft's engines are switched off [523,524]. It is an emerging pushback approach to minimize aircraft fuel consumption (by 50 to 85% reduction) and noise (by 60% reduction) while taxiing [66,523]. Approximately 20 million tonnes of CO₂ emission of the world's airliners are estimated to be reduced during the taxi phase of flights if the TaxiBot is adopted [523]. The Taxibot is in operation at Schiphol [525], Delhi and Bangalore airports [526], and serves Lufthansa [524]. Currently, it is powered whether by electric or diesel engines [525], but the vision is to power them with 100% batteries or hydrogen in the future [30,527].

2.14 Supplementary materials

Two supplementary materials (SM) are provided to access all relevant data but are not included in **Chapter 2**. SM 2.1 can be retrieved from this document. SM 2.2, consisting of calculation procedures and other supporting datasets, can be accessed via <https://doi.org/10.48531/JBRU.CALMIP/MIGWAL>.

Supplementary material 2.1 (SM 2.1)

This document presents additional and more detailed aspects not covered but referred to within **Chapter 2**.

1. Aviation biofuel production technologies

1.1 Aqueous phase reforming (APR)

In the study of [528], an aqueous sucrose solution was hydrogenated over a Ru/C catalyst into a sorbitol/mannitol mixture. The obtained intermediate phase, including alcohols, ketones, acids, and cyclized compounds, was a precursor for condensation to longer-chain hydrocarbons. The aviation fuel was obtained from biomass-based sugars with a yield of 32 wt% (from sorbitol) with an aqueous-phase catalytic process in the presence of 10%Ni-supported HZSM-5/MCM-41. The catalytic process was conducted under the operating pressure of hydrogen of 40 bar, temperature 280 °C, weight (weight hourly space velocity; WHSV) 1.25 h⁻¹, and gas (gas hourly space velocity; GHSV) hourly space velocity 2500 h⁻¹. The resulting liquid products consisted of approximately 72 wt% aromatics and naphthenes, tailored as blending components with other bio-based aviation fuels [94]. Additionally, the study of [455] investigated the composition of the hydrocarbon obtained from sorbitol (biomass-based) through the aqueous catalytic process using the Ni-HZSM-5/SBA-15 catalyst. The catalytic process was performed under 320 °C, WHSV 0.75 h⁻¹, GHSV 2500 h⁻¹, and 40 bar hydrogen pressure. The Ni-HZSM-5/SBA-15 catalyst exhibited high selectivity to cycloalkanes and aromatics with a maximum oil yield of 40 wt%.

Virent Inc., located in Madison, Wisconsin, U.S., developed Virent's BioForming[®] platform to integrate APR with the conventional catalytic processes to convert water-soluble carbohydrates to renewable liquid fuels [529].

Aqueous solutions from hardwood tress containing hemicellulose were used to produce jet and diesel fuel range hydrocarbons by [81]. The 87% furfural yield was initially generated by using acid-catalyzed biphasic dehydration. The furfural in an aqueous phase was then extracted into a tetrahydrofuran (THF) phase prior to feeding into an aldol condensation leading to the formation of the furfural-acetone-furfural (F-Ac-F) dimer. The dimer generated was hydrogenated at 110-130 °C and 55 bar with a 5 wt% Ru/C catalyst. Hydrodeoxygenation was carried out over 4 wt% Pt/SiO₂-Al₂O₃ catalyst at 260 °C, 62 bar, and liquid hourly velocity (LHSV) 1.1 h⁻¹, to produce the range of alkanes suitable for jet fuel, containing mainly 91% C₁₂ and C₁₃. [115] used maize cob feedstock for catalytic conversion in an aqueous phase. Acid hydrolysis was first conducted as pretreatment, resulting in furfural production (71%). The furfural was hydrogenated to 2-methyl furan (2MF) as high as 89% yield over Raney Ni catalyst at the preheating temperature 150 °C, LHSV 1.0 h⁻¹ under a hydrogen pressure of 3 bar. An intermediate, maximum yield of 95% was obtained for C₁₅ through the hydroxyl-alkylation/alkylation condensation of 2MF and furfural by using sulfuric acid as catalyst, under 55 °C and atmospheric pressure, with 50 vol% water/ethanol. The highest liquid alkane yield (C₈-C₁₅) was 83%, with high selectivity of C₁₄/C₁₅ (90%) was reported in the hydrodeoxygenation of the C₁₅ intermediate over 10 wt%Ni/ZrO₂-SiO₂ catalyst under 250 °C, LHSV 0.75 h⁻¹ and 50 bar hydrogen pressure; the product was suitable for direct application as aviation fuel. The hemicellulose derived from the maize cob can produce 0.149 tons aviation fuel/ton maize cob with the mentioned processes. The study of an aqueous phase hydrodeoxygenation into the desired hydrocarbons range was reported by [167]. The lignin derived from maize stover was firstly extracted by using the dilute alkali. The liquid phase undergoes hydrodeoxygenation with the combination of Ru/Al₂O₃ and H⁺-Y acidic zeolite catalysts producing C₁₂-C₁₈ cyclic hydrocarbons for jet fuel. The operating condition was at 250 °C under 40 bar hydrogen pressure with a reaction time of 4 h. [530] researched the aviation biofuel production from *Grindelia squarrosa* (the curly gumweed) by aqueous phase hydrodeoxygenation. A heterogeneous bi-functional catalyst was used in the conversion (1% Pd/W-ZrO₂ catalyst) via the hydrodeoxygenation at the elevated temperature (> 200 °C) and an initial hydrogen pressure of 28 bar, with 1 hour reaction time. The resulting products can be used to synthesize high-density cyclic hydrocarbons containing C₁₄-C₁₆ used as additives in aviation biofuel. The oil phase products provided a high heating value (HHV) of 42.8 MJ kg⁻¹. The APR technology has vested interest due to the achievements in bio-based aviation fuel productions with aromatic content [115,455].

SAK and SK (denoted herein as SC) were developed by Virent and were tested against ASTM specifications [99]. They have excellent freeze point (< -70 °C) and thermal stability relative to conventional aviation fuel in the laboratory and fit-for-purpose testing [528]. Virent SAK aviation fuel was tested in a demonstration flight as a fuel blending component, providing a reduction in particulate matter and GHG emissions.

1.2 Direct sugar to hydrocarbon (DSHC)

Amyris Inc. is currently working with the U.S. National Advanced Biofuels Consortium to employ the complex lignocellulosic sugar streams, including cellulosic wastes and residues in the fermentation technology.

After the fermentation, a two-stage centrifugation technology is employed to recover farnesene from the fermentation broth, achieving 97% recovery efficiency in removing trace metals and high boiling point impurities [531].

1.3 Sugar fermentation and alcohol upgrading (SuF)

Generally, the production of long-chain hydrocarbons (compatible with jet fuels) from alcohol intermediates requires four major steps: dehydration, oligomerization, distillation, and hydrogenation. After the fermentation, the alcohol is firstly dehydrated to form the unsaturated compounds known as olefins. The generated olefins are subsequently oligomerized to produce the longer-range hydrocarbon compounds and then hydrogenated, resulting in saturated compound structures as components of the aviation fuels. For bioethanol fermentation, numerous studies investigated microorganisms with strong tolerance to various stress conditions (e.g. acid condition, product inhibition, etc.) for enhancing the bio-alcohol yields. [106] revealed an acid-tolerant *Zymomonas mobilis* able to produce as high as 99.78 g ethanol L⁻¹, using an initial glucose concentration of 200 g L⁻¹, with a pH value around 4.0. Engineered *Saccharomyces cerevisiae* is capable of producing bioethanol at 50 g L⁻¹, using 70 g L glucose⁻¹

and 40 g L xylose⁻¹ as substrates, within 72 h [532]. A recent study of [533] presented the bioethanol production derived from the co-culture of *Escherichia coli* and *S. cerevisiae*, using sugarcane bagasse slurry as substrate. They obtained an ethanol production of 48.6 g L⁻¹, with a solid loading of 20% in less than 30 h. These aforementioned researches can be applied to produce bioethanol for further applications such as long-chain hydrocarbons compatible as blending components with the conventional kerosene.

Butanol, as four-carbon alcohol, has higher energy density and burning efficiency as ethanol, and is required for use in heavy-duty vehicles, ships, and aviation for longer distances [534]. For example, *S. cerevisiae* was used for the production of isobutanol [113]. The ATJ-SPK is allowed to be used as a blending component up to 50% with traditional aviation fuel [535]. During the production process, the isobutanol is separated from the fermentation broth using low-pressure evaporation, concentration, and purification. The isobutanol is dehydrated into isobutylene as a C₄ building block, which then undergoes oligomerization, resulting in the C₈ and C₁₂ olefins. The olefins are hydrogenated leading to C₈ to C₁₂ saturated alkanes serving as jet fuel blendstock. Additionally, the isooctane as another marketable product could be optionally produce through the isobutanol upgrading steps (as mentioned below). The fermentation route has high product selectivity with less toxic compounds generation. The fermentation operating conditions have been usually conducted at mild conditions.

As mentioned about the butanol dehydration, a novel catalyst composed of Zn-Mn-Co modified γ -Al₂O₃ was reported for dehydration of high n-butanol concentration (620 g L n-butanol⁻¹) solutions, to form butenes [536]. The complete n-butanol conversion was observed under a reaction temperature of 375 °C, with 1.67 h⁻¹ weight hourly space velocity (WHSV), achieving 90% total butane selectivity. It was observed that dibutyl-ether and some other hydrocarbons such as methane, ethylene, propylene were formed at lower and higher reaction temperatures, respectively. This modified catalyst also exhibited excellent activity, high stability with a longer lifetime (180 h) relative to the unmodified γ -Al₂O₃. The resulting olefins were subsequently oligomerized and water was removed.

According to [537], the butane oligomerization (~95% or greater) is achievable with a transition-metal catalyst in the presence of methylaluminoxane (MAO). The 2-ethyl-1-hexene as the specific dimer produced, can be converted into mono-unsaturated C₁₆ compounds (using an acid catalyst). The generated products comply with the hydrocarbon-range for aviation fuels. The oligomerization of butane has also been investigated over nickel oxide supported on mesoporous aluminosilicate (NiO/MMZ_{ZSM-5}) catalyst. A higher yield for C₈-C₁₆ olefins (~63%) was reported with 90% butane conversion in comparison to ZSM-5 and MMZ_{ZSM-5} catalysts [538].

In order to improve the production yield and the fuel quality, the C₈ olefin fraction remaining after oligomerization could be removed or hydrogenated and subsequently dimerized, producing additional C₁₆ hydrocarbons. Similarly, the larger oligomers (C₂₀₊) may be separated as a lubricant or cracked to form additional C₁₀-C₁₆ paraffin leading to desired hydrocarbons for aviation fuel [539]. The catalytic hydrogenation of produced olefins can be achieved with PtO₂ as a catalyst, leading to 100% saturated hydrocarbon fuels, meeting the requirements of ASTM 445 [537].

Gevo Inc. (USA) developed a process using the isobutanol generated from the fermentation of biomass into isobutene and paraffinic kerosene [539], as further detailed in Table S2.2. Gevo demonstrated the isobutanol production using its proprietary yeasts and fermentable sugars (e.g. sugar cane, sugar beet), without other co-products and with a novel continuous separation technology avoiding microbial inhibitions (Table S2.2). According to Gevo Integrated Fermentation Technology (GIFT), isobutanol was continuously removed from the bioreactor during fermentation, to maintain the optimum concentration in the gaseous phase, followed by the condensation of the isobutanol rich phase and by a purification phase. The product was used directly as gasoline blending stock and as a building block in the hydrocarbon production for gasoline, kerosene, and diesel fuels. The isobutanol could be dehydrated into isobutene which is used as raw material for many industrial products as aforementioned [539].

1.4 Biomass gasification

Many parameters have an influence on biomass gasification efficiencies such as biomass type, particle size, moisture content, gasification temperature, pressure, gasifying agent, etc., (e.g. higher CO₂ with lower H₂ and CO contents occur under high moisture conditions) [131]. During the pyrolysis process, dried biomass is decomposed at a temperature ranging between 200-700 °C, in the absence of oxygen. Low temperatures (< 500 °C) and long

residence time is preferred for the production of solid char while the gaseous production occurs at higher temperature (700-1,100 °C) with short retention time in an O₂-deficient condition. Condensable gases, tar, and char are obtained [540]. The obtained products are combusted to generate heat for drying, pyrolysis, and other endothermic reactions during the process. The combustion is performed at operating temperatures between 800-1400 °C, leading to the formation of carbon monoxide (CO) and carbon dioxide (CO₂) with released heat. Reduction reactions occur including Boudouard coking ($C + CO_2 \rightarrow 2CO \Delta H^\circ = +172 \text{ kJ mol}^{-1}$), char reforming ($C + H_2O \rightarrow CO + H_2 \Delta H^\circ = +131 \text{ kJ mol}^{-1}$), water-gas shift ($CO_2 + H_2 \rightarrow CO + H_2O \Delta H^\circ = -39.2 \text{ kJ mol}^{-1}$) and methanation ($C + 2H_2 \rightarrow CH_4 \Delta H^\circ = -75 \text{ kJ mol}^{-1}$) [541,542]. High concentrations of H₂ and CO are obtained at high temperatures with favorable char gasification and water gas shift reactions.

As mentioned about syngas conditioning and cleanup for further FT synthesis, tars are the most problematic in biomass gasification. The tar formation depends on the biomass feedstock, operating conditions, gasifier type. The tar, as a complex mixture of condensable hydrocarbons, must be either removed or reformed to prevent problems in downstream processes such as fouling of equipment, clogging, or deposition on the surface. Tar compounds can be removed with several approaches including wet scrubbing, thermal cracking, hydrocracking, steam, or dry reforming. Tar is thermally cracked at elevated temperatures (> 1100 °C) without a catalyst. Solid acid catalysts such as silica-alumina, or zeolites can be used at operating temperatures above 200 °C [156,540]. The tar decomposition can also be done by catalytic cracking of mixed oxygenated compounds (e.g. heterocyclic aromatics, light aromatic, polycyclic aromatic hydrocarbons (PAH)) into light hydrocarbons, at temperatures increasing from 400 °C to 900 °C [543]. Concerning nitrogen-containing contaminants, they are converted to ammonia (NH₃), hydrogen cyanide (HCN), and nitrogen oxides (NO, NO₂, N₂O, and other NO_x). The wet scrubbing is a conventional approach for cleanup of nitrogen-containing contaminants by e.g. precipitation as ammonia salt. Furthermore, the ammonia from hot stream syngas can be decomposed in the presence of catalysts such as Ni, Co, Ru, Fe [134,156]. The sulfur existent in the biomass feedstock is converted to hydrogen sulfide (H₂S), carbonyl sulfide (COS), carbon disulfide (CS₂). Sulfur removal is achieved with sorbents such as metal oxides (e.g. ZnO or CuO), resulting in the formation of a metal sulfide (as often referred to as the desulfurization process). [134]. Sulfur contaminants are also removed by the addition of CaCO₃ into the gasifier [544]. Apart from the abovementioned contaminants, hydrogen halides could be removed via dehydro-halogenation with alkaline (Li, Na, K) and alkali earth (Mg, Ca, Sr, Ba), and metal oxides, at an operating temperature greater than 500 °C. Considering the mentioned reaction, trace metals such as sodium, potassium, etc. are conjointly removed as halide salts [134]. The excess of CO₂ is removed either with compatible solvents like the aqueous solutions of alkanolamines. Additionally, [133] found that char could be a good candidate as a catalyst for the reduction of tar production and increasing the syngas yield.

1.5 Syngas fermentation and alcohol upgrading (SF)

During the catalytic thermochemical route denoted as mixed alcohol synthesis, the reaction performs at the operating temperatures above 300 °C and at 200 bar. The produced effluents are composed of oxygenated compounds (e.g. propanol, butanol), gaseous by-products (e.g. methane, CO₂), and unconverted syngas. The effluent stream is then condensed for alcohol separation. The unreacted syngas could be either utilized as fuel or recycled to the mixed alcohol synthesis reactor. The mixed alcohols are transferred to the distillation system to separate the methanol and ethanol from the higher alcohols [133]. This existing technology provides the lower fuel yield per biomass with the higher carbon emissions in comparison with the biochemical syngas fermentation to alcohols.

The acetogenic microorganisms such as *Clostridium propionicum*, *C. aceticum*, *Acetobacterium woodii*, are capable of consuming CO and H₂ to produce ethanol, 2,3-butanediol (2,3-BDO), poly-3-hydroxybutyrate (PHB) in the absence of oxygen, resulting in a minimization of microbial contamination in comparison with utilizing carbohydrate-based feedstock [116].

For bioethanol dehydration, the use of molecular sieve catalysts such as HZSM-5 zeolite, SAPO (Si-Al-phosphate) is required at lower reaction temperature (300-400°C). According to [545], NiAPSO-34 as Ni-substituted SAPO-34 molecular sieve is a suitable catalyst in the ethanol dehydration into ethylene. The ethanol conversion was 96.5% at the operating temperature of 375 °C. With the HZSM-5 catalyst, good performance at lower reaction temperature and higher ethylene yield were expected; the ethanol conversion was 97.3% at 325 °C. In addition to

mentioned catalysts, the silicotungstic acid (STA) was active in ethanol dehydration producing ethylene and diethyl ether as an intermediate ($2\text{C}_2\text{H}_5\text{OH} \rightarrow \text{C}_2\text{H}_5\text{OC}_2\text{H}_5 + \text{H}_2\text{O}$ $\Delta H^\circ = -25.1 \text{ kJ mol}^{-1}$) at temperatures higher than 200 °C [546]. Other properties balancing the choice of the catalyst materials are the stability in time and the anti-coking ability. Diethyl ether, acetaldehyde, propane, and butane are the main by-products in the ethanol dehydration process [144].

In the case of ethanol oligomerization, [547] stated that the maximum ethylene conversion has been reached at the reaction temperature of 150 °C and pressure 35 bars, using Ni-MSA30 (Ni-mesostructured silica-alumina material) as a catalyst; the obtained product contains mainly C₄-C₁₂ olefins. The above result corroborated the study of [548]. They reported that the Ni-MCM41 mesoporous material as catalyst provided high activity and stability over 170 hours of functioning, with 95% ethylene conversion efficiency. The major product obtained mainly consisted of C₆-C₁₀ olefins. Furthermore, the Ni-ALSBA-15 catalyst was used in ethylene oligomerization at temperature 150 °C and pressure 35 bar, considered as mild conditions, with high catalytic activity and selectivity. The major products were C₄, C₆, C₈, and C₁₀ olefins with a small amount of C₁₂ olefins [549].

For the Gulf process, the olefins C₄, C₆ to C₁₀, and C₁₂ to C₁₆ are fractionated for hydrogenation. Furthermore, the C₄ fraction is subsequently processed by trans-alkylation for increasing the longer-chain olefin yields. The fractionation is performed to separate the hydrogen, further used for hydrogenation of the liquid product streams. The olefins produced are unstable and undesired in order to avoid gum formation in aviation fuels [144].

Considering the LanzaTech syngas fermentation process, the syngas stream generated is firstly cooled, cleaned, and injected into a fermentation vessel containing engineered microorganisms in the liquid media. Microorganisms utilize these gas streams (CO, CO₂, H₂) for their growth leading to the production of ethanol. The ethanol is separated from the fermentation broth and upgraded to hydrocarbon fuels as substitute of gasoline, jet fuel, and diesel. 2,3-BDO is obtained as a co-product of the thermochemical catalytic process (developed by the U.S. Department of Energy's Pacific Northwest National Laboratory PNNL). Other ethanol sources such as commercial ethanol were also employed as input in the aviation fuel production process. In this case, the ethanol is preliminarily dehydrated leading to the ethylene in the presence of aluminum oxide with 99.9% selectivity and high stability. Ethylene is converted to a mixture of C₄-C₆ olefins, which are then oligomerized to desired longer-chain olefins, avoiding polymerization. The developed oligomerization catalyst by PNNL was used with two regenerations during the functioning period (2,000 hours), under mild conditions (85 °C). The global process provides high conversion and selectivity [550].

1.6 The Fischer-Tropsch (FT) process

Syngas undergoes purification prior to the FT synthesis. The crude syngas is initially cleaned from acid gas including CO₂, H₂S, and sulfide (avoiding poisoning of the synthesis catalyst), and adjusted for the appropriate ratio of H₂/CO which is considered as a crucial parameter in FT technology (a high H₂/CO ratio is preferred). Low H₂/CO ratios (< 2.0) reduce the reaction yield and favor the carbon deposition in the FT equipment. Additionally, methane and other small hydrocarbon molecules can become the main products if an excessive amount of hydrogen is present in the syngas [131]. The syngas derived from biomass typically contains a low proportion of hydrogen with the H₂/CO ratio close to one or lower. The water-gas shift reaction is usually achieved by reaching a favorable H₂/CO ratio (~2.0) for the FT process. The suitable H₂/CO ratio for a large proportion of gasoline and diesel production is 2.0, with operating temperatures of 340 and 240 °C, respectively, under pressures of 25-50 bar, with a Co-based catalyst [544].

Ru (ruthenium) catalyst is the most effective in the production of paraffin under high pressures, as the most expensive option. Iron-based catalyst is appropriate for low hydrogen contents (H₂/CO ratio < 1) as a more economical option, but provides lower CO-conversion than a cobalt-based catalyst. The water-gas shift reaction might therefore be favored to enhance the productivity using Fe-based catalyst. Cobalt-based catalyst with support materials such as SiO₂, TiO₂, Al₂O₃ provides a high conversion level, with an affordable price for the production of paraffin and wax from high hydrogen content (H₂/CO ratio > 1) syngas. Fe-based catalyst is more resistant to sulfur and ammonia compounds compared to Co-based catalyst [162,544]. The reduction in the amounts of tar, methane, and light hydrocarbon compounds has been reported with alumina-supported nickel (Ni- γ -Al₂O₃) as an artificial catalyst [551]. Promoters such as manganese, alumina, or copper support the desirable reactions. Copper

(Cu) is added to the iron-based catalyst for enabling reduction reactions. A small amount of gold can enhance the activity of the Co/TiO₂ catalyst [52,162,552].

Other processes have been performed to increase the kerosene yield. For example, the C₃-C₄ olefin produced is converted by oligomerization into iso-paraffinic kerosene (IPK) consisting of highly branched aliphatic hydrocarbon (C₈-C₁₂), by using a solid phosphoric acid (SPA) catalyst in HTFT process [552]. Naphtha can be converted into paraffin through oligomerization and aromatic alkylation using an acid catalyst such as amorphous silica-alumina (ASA), H-form zeolite socony mobil-5 (H-ZSM-5) in the LTFT process. The linear hydrocarbons could further be isomerized to kerosene. The combined SPA alkylation and oligomerization in HTFT improve the production and the quality of the gasoline fraction. The LTFT process provides more straight-chained hydrocarbons in the kerosene with fewer aromatics, olefins, and oxygenated compounds relative to the HTFT process. The aforementioned conversion from syncrude FT reached the maximum aviation fuel production through the FT technology with an improvement of the carbon efficiency of the overall process [553].

1.7 Hydrotreated depolymerized cellulosic jet (HDCJ)

Fast pyrolysis is known to generate predominantly liquid products (bio-crude oil), and valuable chemicals in the absence of oxygen [171]. This process breaks organic materials into mostly liquid products that are rapidly cooled or quenched from the pyrolysis operating temperatures [177]. This approach can be applied in bio-oil productions from a wide variety of feedstocks like lignocellulosic biomass, energy crops, industrial wastes, and by-products. The bio-crude oil produced from pyrolysis generally has an oxygen content between 15-40%, contains hydrocarbons, water, and a small amount of ash [554].

For the bio-crude oil production by hydrothermal liquefaction (HTL), the operating temperature is the most significant parameter affecting the bio-crude yield and properties. This technology can be employed to produce bio-crude oil derived from several feedstocks including municipal wastes, agricultural residue, forest residue, microalgae, etc. [176]. Numerous reactions take place: hydrolysis, dehydration and decarboxylation, condensation, cyclization, and polymerization. Alkaline catalysts have been employed for yield improvement and bio-crude quality from lignocellulosic biomass [99]. The HTL approach generates an aqueous phase containing organic compounds such as oxygenates, a solid residue (known as char), and a gaseous phase containing carbon monoxide, and carbon dioxide. This facilitates the separation of the bio-crude oil from the other product streams [171,554]. The solid residue yield decreases with increasing the residence time.

For the bio-crude oil upgrading process, [555] investigated solvent extraction by the addition of water and organic solvents (hexadecane and octane). The bio-crude oil neutralization (approximately pH 6) in the combined extraction provided good quality bio-oil with less oxygen content and increased heating value relative to the separation process by centrifugation. Furthermore, the 2-propanol was employed as the hydrogen donor solvent through the catalytic hydrogenation from waste cooking oil (WCO) [556]. The optimum yield of liquid hydrocarbon (72%) was obtained at 380 °C and pressure 2 bar with WHSV 6.7 h⁻¹. The obtained liquid product consisted of alkanes, aromatics, and alkenes using 0.42 L 2-propanol L WCO⁻¹ with 0.53 kg jet fuel kg WCO⁻¹. Apart from the prevention of bio-oil degradation, biofuel properties can be improved through hydrogenation as described in the previous section (see the SuF pathway). This process facilitates bio-crude oil stability and low char production. Also, little coke formation avoids catalyst deactivation resulting in higher bio-crude oil yield. The bio-crude oil generated from pyrolysis of pine sawdust was performed by hydrotreatment over Ru/γ-Al₂O₃ as a catalyst at 30 bar hydrogen pressure [557]. The bio-crude oil quality was improved by decreasing the acidity, and a higher C/H content and heating value.

Hydrodeoxygenation is another upgrading step consisting of the hydrogenation and oxygen-removal processes. The cobalt-molybdenum (CoMo) and nickel-molybdenum (NiMo) catalysts are commercially deployable in the hydrodeoxygenation process in petroleum refineries. This bio-crude oil is treated for oxygen removal via hydrodeoxygenation where the operating temperature (250 °C) and pressures (< 25 bar) are controlled in the presence of a catalyst [171]. The hydrodeoxygenation process was investigated [558], over Pt/HY catalyst, for lignin-derived bio-oil formation by fast pyrolysis. This process generated the maximum of cyclohexane and alkylated cyclohexane, appropriate as blending stock for the conventional transportation fuel. The combined Ni/ZrO₂ catalyst in the supercritical cyclohexane was applied in the hydrotreating process in order to improve bio-oil obtained by HTL of maize stalks [559]. This catalyst exhibited high activity and selectivity for diesel- and

aviation-range hydrocarbons. The authors demonstrated that high hydrocarbon yield (82%), composing 90% of diesel- and aviation fuel, is reached under mild conditions (300 °C, 50 bar H₂). The polymerization of bio-oil was not observed in the supercritical cyclohexane providing a high-quality liquid biofuel. The hydrotreatment of bio-oil from the fast pyrolysis was also investigated in the presence of carbide catalysts (Mo₂C and WC) [560]. Mo₂C/ γ -Al₂O₃ and Pt/ γ -Al₂O₃ catalysts showed good catalytic activity for the formation of the aliphatic and aromatic hydrocarbons (60%) at 500 °C under atmospheric pressure. The highest bio-oil yield (roughly up to 60%) was obtained over the Ru/C catalyst. The upgraded bio-oil had less acidity, less water, and increased heating value (about 40 MJ kg⁻¹) compared to the original pyrolysis oil. The higher amount of aromatics and alkanes were reported to be used as precursors of the possible biofuels from pyrolysis oil [561]. In addition to the improvement of bio-crude oil by the olefins saturation and heteroatom removal processes, the heavier product fraction could be processed into lighter products through the cracking process. Catalytic cracking can be applied for decreasing the undesirable products (e.g. gases, coke) at the operating temperature of 350-400 °C. [562] studied the catalytic cracking of bio-oil derived from fast pyrolysis of the straw stalk, for aviation and diesel fuels. The bio-crude oil was initially cracked into C₆-C₈ low-carbon aromatics and C₂-C₄ light olefins in the presence of an HZSM-5 catalyst. These low hydrocarbons were transformed to meet the requirement of aviation fuel by low-temperature alkylation into C₈-C₁₅ aromatic hydrocarbons, using [bmim]Cl-2AlCl₃ ionic liquid. The hydrogenation of C₈-C₁₅ olefins is then performed in order to produce C₈-C₁₅ alkanes in the presence of the Pd/AC catalyst. The developed transformation process has a potential for the production of cycloparaffinic and aromatic compounds as blending components in the aviation fuel range, overcoming the lack of or low aromatic contents. The product streams could be further refined to various fractions of biofuels including gasoline, jet, and diesel fuels. The catalytic hydrotreatment was also reported as the upgrading step for the pyrolysis oil obtained from beech wood with heterogeneous noble-metal catalysts. Licella Inc. is developing the HDCJ renewable aviation fuel. Licella has signed the memoranda of understanding with Virgin Australia and Air New Zealand in the development of the conversion process of the woody biomass into sustainable aviation fuel in 2011. The HDCJ aviation fuel is under tests following the ASTM specification [99,563].

1.8 Hydroprocessed esters and fatty acids (HEFA)

HEFA process parameters have been investigated [190] for diesel and aviation fuels production with aromatics content. The polyunsaturated fatty acids in the vegetable oil (e.g. soybean, sunflower, and camelina oils) are essential in the production of high aromatic content, with the novel Pt/Al₂O₃/SAPO-11 catalyst. [186] found that the optimal reaction temperature was 400 °C for the jet fuel production from waste cooking oil, with Ni/Meso-Y catalyst, obtaining high alkane (40.5%) and suitable aromatic (11.3%) contents. The study of [564] on hydrocracking palm oil, showed that the reaction temperature has an impact on the production of bio-jet fuel yield in the presence of Ni/SAPO-34 as a catalyst. The increasing temperature from 370 to 390 °C under the pressure of 30 bar provided the increase in bio-jet fuel yields from 21.1 to 42.0% along with the increase of the selectivity for jet fuel. [565] studied the catalytic cracking of vegetable oil in the production of cycloparaffinic and aromatic components in jet fuels. The triglyceride-based oil was firstly cracked in the presence of zeolite (HZSM-5) leading to the formation of C₆-C₉ aromatic hydrocarbons and C₂-C₄ light olefins as a by-product, at a temperature around 500 °C. The alkylation of light aromatics obtained from the previous step was processed using an ionic liquid [bmim] Cl-2AlCl₃. The 86.2 wt% C₈-C₁₅ aromatics in the aviation fuel was reached at the atmospheric pressure and alkylation temperature, within 30 minutes, providing the desired C₁₁ and C₁₂ monocyclic aromatic hydrocarbons. The synthesis of C₈-C₁₅ cycloparaffins, which generally account for 20-50 wt% of fossil-based jet fuels, was performed through the hydrogenation of aromatics with Pd/Ac catalyst. The aromatics were hydrogenated into saturated cycloparaffinics at 200 °C and 50 bar within 6 h reaction time. The products obtained could basically meet the aviation fuel standard requirement. The process could be a practical approach for bio-derived aviation fuels from triglycerides-based oils. In addition to the catalytic cracking approach, [566] investigated the catalytic hydrocracking approach for the kerosene production from fresh and WCO. The authors have noticed that the higher kerosene/naphtha ratios and naphtha selectivity were obtained at the hydrocracking temperature of 350 °C at 138 bar with LHSV 1.5 h⁻¹ and H₂-to-liquid feed ratio (H₂/oil) 1068 nm³/m³ in the presence of di-methyl-disulfide (DMDS) and tetra-butyl-amine (TBA) as catalysts.

For the production of jet fuel range, the soybean oil was firstly transformed by hydrodeoxygenation and reforming in the presence of 1%Pt/Al₂O₃/SAPO-11 at 375-380 °C, 30 bar with liquid hourly space velocity (LHSV) 1 h⁻¹.

The produced hydrocarbons were converted by hydrocracking on the Ni₂P/HY catalyst and by additional isomerization with 0.5%Pt/Al₂O₃/SAPO-11. 42-48 wt% aviation fuel yield with 12% aromatics was achieved as the basic production of drop-in diesel and jet fuel. Following the study of [188], the non-edible *Jatropha* oil was transformed in a hydroprocessing step with sulfided NiMo/SAPO-11 and NiW/SAPO-11 catalysts. The 40% aviation kerosene (C₉-C₁₄) was obtained providing the approximate density and viscosity with low sulfur content. The maximum kerosene yield was reached at 425 °C, 60-80 bar, and space velocity 1 h⁻¹ for all catalysts. The obtained kerosene provided the desirable aromatic content with the reduction of hydrogen consumption of about 10%. [186] reported the production of jet fuel derived from waste cooking oil over nickel-loaded zeolites. Ni/Meso-Y exhibited high jet fuel selectivity (53%) with the proper aviation range aromatic hydrocarbon selectivity. The formation of jet fuel ranging hydrocarbon yield of 40.5% was observed at the operating temperature of 400 °C. They stated that waste cooking oil was initially transformed by decarbonylation leading to the generation of long-chain hydrocarbons (C₁₅-C₁₇). These long-chain alkanes were cracked into jet range hydrocarbons (C₈-C₁₆). [567] reported the conversion of palm kernel oil into jet fuel ranging hydrocarbons with NiMoS₂/γ-Al₂O₃. This catalyst exhibited the 58% selectivity of jet fuel hydrocarbon. The desirable product with C₁₀-C₁₂ jet fuel hydrocarbons (approximately 92%) was obtained at 330 °C, 50 bar hydrogen pressure with LHSV 1 h⁻¹. The hydroprocessing of waste cooking oil (WCO) containing mainly unsaturated compounds into the straight alkanes has been studied over two different catalysts including NiMo/γ-Al₂O₃ and Pd/C [568]. The high concentration of long-chained hydrocarbons (C₁₅-C₁₈) was achieved over Pd/C. Pd/C had better performance relative to NiMo/γ-Al₂O₃ with lower pressure (48 bar) and reaction temperature (300 °C), lower H₂ to oil ratios (750), and LHSV (0.5 h⁻¹). Also, the alkane range C₁₅-C₁₈ hydrocarbons in jet fuel were greater than for NiMo/γ-Al₂O₃ catalyst. These alkane products could further be transformed by cracking and isomerizing into bio-based aviation fuel.

In addition to the aforementioned studies, [222] addressed the direct production of jet fuel derived from non-edible oil including waste soy bean oil (SOB) and palm fatty acid distillate (PFAD) within a single-step conversion. The catalytic conversion was conducted over Pb/beta-zeolite at temperature 270 °C, without additional hydrogen, providing a large portion of the liquid product within the jet fuel range C₁₂-C₁₈. The jet fuel ranged hydrocarbons was 69.3% containing straight, branched, and aromatic hydrocarbons. The high degree of oxygen removal (95%) was reached. The obtained results demonstrated the production of aviation fuel from non-edible oils without supplementary hydrogen and further upgrading process. [569] studied the one-step hydrotreatment of catalytic *Jatropha* oil for kerosene production, using the response surface methodology for the process optimization. The authors found that the optimum condition reaching the highest C₈-C₁₆ was achieved at 410 °C, under 50 bar, LHSV 1.2 h⁻¹ and the H₂/oil ratio of 1000 mL mL⁻¹ by using the SDBS-Pt/SAPO-11 catalyst. This new modified catalyst provided high selectivity for C₈-C₁₆ hydrocarbon, i.e. 59.51%.

1.9 Catalytic hydrothermolysis jet (CHJ)

This process requires a pre-conditioning stage for the removal of contaminants including metals, soaps, phospholipids, and other compounds avoiding the coke formation in downstream equipment and the fouling of catalysts, leading to a clean proper free fatty acid feedstock [570]. According to the study of [201], the bio-derived aviation fuels from the tung oil consisted significantly of high-density aromatic benzene up to 60%, serving as a desirable component for fuel blend stock for other SPK and/or commercial jet fuel.

CHJ process was used to develop ReadJet[®] biofuel by Applied Research Associate (ARA) and Chevron Lummus Global, with the Biofuels ISOCONVERSION (BIC) process. The 100% drop-in ReadJet[®] was used with the Falcon 20 aircraft (2016), is providing a 50% reduction in particulate emission, lower GHG emission, and better fuel efficiency than petroleum aviation fuel [201,571]. The CHCJ-5 exhibited similar performance as petroleum-jet fuel JP-5, with similar physical properties, and energy content without compromising engine performances, having an identical molecular composition as the petroleum counterpart [570]. ReadJet[®] jet fuel is being certified for commercial applications through the ASTM D4054 process. The approach led by BP, Chevron, and Phillips 66 collaborations is based on the processing of fats, oils, and greases as intermediates from numerous SAF conversion technologies such as CHJ, HRJ/HEFA, FT existing in the traditional petroleum refinery. This approach leverages existing refinery infrastructure for hydrotreating and hydrocracking providing cost-saving through refinery integration [572,573]. The insertion points in refinery processes are required depending on bio-based intermediate characteristics and products specification. For instance, oxygen removal and hydrocracking processes

are mandatory for upgrading HTL biocrudes while the Fluid Catalytic Cracker (FCC) as an insertion point is mandatory for the production of gasoline and propylene [574]. They could therefore be combined in a conventional refinery updated to ASTM D1655 allowing a maximum 5% by volume insertion of vegetable oil with middle distillates in hydroprocessing [573,574].

2. Aviation liquid electrofuels

Electrofuels have been pinpointed as a possible sustainable alternative fuel for the large-scale production from renewable electricity (such as on-shore and offshore wind, solar photovoltaic powers, etc.), water, and captured CO₂ as carbon source. The production of electrofuel is independent of the availability of arable land avoiding the risk of energy and food production competitiveness, or deforestation, with lower water demand. There is a considerable reduction of GHG emission and particulate matter emission during combustion in comparison with petroleum-based fuel. The non-CO₂ greenhouse gases released at high altitudes are also mitigated. Details about technologies involved in synthetic aviation fuels production are described in this section.

2.1 Hydrogen supply

Three different water electrolysis technologies have been applied in the production of green hydrogen. Alkaline electrolysis uses two electrodes separated by a diaphragm and immersed in an aqueous alkaline electrolyte solution (KOH, NaOH, or NaCl) at 25-30% by weight for maximizing ionic conductivity. Typical temperatures are 65-100 °C under atmospheric pressure. This technology is less energy-intensive, low capital cost with large plant availability and long lifetimes. However, various drawbacks were observed, like cross-diffusion leading to a reduction in the electrolyzer efficiency, limited current density due to the ohmic loss, inability to operate at high pressure, and also corrosive character [575]. PEM electrolysis is based on a solid polymer electrolyte developed to overcome the drawback of previous electrolysis. The functional group of sulfonic acid (-SO₃H) within a cross-linked membrane can lead to a strongly acid character and is responsible for the proton conductivity through an ion-exchange mechanism. PEM electrolyzers can operate at much higher current densities (in comparison with alkaline electrolysis) resulting in operational and overall costs reduction. PEM electrolysis has drawbacks including high investment costs associated with membrane and noble metal-based electrodes, and a short life span [221,575]. Solid oxide electrolysis (SOE) using a supported tubular electrolyte is still developed at the laboratory scale. A typical single-cell SOE is composed of a dense electrolyte layer between two porous electrodes as sandwiched structure. The advanced concept applies water or steam electrolysis at high temperatures 600-1000 °C, providing the sufficient ionic conductivity of the electrolyte. The most typically used electrolyte material is yttria (Y₂O₃)-stabilized zirconia (ZrO₂) (YSZ) with good ionic conductivity at the prevailing high operating temperatures [576]. This technology can operate at a high current density for large production of hydrogen. SOE could be used for electrolysis [223], and for co-electrolysis of H₂O/CO₂ to H₂/CO for syngas production [221]. High-temperature SOE has gained an interest in hydrogen production due to enhanced energy efficiency relative to the thermodynamically favored process in water splitting leading to a reduction in the electricity demand [577]. The waste heat from SOE electrolysis can be used for steam generation in power plants or in any industrial process. High-temperature SOE electrolysis thus demonstrates an increase in the production potential and efficiency [578]. The major limitation in the industrial application of SOE is the limited long-term stability [575]. Among the three different electrolysis processes, alkaline and PEM electrolysis have currently great potential in hydrogen production with large capacity at significant rates. The emerging process SOE is less mature but also promises an interesting aspect in future applications for renewable hydrogen production.

2.2 Carbon sourcing

The carbon capture and storage (CCS) and carbon capture and utilization (CCU) technologies were implemented for a decade in many industries such as power generation plants, petroleum, and chemical plants, cement factories, steel industries, etc. The CO₂ concentration at the point sources has an influence on the appropriate technology selected and on its efficiency. CO₂ extracted is transported and trapped underground within geological formations for enhancement of oil extraction, as a commercial solvent, and as a carbon source to be transformed into other useful products including aviation fuels. Industrial processing of CO₂ concentrated at the point sources is performed through several available technologies including solid-adsorption, adsorption with a liquid solvent, etc. Moreover, the capture technologies have been applied depending on the industrial combustion process including

post-, pre-, and oxy-combustion capture phases. The major aspect of all three systems is the generation of a CO₂ stream that can be further sequestered or used.

In the case of the post-combustion capture, the exhaust gases nearing the atmospheric pressure contain various amounts of CO₂, for example, 3-6 % by volume in the natural gas-fired boiler, 12-14% in coal-fired power plants [579]. The adsorption/desorption technology is the separation of CO₂ from exhaust flue gases produced in the industrial processes by using chemicals such as amine solution and, alkaline solvents. The amine scrubbing process is the most promising method of CO₂ removal from flue gas of power plants (fossil fuel and natural gas-fired power plants). The CO₂-laden solvent is then heated at 120 °C and 2 bar for desorption (known as solvent regeneration) resulting in the concentrated CO₂ gas stream that is further compressed, stored, or transported to the user. The regenerated solvent is recycled in the absorption process. This technology is mature and easy to implement in commercial plants [580]. The high regeneration energy requirement and diluted CO₂ stream are the major drawback associated with the large-scale power plants and increased operational cost. Many solvents have been developed namely bi-phasic-based, salts-based, water lean meeting the lower energy requirement for the regeneration stage with better adsorption characteristics [578]. Due to the relatively low pressure, compression of CO₂ stream is mandatory to meet the requirement for transport and storage leading to increasing operational cost [581]. Another promising post-combustion capture system is the calcium looping process (CaL) as the reversible gas-solid reaction. It has been investigated for post-combustion CO₂ capture in various pilot-scale tests particularly in the cement industries [582–584], and coal-fired power plants [585]. In this process, the flue gas containing CO₂ reacts with the solid sorbents (such as limestone) at operating temperatures between 600-700 °C, resulting in the formation of solid CaCO₃ (saturated sorbent). The CO₂-saturated sorbent is reversely transformed to the CaO-sorbent (recirculated in the process) and highly concentrated CO₂. The CO₂-rich atmosphere is further purified and compressed. The thermal input for the endothermic calcination at a temperature above 900 °C is typically obtained from the fuel-burning chamber under the oxygen-rich condition in order to produce a highly concentrated CO₂ stream. The main advantage of this technology is the employment of widely available and inexpensive sorbent and the high-energy efficiency [584,586]. Even though this capture technology requires a large energy consumption with both high-temperature reactions, it is possible to recover the thermal input from the calcination reaction [581,583]. Considering the pre-combustion technology capturing carbon prior to the burned fuel, the carbon dioxide concentration is relatively high 40% by volume (10-12 bar) [41]. This technology is known as integrated gasification combined cycle (IGCC) power plants for purified gas and electricity production. In this process, coal-based fuel is gasified to syngas under elevated pressure prior to the power generation. The syngas is cleaned and superheated steam is generated to produce electricity. CO in the syngas is subsequently converted to CO₂ through a water-gas shift reaction. The physical or chemical absorption-based solvent is used to capture the CO₂, depending on the syngas characteristics. The remaining stream of hydrogen is burned to generate electricity. Though this pre-combustion system is more complex and costlier, relative to traditional coal combustion plants. CO₂ separation is much easier and inexpensive due to the high operating pressure suitable for CO₂ storage. IGCC has many advantages including the improvement in thermal efficiency, and low pollutant emissions from the coal power plant [41]. In a third approach, oxy-fuel combustion was developed for coal-fired power plants. The fuel is initially combusted with pure oxygen rather than air. The produced gas contains mostly water vapor and a high concentration of CO₂ that facilitates the capturing process. After the SO₂, NO_x, and particulate matter are removed, the CO₂-rich stream is liquefied for further sequestration [587]. Oxy-combustion system provides higher CO₂ removal efficiencies exceeding 95%. However, this capturing technology requires the air separation unit to generate high oxygen content (95-99%) [588,589]. According to the aforementioned technologies, various industrial sectors especially fossil-based fuel-fired power plants can reduce their CO₂ emissions through carbon sequestration. The use of industrial captured CO₂ with high concentration for the electrofuel production is environmentally preferable for the minimization of the overall GHG emissions from the industrial processes and power generation plants in the near-term future.

The Carbon Engineering (CE) company (Canada) has been developing the aqueous-based absorption of CO₂ (DAC) since 2009. CE is the first company in aviation fuel production from atmospheric CO₂ capture, water, and renewable electricity. This developed DAC is carried out based on an aqueous KOH sorbent coupled with a CaL recovery technology [38]. The large quantities of air horizontally fly through contactors based on the cooling-tower technology. The air contacts the alkaline solution containing 1.0 M OH⁻, 0.5 M CO₃²⁻ and 2.0 M K⁺ to form potassium carbonate: $(2\text{KOH}(\text{aq}) + \text{CO}_2(\text{g}) \rightarrow \text{K}_2\text{CO}_3 + \text{H}_2\text{O} \Delta H^\circ = -95.8 \text{ kJ mol}^{-1})$. These compounds are

precipitated with high ionic strength solutions of 30% $\text{Ca}(\text{OH})_2$ generating calcium carbonate (CaCO_3) pellets simultaneously with KOH that can be reused ($\text{K}_2\text{CO}_3(\text{aq}) + \text{Ca}(\text{OH})_2(\text{s}) \rightarrow \text{CaCO}_3(\text{s}) + 2\text{KOH}(\text{aq}) \Delta H^\circ = -5.8 \text{ kJ mol}^{-1}$). The produced CaCO_3 is subsequently calcined resulting in calcium oxide and CO_2 in supercritical form ($\text{CaCO}_3(\text{s}) \rightarrow \text{CaO}(\text{s}) + \text{CO}_2(\text{g}) \Delta H^\circ = +179.2 \text{ kJ mol}^{-1}$). It is an energy-intensive step at temperatures above 700°C . The recovered superheated steam derived from the CaO pellets could be used for power generation to maximize energy efficiency. The generated calcium oxide is hydrated at the operating temperature 300°C forming $\text{Ca}(\text{OH})_2$ ($\text{CaO}(\text{s}) + \text{H}_2\text{O}(\text{l}) \rightarrow \text{Ca}(\text{OH})_2 \Delta H^\circ = -64.5 \text{ kJ mol}^{-1}$). The captured CO_2 as a concentrated stream is subsequently cleaned and compressed from atmospheric to 15 MPa at 45°C .

The Climeworks company (Switzerland) proposed to use a porous granulated material modified with amines (solid-sorbent system) to capture CO_2 from the atmospheric air. Preliminary, the ambient air is transferred to a filter containing modified supported-amine. The CO_2 captured that is chemically bounded to the saturated filter is released from the solid support at a temperature of 100°C ensured by low-grade/waste heat as an energy source, and pumped out as concentrated CO_2 [590]. The project partners (Climeworks, Ineratec, Sunfire, and KIT) have launched the Power-to-X (P2X) Kopernikus project to produce carbon-neutral fuels from air-captured carbon dioxide and using green power by a combination of advanced technologies to produce liquid fuels with maximum efficiency. For the Power-to-X project, the co-electrolysis is applied to split simultaneously carbon dioxide and water vapor as syngas in a single process (by Sunfire venture). The FT process is applied to convert the produced syngas into long-chain hydrocarbon molecules as a precursor for fuel production by Ineratec (a spinoff of KIT), and fuel quality and yield are further optimized via the hydrocracking process by Karlsruhe Institute of Technology (KIT) [590]. Additionally, Global Thermostat as the start-up for DAC technology (U.S.) has developed amine-modified monolith technology. Two pilot facilities of Global Thermostat are capable of removing 3,000 to 4,000 tonnes of CO_2 per annum by each facility. The technology developed is firstly flown for maximizing the amount of air over the contactor by pushing the air through narrow channels with high contact surface area enabling the adsorption in a short period of time. The cost was estimated at around $\$100/\text{ton CO}_2$ captured. Collaboration with ExxonMobil was foreseen to scale up direct DAC and industrial capture technologies from August 2019 aiming to mitigate 1 billion tonnes of CO_2 each year [591]. Even though emerging technologies are raising great attention allowing negative global CO_2 emissions, the low concentration of carbon dioxide in the ambient air (roughly estimated 400 ppm in 2018) is still the major issue meaning that a large energy amount input and material cost are still necessary for capturing large quantities of air. [592] claimed that 2 to 4 times energy consumption is required for CO_2 captured from the air in comparison with CO_2 captured from flue gases. The development in DAC technology for the reduction of operational costs could provide this alternative option in the competition with the fossil-based liquid fuel in the future.

2.3 Liquid hydrocarbon synthesis

In the FT route, CO_2 from concentrated sources or air extraction is used as a carbon source as mentioned above. A fraction of the electrolytic hydrogen is initially required to reduce carbon dioxide to carbon monoxide via the reverse water gas shift reaction ($\text{H}_2 + \text{CO}_2 \rightarrow \text{CO} + \text{H}_2\text{O} \Delta H_{573\text{K}} = +39.2 \text{ kJ mol}^{-1}$). Then it is combined with the additional hydrogen forming syngas as the precursor for FT synthesis. The syngas produced through this pathway is relatively clean compared to the syngas produced from biomass or fossil fuel gasification. The operating conditions (e.g. H_2/CO ratio, temperature, partial gas pressure, the catalyst used) in FT are of great importance to generate the desired product fractions. The FT synthesis requires similar stages as addressed in previous sections. The FT-derived hydrocarbon molecules with different lengths are upgraded in several process steps including hydrocracking, isomerization, and distillation. The full system integration for power-to-liquid production is demonstrated by Sunfire in Dresden, Germany. Sunfire demonstration plant applies the high-temperature co-electrolysis SOE for the production of synthesis gas in a single step, which reduces the investment and operating costs and increases the production efficiency for the P2X project [593].

In February 2019, Lufthansa has announced to start using low-carbon kerosene (sometimes denoted as electrofuel) generated from the Heide refinery in Germany, which aims to supply 5% of the fuel at Hamburg airport reaching almost zero-(fossil) carbon fuels within five years as a part of the KEROSyN100 project [594]. In this project, the first power-to-jet fuel plant at a commercial demonstration will be developed. The wind power will be used to power a 30 MW alkaline electrolyzer to produce hydrogen while the CO_2 will be captured from the nearby cement plant. The H_2 and CO_2 captured are then combined through the methanol synthesis which is further converted into

synthetic kerosene. According to the study of [595], the electrofuels are not cost-effective options with respect to other fuels, the process is energy-intensive and limited by carbon storage. Reaching the CNG by 2020 in the aviation sector, the KEROGREEN project supported by Europe (Horizon 2020) is developed (2018 to 2022). The project aims to develop a novel conversion route in the production of sustainably synthetic kerosene derived from non-biomass sources. Renewable electricity and CO₂ captured from air and fuel usage have been served as the feedstock. The plasma driven CO₂ dissociation, solid oxide membrane, CO₂ capturing technology and FT process are integrated in compact-sized equipment producing 1 kg kerosene/hour. If successful, this project will provide a remarkable solution. The equipment developed will be used to produce carbon-neutral liquid fuels on-site, with an offshore wind turbine or remote solar array without the requirement of expensive electricity infrastructure [596]. The collaboration between industrial and governmental sectors is a solid premise to foster the development and production of kerosene derived from non-biomass resources.

3. Co-products generation in liquid fuels production pathways (biofuels and electrofuels)

3.1 2,3-Butanediol (optional)

According to LanzaTech Inc., the engineered microorganisms of the family of clostridium, including *Clostridium autoethanogenum*, have been used with carbohydrate substrates like fructose and/or sucrose and gas containing CO. The results showed that increasing the amount of CO provided led to the enhancement of the overall 2,3-BDO productivity. The desirable co-products (such as butanediol) are consequently recovered from fermentation broth using fractional distillation, pervaporation, and extractive fermentation whereas alcohols and acids might be recovered with different separation techniques [597]. [598] have studied the upscaling of 2,3-BDO productions with 150 L bioreactor using high-yield strain *Enterobacter cloacae* TERI BD 18 using commercial grade glucose as substrate. Two-stage pH and dual agitation control strategy can enhance the 2,3-BDO productivity as much as 1.73 g L⁻¹ h⁻¹ with the maximum yield of 0.48 g 2,3-BDO g glucose⁻¹ achieved in 50 h.

LanzaTech pilot plant has a capacity of 15,000 gallons per year commissioned since November 2008. Furthermore, LanzaTech constructed a demonstration plant in China for the conversion of industrial waste gas to 2,3-BDO since 2010. 2,3-BDO derived from the conversion of carbon-rich industrial waste gases as feedstock has been commercialized in 2014. LanzaTech has developed processes with increased production of co-product in particular 2,3-BDO allowing the production of 50% of 2,3-BDO.

3.2 Isobutene (optional)

Lanxess and Gevo have signed an agreement to purchase isobutanol from Gevo Inc. being supplied as an alternative route to traditional fossil fuels for the next ten years [599]. According to Global Bioenergies Inc., the engineered *E. coli* strain MG1655 comprising of HMG-CoA synthase and mevalonate diphosphate decarboxylase has been used in the isobutene production with glucose feedstock via fermentation. Global Bioenergies' technology has been developed with broad feedstock flexibility including non-biomass derived carbon sources for the isobutene productions. Due to low aqueous stability, isobutene is continuously vaporized and separated from the liquid broth in a gaseous state at ambient temperature and pressure [600]. The industrial pilot plant built in France (Pomacle) with Cristal Union as a partner, has a capacity of 10 tons per annum producing e-gasoline for Audi cars or purified as a valuable commodity chemical for numerous industries such as cosmetics, kerosene, LPG, plastics (since early 2015). The 100 tons/year production capacity was achieved in the demonstration plant at Leuna, Germany, operated since early 2017. The first full-sized plant is foreseen by the year 2020.

In 2015, LanzaTech with its partner INVISTA as the world's largest integrated producer of chemical intermediates, polymers, and fibers, declared the successful development of a metabolic toolkit generating novel metabolic pathway to bio-derived butadiene and precursors such as 1,3-butanediol, 2,3-butanediol. This novel approach results in new direct and two-step processes for butadiene production as a particular product through gas fermentation technology [601]. Lanxess as a leading chemical company based in Germany has collaborated with Gevo in the development of sustainable isobutanol dehydration into isobutene as a material needed in rubber manufacturing since 2010 [599]. Additionally, the isobutene derived production from renewable feedstocks (e.g. residual sugars, crops, agricultural and forestry wastes) was announced by Global Bioenergies company (France) [600]. Furthermore, Global Bioenergies and LanzaTech have announced a new collaboration (in 2016) in order to directly transform the waste gas into isobutene [602].

3.3 Propane

The renewable propane produced by Neste Corporation will be supplied to its collaborator SHV Energy, the global leader in LPG distribution, 160,000 tonnes over a four-year period, sold as BioLPG for transportation applications in Europe. BioLPG can be used in various ranges of applications such as transportation without compromise on performance, commercial heating to retail leisure cylinders resulting in notable carbon footprint saving up to 80% [603]. In June 2019, KLM, SkyNRG, and SHV Energy have announced the first European production plant for sustainable aviation fuel in Delfzijl scheduled to operate in 2022 combining local waste streams and hydrogen from electrolysis. This facility, as part of the SkyNRG project called DSL-01, will annually produce 100,000 tonnes of SAF and 15,000 tonnes of BioLPG as a by-product. The waste and residue streams coming from regional industries will serve as feedstock ensuring the negative impact on food supply and environment, to meet the sustainability standards for sustainable fuels. Corresponding with this statement, KLM will purchase 75,000 tonnes SAF y^{-1} saving more than 200,000 tonnes of CO₂ emission per annum whereas BioLPG products will be purchased by SHV Energy. This project contributes as a significant milestone to the energy transition in the upscaling of the market for sustainable kerosene along with BioLPG (KLM, SkyNRG, and SHV) [604]. AltAir Paramount LLC refinery in California owned by the leader in low-carbon transportation fuels supplier World Energy Inc. since 2018 produced renewable propane along with aviation and diesel fuels from a small number of non-edible vegetable oils and animal tallow. The renewable propane is also applied on-site or exported as process fuel [605].

3.4 Naphtha

The CARB-compliant renewable gasoline (as an alkylate combination) provides an octane number of 91, cleaner combustion and emission reduction meeting more stringent air quality standards. Additionally, World Energy has announced the partnership with Pearson Fuels to purchase renewable naphtha in October 2019. Pearson Fuels as the largest distributor of E85 Flex Fuel in California blends this renewable naphtha with its ethanol allowing delivery of sustainable fuels and energy. This low-carbon, high-octane E85 fuel is up to 55% cleaner in comparison with conventional gasoline and is specified for use in Flexible Fuel Vehicles (FFV's). E85 Flex Fuel generally purchases for 50 to 75 cents gallon⁻¹ less than regular unleaded gasoline driving immediate and positive environmental changes [606]. Neste MY renewable naphtha is generated as a co-product derived from the refining of renewable diesel production through HEFA conversion technology. It could be used as a blending gasoline component or fuel additive due to its high energy density, and serves as a precursor in the production of bioplastics and renewable-based chemicals [607]. The proportion of renewable-based naphtha as a blending component can be determined by the RVP and octane number of both substituents.

3.5 Isooctane

Gevo Inc., a SAF refinery company (SAF from alcoholic fermentation), has announced in February 2019 a 10-y purchase and sale agreement with HCS group, for 10,000 tonnes/year of Gevo's isooctane for high-end applications, for instance, high purity solvents, special fuels under the key brand Haltermann Carless (excluding isooctane use for road transportation fuels) [267]. According to this agreement, isooctane is one of the main products derived from Gevo Inc., coupled with isobutanol and renewable aviation fuels production [267].

Global Bioenergies has also developed an innovative approach in the fermentation process allowing gaseous product separation from the liquid phase through spontaneous evaporation. This process could mitigate the process complexity along with energy intensity in product separation, for isooctane production [602]. The first isobutene batch produced from renewable sources at Global Bioenergies' industrial pilot plant had been delivered to chemical company Arkema in May 2015 and was subsequently converted into isooctane by the Fraunhofer Center for Chemical Biotechnological Processes (CBP). These isooctane produced in collaboration with Audi could be applied as additive fuel or as standalone fuel labeled unleaded 100 [263]. Global Bioenergies has signed an agreement with IBN-One and Lantmännen Aspen for the production of isooctane for specialty fuel applications in early 2020. During this project, isobutene produced from the Global Bioenergies demonstration plant (based in Leuna) will be converted into isooctane prior to starting the commercial plant IBN-One [608]. In addition to bio-based isooctane, Global Bioenergies and its collaborator Audi have announced the production of renewable liquid isooctane denoted as e-Benzin (e-gasoline). This program is devoted to developing innovative technology in the production of renewable isooctane using non-biomass sources such as water and, sunlight. The first production of Audi e-gasoline of 60 L, was achieved for initial engine tests in March 2018 [609].

3.6 Gasoline

Gevo Inc. (Table S2.2), for example, markets a renewable gasoline product generated by blending the isooctane derived from maize-based isobutanol with naphtha and alcohols (ethanol, isobutanol). This product has applications like fuel for Formula One racing, packaged fuels for outdoor equipment, fuel for light-duty city fleet (in Seattle) [265].

3.7 Diesel

Red Rock Biofuel's biorefinery (Oregon) has a production capacity of 7.2 million gallons of aviation fuel coupled with 7.2 million gallons diesel and 3.6 million gallons naphtha per annum in Table S2.2 [610]. Furthermore, Altalto Immingham Limited in collaboration with British Airways, Shell, and Velocys, develops the first European commercial plant to produce sustainable fuels (based in the U.K.) since August 2019. The production of renewable fuels is planned, in particular of SPK, using household and commercial solid waste through the FT process developed by Velocys. British Airline purchases this renewable aviation fuel reaching CNG from 2020. Shell intends to purchase both aviation and road transportation fuels derived from the Altalto project for carbon footprint mitigation [611]. During the bio-based kerosene production through biochemical conversion processes, the diesel range hydrocarbons are cracked and isomerized to form paraffin with the appropriate carbon distribution for the aviation fuel range. Renewable diesel is generated from Gevo Inc. as a by-product from the alcoholic fermentation process providing reductions in CO₂ and particulates emissions. This renewable diesel might facilitate the marine sector to meet new international water regulations starting in 2020, due to notably sulfur reduction, particulates, and CO₂ emissions [612]. Honeywell UOP produces renewable diesel through the HRJ/HEFA pathway coupled with renewable aviation fuels production. The desirable product fractions, either renewable diesel or synthetic paraffinic kerosene (SPK), are significantly dependent on the market demand and price. Honeywell Green Diesel has 44 MJ kg⁻¹ energy density, less sulfur content (< 2 ppm) with a high cetane number of 75-90 and can be utilized at neat form without significant modification in fleet operations. This renewable diesel could be used as blending stock without additional investments or engine modifications.

3.8 Wax

Waxes produced in FT pathways are competitive with fossil oil-based waxes. Due to their purity, they might be sold at around \$1.24 kg⁻¹ while the crude oil-based paraffin waxes are purchased at approximately \$1.03 kg⁻¹ [613]. It appears there is already a market demand for these FT-wax products; for instance, Carbon Engineering, a leading company in Direct Air Capture technology, announced that they will sell some of these heavy alkanes (C₂₁-C₃₀) as industrial lubricant precursors to customers such as Unilever, for the production of synthetic petroleum jelly [613].

4. Electric and Carbon-free aviation

4.1 Electric powered aviation

The limited battery energy density and the improvement of energy storage have been studied for delivering sufficient power to engines. NASA as a part of the X-planes, with Electric Power System (EPS) by Safran Corporate, develop a battery module for the experimental X-57 Maxwell electric aircraft. They are seeking reliable lithium-ion battery modules, lightweight, with advanced battery packing technologies, for efficient flights avoiding overheating and failure. EPS innovates in cell welding and thermal management without additional weights and provided an 850-pound lithium-ion battery pack for NASA's X-57 Maxwell. This innovative approach is capable of stopping thermal runaway at an individual cell level and set a new standard for "packaging overhead" as the ratio of the packaging weight to the weight of the cells [614]. Development of this prototype has been continuously carried out such as a high-aspect-ratio wing, smaller high-lift motors providing better performance and energy efficiency [615]. The modified X-57 Maxwell denoted as Modification IV has been planned for its first test flight in late 2020. As the mentioned successful issue, the eFlyer program created by Bye Aerospace as the world leader and innovator of electric and solar-electric aircraft produced 2-seat eFlyer (eFlyer 2) since February 2014 and also developed 4-seat aircraft model as denoted as eFlyer 4 in July 2017. These electric aircraft are made from composite materials powered by six and ten lithium-ion batteries in eFlyer 2 and eFlyer 4, respectively Bye Aerospace has announced to apply the EPS batteries to power the eFlyer in March 2018. For the first flight, eFlyer 2 consisting of a Siemens SP70D electric motor was demonstrated in April 2018 [616]. Boeing HorizonX Ventures and Safran Corporate Ventures have announced their collaboration in EPS since September 2019 to develop

lightweight energy storage systems providing high-quality power in the aviation sectors at an unprecedented scale. They have unveiled to produce batteries for the urban air mobility at an industrial scale based on the Utah-company in coordination with the U.S. Federal Aviation Administration for testing and developing the safety regulations and testing requirement for electric and hybrid aircraft. Boeing HorizonX Ventures has invested in Cuberg as an advanced lithium metal battery technology. Safran Ventures has invested in OXIS Energy as the leader in lithium-sulfur cell technology for high energy density battery systems [617].

Bell Inc. has designed electric vertical take-off and landing (eVTOL) aircraft with the addition of a purely electric propulsion option in the new demonstrator helicopter Bell Nexus 4EX in 2019, consisting of four ducted fans. This new aircraft demonstrates less drag with more efficiency in the cruise mode providing 10% to 15% energy density improvement by the mid-2020s [618]. Rolls-Royce recently reveals the project Accelerating the Electrification of Flight (ACCEL) with the Aerospace Technology Institute (ATI) as a partner in the development of electric propulsion. They planned to create the fastest all-electric aircraft with a highly powerful battery and with lightweight materials. Rolls-Royce and YASA as a manufacturer of high-power, lightweight electric motors, and controllers, are involved in the development of an electric demonstrator aircraft, supported by Electroflight start-up for high-performance electric powertrains [619]. The ionBird test airframe as the electrical technology propelling the aircraft in the ACCEL project was also unveiled in December 2019. According to Rolls-Royce, the most powerful battery for an aircraft in ACCEL will provide sufficient energy to fly 200 miles on single charges. These 6,000 cells are packaged to minimize weight and maximize thermal protection with an advanced cooling system [620]. Furthermore, Rolls-Royce has participated in the research program with Norwegian airline Widerøe since August 2019 on a zero-emission aviation program. They have planned to replace and electrify its regional fleet of more than 30 planes by 2030, designed for short-haul distances. The investment in electrification is ramping up rapidly to make it become a reality [621]. According to the regulatory approval, and public perception, the Urban Air Mobility (UAM) including package delivery drones, passenger-carrying air taxis, air ambulances, etc. could make profitable as many as 500 million flights for cargo services and 750 million flights per annum for air metro services [622]. However, the prospective for electric longer-range flights is dependent on liquid sustainable aviation fuels for the next few decades.

In addition to all-electric aircraft projects, the E-Fan X hybrid-electric propulsion has been developed by Rolls-Royce, Airbus, and Siemens, launched in 2017 [623]. A first flight was expected in 2021; however, this project was canceled in April 2020 [624].

4.2 Hydrogen aviation

Airports like London Heathrow (LHR), Berlin Brandenburg (BER), Los Angeles International Airport (LAX), Gatwick, Toulouse-Blagnac (TLS) are expected to have installed hydrogen refueling stations by 2020, and to generate hydrogen on-site from renewable energy sources through water electrolysis.

Both liquid and gaseous forms of hydrogen can serve as fuels depending mainly on the developed technologies. Liquid hydrogen contains a higher energy density relative to the compressed gas. However, it increases the aircrafts' weight as it requires cryogenic tanks in accordance with the safety regulation and high energy-intensive process in production. A four-seat passenger HY4 aircraft, with 1500-kilometer range, has been developed by DLR Institute of Engineering and Thermodynamics (Germany) with More Electric Aircraft (MEA) and All Electric Aircraft (AEA). The HY4 fuel cell powered aircraft was flown the first flight from Stuttgart Airport on September 2016. This aircraft is the world's first aircraft powered solely by hydrogen fuel cell system. The powertrain system comprises a hydrogen storage system, and a low-temperature hydrogen fuel cell and lithium battery as energy storage component. The compressed hydrogen is directly converted into electricity, with water vapor and small amount of heat as waste products. Further objective of the DLR Institute of Engineering & Thermodynamics is to improve the fuel cell powertrain in regional aircrafts with up to 19 passenger [625]. ZeroAvia based in Cranfield, U.K. and Hollister, California, U.S. aims to demonstrate hydrogen fuel cell powertrain technology aircrafts for zero-emission aviation [626]. The Piper M-class aircraft with 6-seats in business-class arrangement was successfully conducted for the full test flight with two tons takeoff weight in April 2019. The hydrogen in this airframe is compressed at about 345 bar, similarly to the high-pressure fuel cell system in road vehicles. The development of hydrogen fuel cell powertrain was also the subject of the HyFlyer project of ZeroAvia, granted by the U.K. government, enabling zero emission in commercial aviation. During the project,

the conventional powertrain will be replaced with electric motors, hydrogen fuel cells and gas storage. Intelligent Energy will intervene with ZeroAvia in optimization of evaporative cooling fuel cell technology. Cranfield Aerospace Solutions (CAeS) will support the integrating ZeroAvia's hydrogen powertrain technology into the Piper airframe. Moreover, the project partner European Marine Energy Centre (EMEC) Hydrogen generates the green hydrogen from renewable wind and tidal energy and will supply the hydrogen for the flight test. Their hydrogen-powered planes with as many as 20 seats, are planned to launch commercial operations in 2020, delivering up to 500 miles (~ 8,047 km) regional flights.

Singapore's HES Inc. as the global leader in hydrogen propulsion systems for autonomous aerial vehicles has unveiled Element One as the world's first regional hydrogen-powered passenger aircraft in October 2018. It is expected to be the first prototype to be ready by the year 2025 in Toulouse, France. The Element One aircraft could currently carry four to ten passengers between 500 and 5,000 km for regional flights depending on whether the hydrogen is stored in gaseous or liquid form. The key technology in this aircraft is HES' Aeropak solution merging ultra-light hydrogen fuel cell technologies with a distributed electric aircraft propulsion design as a hybrid hydrogen-electric propulsion system. After which the smaller scale unmanned aircraft with a single Aeropak will begin the test in 2027 [627]. HES has joined the consortium including Aerospace Valley as the global aviation research and development hub in Toulouse, Wingly as a French startup offering flight-sharing services for decentralized and regional air travel, ERGOSUP as a small developer of the innovative electrolyzer capable of producing hydrogen from renewable resources. Industrial-scale hydrogen producers (H_2 derived from renewable solar or wind energy) are involved in the development of the refueling systems in hydrogen-ready airports preparation for large-scale hybrid hydrogen-electric Element One aircraft [627]. Alakai Technologies Corporation (a Massachusetts-based startup) has unveiled the test flight of five-seat multirotor Skai aircraft powered by hydrogen fuel cells in 2019 and is expected to achieve USA Federal Aviation Administration (FAA) certification by 2020. Skai aircraft can range up to 400 miles with 4 hours flight time. This aircraft contains three hydrogen fuel cells, hydrogen cooled into liquid form and stored in double-walled stainless steel fuel tanks under 100 psi pressure [628]. ENABLING Cryogenic Hydrogen-Based CO_2 -free Air Transport (ENABLEH2) has recently been funded (2018-2022) by the European Union's Horizon 2020 research and innovation program, and led by Cranfield University. This project aims to develop the liquid hydrogen (LH_2) based propulsion technology achieving zero-level CO_2 and ultra-low NO_x emissions through several approaches such as combustor design improvement with high energy efficiency, fuel system heat management, infrastructure development, economic sustainability, and community acceptance, etc. The roadmap enables technology development and integration of aircraft and propulsion systems at TRL 6 by 2030-2035. NASA is ongoing the project in the development of a super-cold cryogenic hydrogen fuel cell system for powering electric aircraft since May 2019 [629]. The Center for Cryogenic High-Efficiency Electrical Technologies for Aircraft (CHEETA) program will investigate the practical electric propulsion technology to replace conventional fossil fuel propulsion systems. This program focuses on the development of aircraft powered by cryogenic liquid hydrogen as energy carriers through fuel cells driving the ultra-efficient electric propulsion system. Eight institutions collaborate to overcome the barriers in the practical cryogenic hydrogen applications in the electric propulsion system. The low-temperature requirement for a hydrogen propulsion system is also being investigated by using superconducting energy transmission, and a high-power motor system [630]. Additionally, the collaboration between eCap and Breezer Aircraft companies has set the objective to make aircraft powered by electricity generated from hydrogen in January 2020. The new high-performance electric propulsion system from Breezer Aircraft will be installed in a Breezer B440-6 small aircraft including high-performance battery storage provided by eCap. The fuel cell will be applied in another prototype [631]. In addition, in July 2020, Airbus has been launched the utilization of hydrogen fuel cell to power gas turbines or hybrid-electric combinations as the expected technology for the next decade able to reduce the climate change effects [632].

4.3 Solar aviation

For the solar aviation, photovoltaic (PV) systems serve as (solar) energy converter for electricity generation [633]. this system is similar to all fuel cell electric (Fig. 2.17d), the PV being installed instead of fuel cells. Solar panels installed on the wings convert the solar energy into electricity, which is used to power the electric motor driving a propeller/fan, and charge batteries during daylight time [368]. Excess electricity is stored in batteries to supply overnight power. The limitations are low conversion efficiency of solar panels to electricity, inconsistency for

capturing photons onboard, and vulnerable materials to adverse weather conditions [368]. To date, solar-aviation is focusing on other applications including unmanned aircraft systems/unmanned aerial vehicles (UAS/UAV) as mentioned below. General aviation has also been conducted, for instance, the Solar Impulse project (not for passenger-carrying). The development for greater payload is far as there have been other emerging energy sources to be deployed. However, if successfully, they can provide clean solutions as a long-term perspective for the air transportations. Airbus Defence and Space announced the world's first operational High Altitude Pseudo-Satellite (HAPS) Unmanned Aircraft System/ Unmanned Aerial Vehicle (UAS/UAV) flight (Zephyr project). A first model has completed a maiden flight in 2018 for 26 days straight [634]. Other successful demonstrations for solar powered UAS/UAV include the Odysseus drone (first flight in April 2019; [635]) and the Silent Falcon UAS/UAV (commercialized in 2015 five to seven hours flight; [636]). Notably, Solar Impulse has become the first solar airplane flying more than 40,000 km around the world without fuel, from June 2012 to July 2016; however, it is a one-seat plane (pilot) and was not built to carry passengers [637].

5. Sustainable biomass and alternative potentials

Assumptions and background information for the calculation of sustainable biomass potentials are presented here below.

5.1 Aviation fuel demand and assumptions

Aviation fuel demand has been calculated based on the projected air passenger demands from [638]. In 2045, approximately 22 trillion revenue passenger kilometers (RPKs) is foreseen for domestic and international service segments. The passenger load factor is assumed as 80% corresponding with the actual value before the COVID-19 outbreak. Aircraft's performances derived from Airbus and Boeing manufacturing with the aforementioned parameters have been used to estimate their specific energy consumption as $\text{MJ seat}^{-1} \text{ km}^{-1}$ (flight range dependent). The energy requirement (fossil-based kerosene) in 2045 is approximated at 16.73 EJ y^{-1} . This amount is further used to calculate the sustainable biomass potentials (detail in SM 2.2).

Concerning the global RPKs in 2020, around 2.9 trillion RPKs y^{-1} have been reported [639]. Approximately 2.55 EJ kerosene is needed.

5.2 Biomass required to fulfill the 2045 demand, if 100% bio-kerosene

The meta-study of [640] suggests a maximal residual biomass potential of ca. 200 EJ y^{-1} (equivalent to approx. $10,000\text{-}13,333 \text{ Mtonnes y}^{-1}$ (Mt) considering the biomass energy density of $15\text{-}20 \text{ MJ kg}^{-1}$).

For sustainable bio-kerosene, the biomass gasification-FT process has been considered with carbohydrate- and lignocellulosic-based biomass. The energy density of these biomasses has been estimated using data from [641], i.e., within the range of $15\text{-}20 \text{ MJ kg}^{-1}$. Input (biomass) and output (syngas before the FT process) data are obtained from [642], while the output mass fraction derived from the FT process is retrieved from [553,643]. Residual biomass composition is derived from [644]. From the aforementioned studies, it was considered that 0.183 kg biomass (dry matter) is required to generate 1 MJ FT-SPK .

Therefore, biomass requirements for alternative kerosene production are estimated at approximately $53.29\text{-}71.05 \text{ EJ y}^{-1}$ to reach the projected air passenger demand ($16.73 \text{ EJ kerosene y}^{-1}$) in 2045.

5.3 Biomass potential for bioplastic projection demand

For comparison reasons, the required biomass for bioplastic production is also estimated. Based on [645], about 4.3 million tonnes of biomass is required to supply 3.4 million tonnes bioplastics (with an average bio-based share of 43%). The Ellen MacArthur Foundation forecasts a global consumption (year 2050) of 1,124 million tonnes of plastics y^{-1} [646]. Considering a lower heating value of biomass of 15 GJ tonne^{-1} approximately $20 \text{ EJ biomass y}^{-1}$ is thus demanded just for the future bioplastic demand.

5.4 Biomass potential for maritime fuel projection demand

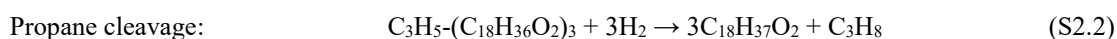
Another example is the forecasted demand for the maritime sector (shipping sector). Numerous energy sources can be applied (e.g., liquefied natural gas (LNG), diesel, ammonia; [339]). The projected maritime fuel in 2050 is about 9.50 EJ , and LNG represents the major share of this [338,339]. Roughly considering that 100% of the 9.50 EJ y^{-1} demand is to be supplied by bio-based LNG, approximately $20 \text{ EJ biomass y}^{-1}$ could be required. This

estimation considers straw (90% dry matter, 90% volatile solids out of total dry matter and 0.22 Nm³ CH₄ per kg volatile solids; [647]), 1,300 Nm³ CH₄ per tonne LNG [648], a LHV of 50 MJ kg⁻¹ LNG [338] and a biomass LHV of 15 GJ tonne⁻¹.

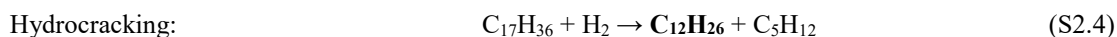
5.5 Waste oil and residual fat potential for HEFA-SPK projection demand

Waste oil and residual fats are one of the promising feedstock as listed in the Renewable Energy Directive (RED II), Annex IV Part B for the eligible fuel productions [19,649]. Moreover, they are considered the primary feedstock for aviation fuel production through the HEFA-SPK from the point of view of sustainability criteria (e.g., food and feed market competition, land-use change impacts). However, their availability is another issue to be discussed. This section, therefore, provides key assumptions for calculating their estimated potential according to the reported HEFA-SPK production capacity (by Neste) and the projected demands.

According to the literature (e.g., [650–653]), the oleic acid (C₁₈H₃₄O₂) is the main fatty acid of triglyceride compounds, the major component of the oleochemical wastes. Therefore, glyceryl tri-oleate was chosen as the representative compound to apply in the hydro-deoxygenation (HDD) and hydrocracking units. During the HDD process, the triglyceride molecule is converted into the paraffinic compounds via three main reactions [568,654,655]:



Subsequently, the paraffinic compounds (herein referred to as C₁₇H₃₆) are converted into the HEFA-SPK in the hydrocracking unit. For simplicity, C₁₂H₂₆ is considered as the representative SPK (hydrocarbon ranges between C₈-C₁₆ in kerosene [656]).

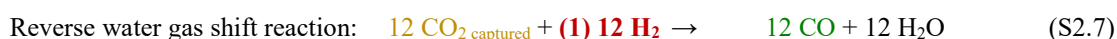
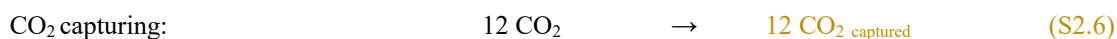
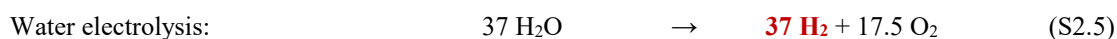


It is assumed that other compounds such as phospholipids are negligible in the waste oils and residual fat feedstock. A lower heating value (LHV) of waste oil/residual fat and the produced HEFA-SPK of about 40 MJ kg⁻¹ [657,658] and 45 MJ kg⁻¹ [659], respectively, are applied.

From the abovementioned assumptions, approximately 0.12 kg of waste oils and residual fats are required to produce 1 MJ HEFA-SPK. As reported by Neste, it is demonstrated that around 0.02 EJ oleochemical waste is needed to produce 100,000 tonnes of HEFA-SPK [660]. To produce 16.73 EJ aviation energy demand, considered to be only derived from the HEFA process, about 77.41 EJ waste oils and fats are required.

5.6 Theoretical hydrogen, water, and CO₂ needs to supply future aviation demand by 100% electrofuels

According to the carbon distribution in kerosene in the range of 8 and 16, an average carbon number of 12 corresponding to C₁₂H₂₆ is assumed as the major component in the aviation electrofuel. Gravimetric energy density of kerosene is 43.0 MJ kg⁻¹ [553,659]. Hydrogen is considered to be obtained through water electrolysis. The electricity requirement for water splitting can be retrieved in Table S2.4. Reverse water gas shift reaction is required for syngas composition adjustment. Electricity for DAC technologies varies, with 0.23 and 0.45 kWh kg⁻¹ CO₂ captured for physical absorption in liquid media and solid adsorption, respectively [38,39]. It is assumed that captured carbon and hydrogen are directly used without compression and storage. Generic chemical reactions for this production process are given below.



For the aforementioned reactions and assumptions, to produce 16.73 EJ aviation kerosene ($C_{12}H_{26}$) for 2045, 169 Mt hydrogen and 1,200 Mt CO_2 are needed, which request approximately 5,900-11,000 TWh electricity. Approximately 1,500 Mt of water is required to produce the mentioned hydrogen amount. The detailed calculation can be retrieved in SM 2.2: excel spreadsheet.

5.7 Liquid hydrogen production

Water electrolysis is put forward as a key “green hydrogen” production technology. Electricity consumption for water splitting varies depending on the technology as demonstrated in Table S2.4. The generated hydrogen must be compressed for its use in the plane, which needs additional electricity consumption. Herein, gaseous hydrogen is compressed to liquid with approximately 7 kWh kg H_2^{-1} [661]. To reach the 16.73 EJ aviation demand in 2045, about 5,500-9,300 TWh electricity including liquefaction is needed, as well as approximately 1,250 Mt water required for water electrolysis. The further detailed calculation can be retrieved in SM 2.2: excel spreadsheet.

6. Table S2.1 Aviation biofuels characteristics from different conversion technologies

Technological conversion	Feedstock	Fuels produced and blending ratio by volume	Aviation biofuels characteristics	Limitations	Commercial use ^d
Aqueous Phase Reforming (APR) [34,99,148,187,662]	Carbohydrate and lignocellulosic-based biomass	SKA and SK: Unknown; still under certification	<ul style="list-style-type: none"> • High cyclic hydrocarbon and suitable aromatic content^a allowing to increase the content of bio-based fuel in the blending • A likely broader range of hydrocarbons than other bio-based alternatives • Reduction (50-80%) in particulate matters compared to conventional jet fuels • Good cold flow properties^b and thermal stability^c 	<ul style="list-style-type: none"> • Expensive and short-lived (deactivation) catalysts 	TRL 4-5 FRL ^d of 6 according to Virent's APR technology in demonstration facilities
Direct Sugar to Hydrocarbon (DSHC), also referred to as Hydroprocessed fermented sugar (HFS) [34,99,201,531,663]	Carbohydrate and lignocellulosic-based biomass	SIP: Up to 10% (certified in 2014) (Amyris and Total)	<ul style="list-style-type: none"> • Mainly comprising of iso-paraffin (97% by weight farnesane), which results in low freezing point • High energy contents (47.5 MJ kg⁻¹) • High flash point (51.3 °C) due to long-chain hydrocarbons • No sulfur and particulate matters 	<ul style="list-style-type: none"> • Long-chain hydrocarbon (as farnesane C₁₅H₃₂) resulting in a high viscosity causing poor combustion performance, poor lubricity, and pumping difficulties • Absence of aromatics leading to elastomers being shrunk and fuel leakage • Incomplete mixture of hydrocarbons, as uncovered by a continuous distillation curve (ASTM D7566 Annex A3) • Alternative high-value markets for farnesane 	TRL 7-8 for sugar feedstock TRL 5 for cellulosic biomass FRL 7-8 according to Amyris technology
Alcohol-to-Jet (ATJ): Sugar fermentation and alcohol upgrading (SuF) [34,144,273,664]	Carbohydrate-based and lignocellulosic biomass	ATJ-SPK from isobutanol: up to 50% (certified in 2018) ATJ-SK: unknown; under certification	<ul style="list-style-type: none"> • Mixture of C₁₂ and C₁₆ iso-paraffinic hydrocarbons derived from iso-butanol based • High energy density (43.2 MJ kg⁻¹) and good thermal stability^c • High flash point (48 °C) • Low total sulfur content (<0.01%) with low soot formations 	<ul style="list-style-type: none"> • Absence of aromatics leading to elastomer shrinkage and fuel leakage • Requirement for upgrading processes to longer-chained hydrocarbons with higher energy density • Low reactivity resulting from the high fraction of branched hydrocarbons • In a complete mixture of hydrocarbons, as uncovered by a continuous distillation curve (ASTM D7566 Annex A5) 	TRL 5-6 FRL 4-6

Alcohol-to-Jet (ATJ): Syngas fermentation and alcohol upgrading (SF) [34,186,665,666]	Industrial off gases ^c , syngas or biogas generated from biomass resource	ATJ-SPK: up to 50% (certified in 2018) derived from renewable ethanol	<ul style="list-style-type: none"> • High content of iso-paraffinic hydrocarbons without the formation of aromatics and cycloalkanes • Wide-boiling iso-paraffinic kerosene similar to HEPA-SPK and conventional jet fuel • Good thermal stability^b and low amount of contaminants • Optimum flash point (≥ 38 °C) • Freezing point (-61 °C) well below ASTM standard 	<ul style="list-style-type: none"> • Low solubility of syngas in fermentation media with limiting gas conversion efficiency • Requirement of the upgrading processes to longer-chained hydrocarbons with higher energy density • Low aromatic content resulting in poor lubricity 	TRL 5-6 FRL 4-6
Fischer-Tropsch (FT) process [34,145,187,667,668]	Lignocellulosic biomass (e.g. forestry residue, crop residues)	FT-SPK: up to 50% (certified in 2009)	<ul style="list-style-type: none"> • Mostly composed of n- and iso-paraffins conferring a good thermal stability and cold flow properties^b • High cetane number leading to complete combustion with a shorter ignition delay time • Low nitrogen, sulfur, and cyclic hydrocarbon content 	<ul style="list-style-type: none"> • High production cost with process efficiency between 25-50 % • Low lubricity because of the absence of occurring oxygen, nitrogen, and sulfur-containing compounds • Low aromatic content resulting in some fuel leakage problems • Extensive gas cleanup and conditioning requirement of syngas properties prior to the FT unit 	TRL 5-6 FRL 7-8 corresponding with biomass-to-liquid FT
Integrated hydrolysis and hydroconversion (IH ²) [34,181]	Lignocellulosic biomass	Unknown; under certification	<ul style="list-style-type: none"> • High aromatic content (around 92 vol.%) exceeding the ASTM D1655 (max. 25 vol.%) 	<ul style="list-style-type: none"> • Low values in terms of the net heat of combustion, smoke point, naphthalenes, etc. • Low catalysts lifetime 	TRL 6
Hydrotreated depolymerized cellulosic jet (HDCJ) [34,99,563,669]	Lignocellulosic biomass	Unknown; still under research and development	<ul style="list-style-type: none"> • High energy density of bio-crude oil (from pilot-scale results) • Low sulfur content • High lubricity 	<ul style="list-style-type: none"> • Intensive bio-oil upgrading processes in particular pyrolysis bio-oil 	TRL 6 FRL 6 according to Licella's Cat-HTR technology
Hydroprocessed renewable jet (HRJ) also referred to as Hydroprocessed esters and fatty acids (HEFA) [34,184,188,668,670]	Oil-based biomass such as animal fat used cooking oils	HEFA-SPK: up to 50% (certified in 2011) HC HEFA-SPK: up to 10% (certified in 2020) HEFA-SK: unknown; under consideration	<ul style="list-style-type: none"> • Composed mainly of linear and branched alkanes (C₉-C₁₅) with a small fraction of cyclic hydrocarbons • High cetane number, which causes a short ignition time delay and good combustion performance • Free of aromatics and sulfur • Good thermal stability^b due to the absence of aromatics • Ash-free fuel combustion • Low soot formation 	<ul style="list-style-type: none"> • Low lubricity due to the absence of oxygen, nitrogen, and sulfur-containing compounds • High paraffin contents affecting the cold flow properties • Low oxidative stability^f due to the absence of cyclic compounds and/or antioxidants • Different feedstock used providing different cetane numbers resulting in the fuel ignition engine • High hydrogen requirement • High vulnerability on feedstock cost 	TRL 8 (vegetable and lipids) TRL 5 (micro algal oils) FRL 9; the technology is mature and deployed at commercial scale

Catalytic hydrothermolysis jet (CHJ) [34,562, 570]	Oil-based biomass such as animal fat, waste oils	CH-SK: up to 50% (certified in 2020)	<ul style="list-style-type: none">• CH-SK consists of aromatic, cyclo-paraffinic, and iso-paraffinic hydrocarbons suitable for use as a 100% drop-in fuel• 20% Aromatic content	<ul style="list-style-type: none">• Low smoke point
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7. Table S2.2 Aviation biofuel developers and their partnerships^a

Developers	Plant location	Feedstock	Technology/ process involved	Partnerships	Production capacity ^a
LanzaTech [671–673]	Asia/Europe/USA (expansion) China (commercial plant)	<ul style="list-style-type: none"> Industrial off-gases, syngas generated from biomass resource, hydrogen from reformed biogas Lignocellulosic biomass such as agricultural residues 	<ul style="list-style-type: none"> Syngas fermentation to ethanol Upgrading of ethanol processes to ATJ-SPK Fractional distillation 	<ul style="list-style-type: none"> PNNL^b developed a catalytic process for converting ethanol into ATJ-SPK First commercial flight by Virgin Atlantic airline from Orlando to London Gatwick with Boeing 747 aircraft in October 2019 An offtake agreement with ANA, Japan's largest airline in June 2020 	125 million gallons of ATJ-SPK year ⁻¹ (expected from UK plants by 2025)
Gevo [674–677]	USA	<ul style="list-style-type: none"> Carbohydrate-rich biomass such as industrial maize Lignocellulosic-based biomass such as crop and forestry residues or cellulosic municipal solid waste 	<ul style="list-style-type: none"> Pretreatment of lignocellulosic feedstock and to hydrolyze sugars Fermentation to isobutanol using GIFT® (Gevo Integrated Fermentation Technology) Isobutanol upgrading processes to ATJ-SPK Fractional distillation 	<ul style="list-style-type: none"> A long-term offtake agreement with Delta airline; 10 million gallons/year in December 2019 Collaboration with Avfuel delivering ATJ-SPK to Bombardier's aircraft facility since November 2019 Fuel sale agreement with Scandinavian Airline System (SAS) planned in November 2020 Partnership agreement supplying fuel to Air TOTAL International in September 2019 	8 million gallons year ⁻¹
BYOGY Renewables [678,679]	USA	<ul style="list-style-type: none"> Sugar- and cellulosic-rich feedstock 	<ul style="list-style-type: none"> Pretreatment of feedstock Fermentation to ethanol and distillation Ethanol upgrading processes via the developed catalytic synthesis technology with molecular adjustment of the fuel to required properties Product fractionation into ATJ-SPK and gasoline 	<ul style="list-style-type: none"> Partnership with AusAgave Australia to develop production from low-cost sugar feedstock since 2014 Initiative launched in collaboration with Avianca Brazil in 2014 testing the first full replacement with ATJ-SPK Qatar Airway invested in Byogy Renewables; offtake agreement with Qatar Airway in 2012 	-
Fulcrum BioEnergy [680]	USA (expansion)	<ul style="list-style-type: none"> Municipal solid wastes (MSW) 	<ul style="list-style-type: none"> MSW conversion to syngas with gasification FT process converting gas to liquid hydrocarbons Hydroprocessing refinery process to naphtha, aviation- and diesel fuels 	<ul style="list-style-type: none"> ThermoChem Recovery International, Inc. (TRI) developed a gasification system BP and Johnson Matthey (JM) technologies developed for the FT process and needed catalyst Long-term fuel offtake agreement with United Airlines providing 90 million gallons/year 	10-60 million gallon year ⁻¹ plant ⁻¹

Red Rock Biofuels [681,682]	USA	<ul style="list-style-type: none"> • Lignocellulosic biomass such as forest and sawmill residues 	<ul style="list-style-type: none"> • Woody biomass gasification to synthesis gas • FT process converting gas to liquid hydrocarbon • Hydroprocessing refinery process to naphtha, aviation and diesel fuels 	<ul style="list-style-type: none"> • Lakeview Project (Oregon): converting wood waste into 15.1 million gallons year⁻¹ of renewable fuel since 2018 • Agreement with FedEx: supplying 7 million gallons year⁻¹ between 2017 and 2024 • Agreement with Southwest Airlines: purchasing 3 million gallons year⁻¹ in 2014 (the first delivery expected in 2016) 	<ul style="list-style-type: none"> • 15.1 million gallons year⁻¹ of renewable gasoline, aviation and diesel fuels
Velocys [683,684]	UK	<ul style="list-style-type: none"> • Lignocellulosic biomass such as forest residues and household wastes 	<ul style="list-style-type: none"> • Gasification • FT process converting gas to liquid hydrocarbon • Hydroprocessing refinery process to naphtha, aviation and diesel fuels • the NEXBTL™ as the hydrotreatment process (HEFA) 	<ul style="list-style-type: none"> • Altalto project (due July 2019): Commercial plant in Immingham (UK), in partnership with British Airways and Shell 	<ul style="list-style-type: none"> • 20 million gallons year⁻¹ of aviation fuel and naphtha in Altalto project
Neste [685]	Finland, the Netherland Singapore (expansion)	<ul style="list-style-type: none"> • Oil-based biomass such as animal fat from food processing wastes, vegetable oil residues, inedible tall oil pitch 	<ul style="list-style-type: none"> • the NEXBTL™ as the hydrotreatment process (HEFA) 	<ul style="list-style-type: none"> • First commercial flight with Lufthansa between Frankfurt and Hamburg in 2011 • Intercontinental flight with Lufthansa airline between Frankfurt and Washington D.C. in 2012 • First commercial flight in collaboration with Air BP in early 2020 • Collaboration with Lufthansa in Frankfurt airport in 2020 • Supply KLM airline additional ATJ-SPK at Amsterdam Airport Schiphol from December 2020 	<ul style="list-style-type: none"> • 100,000 tonnes SPK year⁻¹ in the US and Europe • Expecting over 1 million tonnes SPK by 2022 in Singapore refinery expansion
Honeywell UOP [686]	USA	<ul style="list-style-type: none"> • Oil-based biomass 	<ul style="list-style-type: none"> • the UOP Renewable jet fuel process™ (HEFA) 	<ul style="list-style-type: none"> • AltAir refinery (both renewable jet- and diesel fuels) started in 2015 • Supply > 1 million gallons HEFA-jet fuels produced for the U.S. military and commercial aviation 	-
World Energy [687,688]	USA (expansion in Paramount, California)	<ul style="list-style-type: none"> • Oil-based biomass derived from waste stream food processing 	<ul style="list-style-type: none"> • the AltAir fuels hydrotreatment process 	<ul style="list-style-type: none"> • Honeywell UOP developed the process technology • Collaboration with United Airlines purchasing up to 10 million gallons over the next two years from May 2020 • A memorandum of understanding between Air France, World Energy, and 	<ul style="list-style-type: none"> • Expecting over 300 million gallons of SPK year⁻¹ at the expanded plant

SkyNRG [604,689, 690]	Netherland	<ul style="list-style-type: none"> • Oil-based feedstock derived from waste streams from food processing 	<ul style="list-style-type: none"> • HEFA technology produced by the World Energy (AltAir fuels) 	<p>Shell to be in effect from 1st June 2020</p> <ul style="list-style-type: none"> • Collaboration with Shell aviation and produced SPK by the U.S. World Energy since January 2019 • Europe's first dedicated sustainable aviation fuel production plant launched in November 2019, in collaboration with Shell, as part of the DSL-01 project • Collaboration with Finnair providing the "Push for change" service allowing customers the choice to fly on SPK since early 2020 • Royal Netherlands Air Force operating with F-16 Fighting Falcons on SPK in January 2019 • First SPK flight of Singapore Airlines (SIA) partnered with the CAAS^c with an Airbus A350-900 in May 2017 • Air Canada partnered with the CAAFCER^d operating with SPK in April 2017 	-
Virent [528,529]	USA	<ul style="list-style-type: none"> • Sugar-rich feedstock such as maize, sugarcane, sugar beet • Lignocellulosic-rich feedstock such as wood and agricultural wastes 	<ul style="list-style-type: none"> • Pretreatment feedstock prior to Virent BioForming[®] process • Feedstock conditioning • APR of soluble carbohydrates into hydrocarbons • Catalytic processes for Virent's SPK and SKA 	<ul style="list-style-type: none"> • Marathon Petroleum Corporation (MPC) has ambitions, together with BP and Johnson Matthey (JM) on scaling up and commercialize Virent's BioForming technology • Demonstration testing of Virent's BioForm[®] SKA by Rolls-Royce supported by FAA^e in 2017 	-
ARA/CLG/ Lummus Global [570,572]	USA	<ul style="list-style-type: none"> • Oil-based feedstock such as waste fats, oils, and greases 	<ul style="list-style-type: none"> • Catalytic hydrothermolysis with supercritical water • Hydrotreating process • Products fractionation to diesel and aviation fuels 	<ul style="list-style-type: none"> • ReadiJet[®] alternative fuel test flight powered by 100% unblended SPK in October 2012 • High aromatic ReadiJet[®] alternative fuel testing program at Rolls-Royce facilities in August 2011 • Feedstock technology for crop improvement by Agrisoma Biosciences • ARA and Chevron Lummus Global (CLG) developed Biofuels ISOCONVERSION (BIC) process as the novel catalytic hydrothermolysis (CH) 	-

Licella [669]	Australia	<ul style="list-style-type: none"> • Lignocellulosic feedstock such as woody biomass, agricultural residues, energy crops, algae etc. • Waste oil and industrial residues 	<ul style="list-style-type: none"> • Catalytic hydrothermal reactor platform (Cat-HTR™) as hydrothermal upgrading plants 	<ul style="list-style-type: none"> • First commercial Cat-HRT plant from biomass raw materials with JV and Canfor Pulp in 2021/2022 • Collaboration with Neste using mixed waste plastics for the production of fuels, chemicals, and new plastics in 2018 • The Australian government supported a commercial demonstration plant for the production of bio-crude to be used as a drop-in fuel for the aviation industry in 2011 • A memorandum of understanding (MOU) with Air New Zealand for converting woody biomass into sustainable aviation biofuels was signed in 2011 • Virgin Australia set an aspirational target of sourcing 5% of aviation fuel from sustainable sources from 2020
Shell/Biozin Holding AS [34]	India Norway	<ul style="list-style-type: none"> • Lignocellulosic biomass such as forestry residue, agricultural residue, etc. 	<ul style="list-style-type: none"> • Catalytic hydrolysis • Hydroconversion • Products fractionation to gasoline, diesel, and aviation fuels 	<ul style="list-style-type: none"> • 584 tonne yr-1, start-up since 2015 (Demonstration: Shell India) • Planned in 2022 with the expected production capacity of 96,000 tonne yr-1 (Biocorde is a target product.)

Notes. ^a units represented as reported in the original references

^b as Pacific Northwest National Laboratory, a U.S. Department of Energy National Laboratory

^c as the Civil Aviation Authority of Singapore; ^d as the Civil Aviation Alternate Fuel Contrail and Emission Research; ^e as the Federal Aviation Administration

8. Table S2.3 Differences and similarities between the FT and methanol synthesis processes for the aviation electrofuel productions

Parameters	FT synthesis	Methanol synthesis	References
Differences			
Operating conditions	HTFT: 310-340 °C LTFT: 210-260 °C 10-40 bars	150-300 °C, 10-100 bar typical condition at 250-260 °C, 50-60 bar	[552,691,692]
Catalysts	Fe, Co, Ni, Ru Fe and Co: commonly used Co preferred for GtL ^a FT	Cu, Zn, Al, Si Copper-containing catalysts: commonly used such as Cu/ZnO/Al ₂ O ₃	[552,692]
Processes involving	Polymerization reactions $2\text{H}_2 + \text{CO} \rightarrow (\text{CH}_2) + \text{H}_2\text{O}$ $(2n+1)\text{H}_2 + n\text{CO} \rightarrow \text{C}_n\text{H}_{2n+2} + n\text{H}_2\text{O}$ $(2n)\text{H}_2 + n\text{CO} \rightarrow \text{C}_n\text{H}_{2n} + n\text{H}_2\text{O}$	$2\text{H}_2 + \text{CO} \rightarrow \text{CH}_3\text{OH}$ $\text{CO}_2 + 3\text{H}_2 \rightarrow \text{CH}_3\text{OH} + \text{H}_2\text{O}$ $\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$	[153,691]
Output from synthesis processes	FT syncrude composition depending on the various parameters (as mentioned below)	Methanol (CH ₃ OH)	[691]
Kerosene upgrading processes	Hydrocracking Oligomerization Hydrotreater Aromatization Alkylation	Methanol-to-kerosene has not been reported on the commercial scale yet (still in the ongoing project KEROSyN100).	[691]
Requirement	<ul style="list-style-type: none"> Adjustment H₂/CO ratio (2.0) avoiding the formation of methane using RWGS^b reaction ($\text{CO}_2 + \text{H}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$) Restriction in the removal of acid gas (NH₃, H₂S) avoiding catalyst deactivation 	<ul style="list-style-type: none"> H₂/CO₂ ≥ 3.0 H₂/CO₂ ≥ 4.0 in case of a fixed-bed reactor 	[131,552,692,693]
Similarities			
<ul style="list-style-type: none"> Both synthesis processes are “exothermic reactions”. Syngas cleanup and conditioning are required. Product yields depend on the catalyst used, reactors, temperatures, pressures, and syngas conditions. 			[131,153,552,691]

Notes. ^a as Gas-to-Liquid

^b as RWGS: Reverse water gas shift reaction

9. Table S2.4 Average energy demand (AED) for water-splitting hydrogen production technologies

Technology	Energy demand (kWh kg H ₂ ⁻¹)			Reference
	Min.	Max.	Average	
1. Electrochemistry				
1.1 Water electrolysis				
1.1.1 Alkaline	50.00	76.40	61.77	[35,221,592,694,695]
1.1.2 PEM	45.00	69.10	57.63	[35,221,696,697]
1.1.3 SOE	33.30	42.70	38.11	[35,593,696,698,699]
1.2 Photo-electrolysis			2.33	[700]
2. Solar-thermochemistry	102.68	104.87	103.78	[700]

Notes. PEM: Proton/polymer exchange membrane; SOE: Solid oxide electrolysis

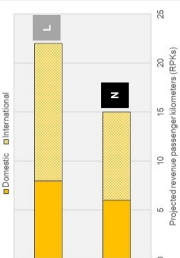
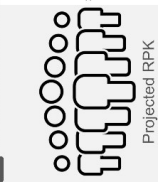
3

Framework for Life Cycle Assessment (LCA) of Sustainable Aviation Systems



“Revenue Passenger Kilometers (RPK) translation to energy requirement”

1 Functional unit



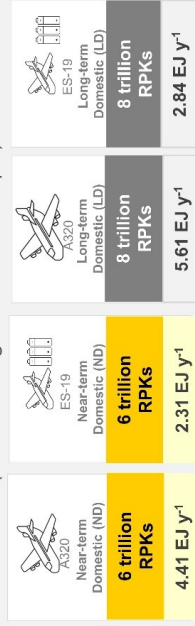
N Near-term scenario (2035) L Long-term scenario (2045)

2 Specific energy consumption* (MJ tonne⁻¹ km⁻¹)

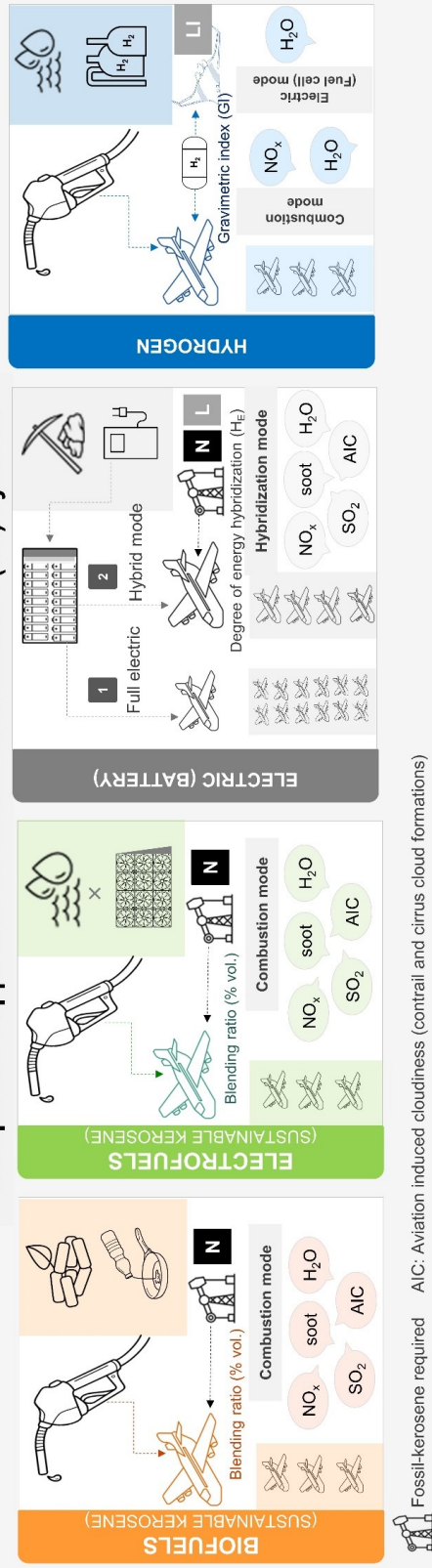


*Calculated based upon the lower heating value (LHV) of fossil kerosene (43 MJ/kg)
BWB: Blended wing body aircraft

Expected energy requirements (Domestic segment as an example)



“Comparative approach for Sustainable Aviation (SA) systems”



Fossil-kerosene required AIC: Aviation induced cloudiness (contrail and cirrus cloud formations)

ABSTRACT

A comprehensive and complete framework is proposed for life cycle assessment (LCA) in the field of commercial aviation (passengers and cargo), capable to ensure transparent comparability when evaluating the overall environmental performances of four emerging sustainable aviation systems, i.e., biofuels, electrofuels, electric, and hydrogen. The aviation service unit is defined as the projected global revenue passenger kilometer (RPK) and is suggested as the functional unit for two timeframes, i.e., 2035 (short-term) and 2045 (long-term), and for two segments, namely domestic and international. The framework proposes a methodology to translate projected RPK into energy requirements for each of the studied sustainable aviation systems. Generic system boundaries are defined with their key activities for all four systems, with the biofuel system being sub-divided into two categories to distinguish whether it stems from residual or land-dependent biomass. The activities are grouped in seven categories: (i) conventional (fossil-based) kerosene activity, (ii) conversion processes from feedstock supply to fuel or energy production for aircraft operation, (iii) counterfactual uses of the feedstock and displacement effects associated to co-products, (iv) aircraft manufacture, (v) aircraft operation, (vi) additional infrastructure needed, and (vii) end-of-life management (applied to aircraft and batteries). The model also includes a methodology to handle: (i) hybridization (the use of more than one source of energy to power an aircraft), (ii) the mass penalty affecting the number of carried passengers, and (iii) impacts stemming from non-CO₂ tailpipe emissions - aspects that are currently neglected in most LCA studies. The proposed methodology includes the most recent knowledge in the field; however, some choices are dependent on current scientific advances concerning e.g., tailpipe emissions and their environmental impacts, new aircraft configuration, etc., and are subject to significant uncertainties. Overall, this framework provides a guideline for LCA practitioners when considering new energy sources for future aviation.

Keywords: Battery, Biofuels, Electrofuels, Energy consumption, Hydrogen, Life Cycle Assessment (LCA), Tailpipe emissions, Revenue Passenger Kilometer (RPK)

HIGHLIGHTS

- Comparative LCA framework is presented for 4 emerging aviation systems
- Calculation methodology translating RPK to energy demand is proposed for all systems
- Mass penalty and hybridization are integrated into the LCA framework
- Non-CO₂ emissions contribute up to 50% to the climate impact of tailpipe emissions

Nomenclature

Symbols	Unit	Definition
B	%	The blending ratio, more especially for alternative hydrocarbon fuels (biofuels/electrofuels), presenting in the unit of % by volume
c	kg passenger ⁻¹	Assumed mass of passenger (including luggage) as 100 kg
CO ₂ -eq.	mass unit	CO ₂ equivalent
D	km	Distance traveled
E	J or Wh	Energy term prefixes include Exa ($\times 10^{18}$) and Mega ($\times 10^6$) to improve readability. Joule and watt-hour are mainly used for hydrocarbon fuels, hydrogen, and battery, respectively.
e	Wh kg ⁻¹	The expected battery (gravimetric) energy density
EC	MJ tonne ⁻¹ km ⁻¹	Energy consumption rate
ED	MJ kg ⁻¹	(Gravimetric) Energy density
EF	g pollutant kg ⁻¹ fuel	Emission factors, commonly represented in the unit of gram pollutant per kg fuel supplied in exception for the case of aviation induced cloudiness where microgram (μg) per kg fuel supplied (in Table 3.6)
F	%	The fraction of freight mass in the unit of % by mass
GI	%	Gravimetric index for H ₂ aviation varies from 0 to 1, representing in the unit of % by mass
H _E	%	The degree of energy hybridization expressed in the term of % by energy
M	kg	Mass
N		Number, the unit is defined depending on the context.
OPE	%	Overall propulsion efficiency
η	%	Battery discharge efficiency is sometimes referred to as Depth (Degree) of Discharge (DoD)
RPK	Revenue passenger km year ⁻¹	The number of (projected) RPK at a particular period
ρ	kg L ⁻¹	Fuel density
SC	%	Percentage of the change in the number of seats available relative to the conventional aircraft's model
TPE	mass unit	Tailpipe emissions express in the unit of mass (e.g., kg, tonne), which is interchangeable.
χ	%	The proportion by energy
Subscripts		Definition
alt		Alternative hydrocarbon fuels, denoted herein as biofuels/electrofuels
bat		Battery
eff		Battery discharge efficiency, sometimes referred as Depth (Degree) of Discharge (DoD)
CCD		Climb, Cruise, and descent phases of flight
F		Fuel, whether conventional (fossil-based) kerosene, biofuels/electrofuels, battery (electric) or hydrogen used to power an aircraft
i		Parameter based on the representative aircraft's model and/or the type of energy source
j		Parameter based on a given segment at a particular period (e.g., domestic in 2035, international in 2045)
L		Landing
LH ₂		Liquid hydrogen
LTO		Landing, Take-off phases of flight
max		Maximum
OE		Operating empty mass of the aircraft
others		Electric (battery): others are defined for the battery management system (BMS), cooling system, and packaging
pax		Passengers
PL		Payload mass fraction including passengers (their luggage) and freight of the aircraft
phase		Phases of flights, clustered into LTO and CCD
pollutant		Emitted compounds during air operations (tailpipe emissions)
% mass		Parameter calculated upon the mass fraction
% energy		Parameter calculated upon the energy fraction

ref	Reference system of energy source, herein the conventional (fossil-based) kerosene is defined.
RF	Reserve fuel
RPK	Parameter based upon revenue passenger kilometer
seat	Seat carrying capacity
system	Additional systems to be considered such as the electrically driven compartments of the aircraft for the alternative propulsion system, the introduction of the hydrogen storage system
TF	Trip fuel
TO	Take-off
vented H ₂	Vented hydrogen (waste as not used) during the use phase in an aircraft
Useable LH ₂	The useable proportion of LH ₂ fuel
ZF	Zero fuel

3.1 Introduction

The last several years have seen the emergence of growing concern, from researchers [701,702], industry [703–705], governments [706–708], and the society [709,710], with respect to reducing the climate impact of aviation. To address this challenge, considerable effort has been devoted to the development of sustainable aviation (SA) technologies and fuels [711]. Such developments include alternative liquid hydrocarbon fuels (biofuel and electrofuel), as well as carbon-free (electric battery and hydrogen) approaches. However, it remains unclear which approach should prevail from an environmental standpoint. While life cycle assessment (LCA) is an acknowledged methodology to quantify and compare the environmental impacts of such emerging alternatives [712], the particular case of SA poses several methodological challenges that need to be addressed to allow meaningful comparisons via LCA.

A variety of LCA studies for SA alternatives have been performed, as shown in Table 3.1. While valuable, these studies have essentially focused on biofuel approaches, particularly the hydroprocessed esters and fatty acids (HEFA) route from oil feedstock (whether cultivated or from a residual lipid source). Accordingly, the most commonly used functional unit to compare scenarios is megajoules of fuel produced or consumed on-board, which poses challenges when comparing alternatives that are not liquid hydrocarbon drop-in fuels, e.g. those involving batteries or fuel cells. Moreover, these liquid hydrocarbon pathways do not, unlike carbon-free alternatives, involve the need to consider additional infrastructure, e.g., charging infrastructure for batteries or storage tanks for hydrogen (whether on-ground or on-board), which remain somewhat overlooked in existing SA LCAs. In addition, many existing LCA studies on sustainable aviation systems are not in compliance with the International Organization for Standardization (ISO) standards (ISO 14040:2006 and ISO 14044:2006), accounting for a single impact only, namely, climate change (Table 3.1). More importantly, it was found no studies in which biofuels, electrofuels, electric (battery), and hydrogen aviation were simultaneously compared. One study [713], however, did simultaneously compare biofuels, batteries, and hydrogen, shedding light on important technical issues such as the need for blending (either with fossil- or another alternative to kerosene), the degree of energy hybridization (H_E , the ratio of the installed propulsion power of electric motors to the total installed propulsion power at the propeller shaft), the gravimetric index (GI, the ratio of the fuel mass to the mass of the full fuel system including the tank), and thus the mass penalty, which are in turn interdependent with aircraft technical specifications, e.g., fundamental aircraft design. Other crucial issues remain disregarded in sustainable aviation LCAs. This includes, among others, the consideration of non-CO₂ tailpipe emissions, e.g., water vapor and aviation soot ([714]. The importance of this latter issue has been stressed in a variety of recent studies (e.g., [715–717]), including the recent Assessment Report 6 (AR6) of the Intergovernmental Panel on Climate Change (IPCC) [718].

To bridge these gaps and to fairly compare and quantify the environmental implications of carbon-based and carbon-free emerging SA systems, the present study proposes a guideline for SA LCAs, addressing each of the previously identified issues.

Table 3.1 Non-exhaustive list of publications presenting an environmental assessment of sustainable aviation (SA)

Reference	Goal and scope (Main contributions)	Technologies included	Data sources (foreground and background)	Functional unit	System boundaries (SBs) and multi-functionality (MF) ^b	LCIA method, impact categories, and LUC
Alternative hydrocarbon liquid fuels						
[719]	<ul style="list-style-type: none"> Investigate the GHG emissions of liquid bio-based fuel and discuss different allocation methods for multi-functionality 	<ul style="list-style-type: none"> HEFA from oilseed crops FT from maize stover, co-feeding with coal Pyrolysis from maize stover 	<ul style="list-style-type: none"> GREET database Literature reviews 	1 MJ fuel combusted	SB: Cradle-to-Gate from feedstock cultivation to fuel combustion in aircraft engine; MF: Both SE and Alloc. (mass and energy)	<ul style="list-style-type: none"> GWP (presumably GWP₁₀₀, but not clearly stated; IPCC AR4), LUC emissions explicitly excluded
[720]	<ul style="list-style-type: none"> Analyze the overall environmental impacts of biodiesel (road) and jet HEFA applying system expansion to handle multi-functionality 	<ul style="list-style-type: none"> HEFA from camelina oil 	<ul style="list-style-type: none"> ecoinvent database Literature reviews 	1 MJ fuel combusted	SB: Cradle-to-Gate from camelina cultivation to diesel or jet fuel production from the transportation of fuel to market to fuel combustion in aircraft engine; MF: SE	<ul style="list-style-type: none"> Impact 2002+ • Climate change and endpoint impacts of the method (human health, ecosystem quality, and resources); LUC emissions not mentioned
[721]	<ul style="list-style-type: none"> Identify the GHG emissions of microalgae-based jet fuels; multi-functionality method explicitly excluded 	<ul style="list-style-type: none"> HTL of microalgae and upgrading via traditional refinery processes 	<ul style="list-style-type: none"> Source of applied background data not specified Experimental data 	1 GJ fuel produced and combusted ^c	SB: Cradle-to-Gate from microalgae production to combustion in aircraft engine; MF: Alloc. (mass)	<ul style="list-style-type: none"> TRACI 2.0 GWP (presumably GWP₁₀₀, but not clearly stated; IPCC AR3); LUC emissions explicitly excluded
[722]	<ul style="list-style-type: none"> GHG emissions of bio-based renewable middle distillate jet fuel and biodiesel (road) from fermentation technologies with different allocation methodologies 	<ul style="list-style-type: none"> Simultaneous saccharification and fermentation of sugar cane, maize grain, and switchgrass and upgrading to MD fuels via the HEFA process 	<ul style="list-style-type: none"> GREET database Literature reviews 	1 MJ middle distillate (referring to diesel and jet fuel) produced and combusted ^c	SB: Cradle-to-Gate from biomass cultivation to MD fuel combustion in aircraft engine; MF: SE, Alloc. (market)	<ul style="list-style-type: none"> GWP₁₀₀^a; IPCC AR5; direct LUC emissions from carbon debt scenarios [723]
[724]	<ul style="list-style-type: none"> Investigate GHG emissions of different biofuels for aviation and compare allocation methods Reveal water consumption 	<ul style="list-style-type: none"> Ethanol-to-jet (ETJ) (biological conversion) from corn and corn stover Sugar-to-jet (STJ) (catalytic conversion) from corn and corn stover 	<ul style="list-style-type: none"> GREET database Literature reviews 	1 MJ fuel combusted and 1-tonne maize stover	SB: Cradle-to-Gate from feedstock cultivation to fuel combustion in aircraft engine; MF: SE, Alloc. (energy)	<ul style="list-style-type: none"> GWP (presumably GWP₁₀₀ and IPCC AR4, but not clearly stated); and LUC-related emissions (domestic and international) from GTAP and CCLUB model of GREET
[336]	<ul style="list-style-type: none"> Analyze and compare GHG emissions of different biofuels for aviation, using both allocation and system expansion 	<ul style="list-style-type: none"> Six conversion technologies: HEFA, FT, HTL, pyrolysis, ATJ, and DSHC with the following biomasses: jatropha, camelina and used cooking oil, willow, poplar and corn stover, forestry residue, corn and corn stover, and sugarcane 	<ul style="list-style-type: none"> GREET database Literature reviews 	1 MJ fuel combusted	SB: Cradle-to-Gate GHG emissions from feedstock cultivation to fuel combustion in aircraft engine; MF: SE, Alloc. (market, energy, and mass)	<ul style="list-style-type: none"> GWP₁₀₀^a (presumably IPCC AR5, but not clearly stated); LUC emissions explicitly excluded
[725]	<ul style="list-style-type: none"> Conduct a techno-economic and environmental assessment (GHG only) of one specific biofuel pathway for aviation 	<ul style="list-style-type: none"> DSHC from sugarcane bagasse (farnesane production) 	<ul style="list-style-type: none"> ecoinvent database Literature reviews 	1 MJ fuel combusted	SB: Cradle-to-Gate from sugarcane cultivation to product end-use; MF: SE, Alloc. (energy)	<ul style="list-style-type: none"> GWP₁₀₀^a (presumably AR5); LUC emissions explicitly excluded

[726]	<ul style="list-style-type: none"> Environmental assessment of one specific biofuel pathway for aviation with both allocation (mass) and system expansion methods 	<ul style="list-style-type: none"> ATJ from residual woody biomass along with the generation of lignosulfonate 	<ul style="list-style-type: none"> ecoinvent database NREL Life Cycle Inventory data for lignocellulosic biomass conversion into ethanol Literature reviews 	1 GJ fuel combusted	SB: Cradle-to-Gate from residual collection to fuel combustion in aircraft engine; MF: SE, Alloc. (mass)	<ul style="list-style-type: none"> TRACI 2.1 ACD, EUT, SMOG, RES, CC, carcinogens, noncarcinogens, and ecotoxicity; LUC emissions not mentioned
[727]	<ul style="list-style-type: none"> Analyze the environmental impacts of 1G/2G feedstock in Brazil for aviation biofuels using the economic allocation method 	<ul style="list-style-type: none"> HEFA, FT, and ATJ with different feedstock generations 	<ul style="list-style-type: none"> ecoinvent, USLCI, and GREET databases Literature reviews 	1 MJ fuel combusted	SB: Cradle-to-Gate from feedstock cultivation to fuel combustion in aircraft engine; MF: Alloc. (market and energy)	<ul style="list-style-type: none"> ReCiPe midpoint (H) method v.1.13; LUC emissions explicitly excluded
[728]	<ul style="list-style-type: none"> LCA (GHG emissions only) for electrofuels (aviation and road) production with C from direct air capture (DAC) 	<ul style="list-style-type: none"> Solvent-based DAC and water electrolysis for hydrogen production, and FT for fuel production 	<ul style="list-style-type: none"> DAC pilot plant data from Carbon Engineering Ltd. Literature reviews 	1 gCO ₂ captured and 1 MJ fuel combusted	SB: Cradle-to-Gate from raw material supply to fuel combustion in aircraft engine; MF: SE, Alloc. (mass and emission)	<ul style="list-style-type: none"> GWP₁₀₀^a; IPCC AR5
[729]	<ul style="list-style-type: none"> Analyze carbon footprint and investigate the economic performance of sugar fermentation through an acetone-butanol-ethanol (ABE) route to jet fuels, derived from agricultural by-products from food processing 	<ul style="list-style-type: none"> ABE fermentation of potato by-product and sugar beet, followed by alcohol condensation and hydrotreatment, to jet fuels 	<ul style="list-style-type: none"> ecoinvent database Experimental data 	1 MJ fuel produced	SB: Cradle-to-Gate from feedstock cultivation to fuel distribution; MF: Alloc. (market, energy, and mass)	<ul style="list-style-type: none"> GWP₁₀₀; IPCC AR5
[730]	<ul style="list-style-type: none"> Environmental assessment of different alternative technologies with various (passenger and freight) aircraft classes 	<ul style="list-style-type: none"> Three conversion technologies: FT with natural gas, coal, and biomass; fast pyrolysis of cellulosic biomass; and HEFA from vegetable and algal oils 	<ul style="list-style-type: none"> GREET database 	MJ fuel combusted, kg of payload for each km of great-circle distance, and number of passengers for each km of great-circle distance	SB: Cradle-to-Gate from aviation fuel productions to fuel combustion in aircraft; MF: SE, Alloc. (mass)	<ul style="list-style-type: none"> GWP₁₀₀ (presumably AR5); LUC emissions not mentioned
Electric aviation (battery-based)						
[731]	<ul style="list-style-type: none"> Environmental assessment of hybrid-electric propulsion 	<ul style="list-style-type: none"> Lithium-based technologies including Li-sulfur and Li-air 	<ul style="list-style-type: none"> ecoinvent database Literature reviews 	<ul style="list-style-type: none"> Flight missions over battery lifetime (charging number = number of missions) 	SB: Cradle-to-grave from raw material extraction, including battery system production, electricity consumption, and hybridization in an aircraft, to the end-of-life of the batteries; MF: SE	<ul style="list-style-type: none"> ReCiPe midpoint (H) method v.1.11 CC, HUT, ACD, EUT, SMOG, PMF, OZD
Hydrogen-powered aviation						
[732]	<ul style="list-style-type: none"> Conceptual design for hydrogen-powered aircraft Environmental assessment of a hydrogen-electric aircraft in comparison with a traditional aircraft 	<ul style="list-style-type: none"> Solid oxide cell water electrolysis and solid oxide fuel cells (H₂ production and electricity generation on-board, respectively) 	<ul style="list-style-type: none"> ecoinvent database Literature reviews Piano-X software for conceptual aircraft design 	MJ energy consumed per km travelled	SB: Cradle-to-Gate from hydrogen production to the use phase with fuel cells in the aircraft; MF: the multi-functionality	<ul style="list-style-type: none"> ReCiPe midpoint (E) method V1.13 GWP, OZD, HTP, PMF, POF, MED

					method is not defined.	
Alternative hydrocarbon liquid fuel, electric (battery), and hydrogen						
[713]	<ul style="list-style-type: none"> • Conceptual aircraft design • Environmental assessment of different alternatives, including alternative liquid fuels, electric (battery), and hydrogen 	<ul style="list-style-type: none"> • Alternative liquid fuels produced via vegetable oil hydration from algae • Natural gas steam reforming for hydrogen production • Li-ion batteries applied in the Ce-Liner electric-aircraft project 	<ul style="list-style-type: none"> • Literature reviews • PrOPerA software for conceptual aircraft design 	<ul style="list-style-type: none"> • Passenger kilometer 	SB: Cradle-to-grave from energy sourcing production to the use phase in the aircraft; MF: the multi-functionality method is not defined.	ReCiPe method (perspective used, whether individualist, hierarchical, or egalitarian, is not specified.); LUC emissions not mentioned

^a Non-CO₂ emissions from aviation fuel combustion are stated as being excluded in the study. ^b The displacement accounts for the system expansion method.

^c The “and combustion” portion is not expressively phrased by the authors of the original study, but the results shown were included in the functional unit

Acronyms for:

(I) Production technologies: ATJ: Alcohol-to-Jet; DSHC: Direct sugar to hydrocarbon; FT: Fischer–Tropsch process; HEFA: Hydroprocessed esters and fatty acids;

HTL: Hydrothermal liquefaction;

(II) Impact categories: ACD: Acidification potential; CC: Climate change; EUT: Eutrophication potential; HUT: Human toxicity; GWP: Global warming potential;

GWP₁₀₀: Global warming potential on a 100-year horizon; MED: Metal depletion; OZD: Ozone depletion; PMF: Particle matter formation;

POF: Photochemical oxidant formation;

RESP: Respiratory effects; SMOG: Smog formation;

(III) Others: AR: Assessment Report; CCLUB: Carbon Calculator for Land Use Change; GHG: Greenhouse gases;

GREET: Greenhouse gases, Regulated Emissions, and Energy use in Transportation;

GTAP: Global Trade Analysis Project; USLCI: U.S. Life Cycle Inventory; IPCC: Intergovernmental Panel on Climate Change; LCIA: Life Cycle Impact Assessment;

LUC: Land use change; NREL: National Renewable Energy Laboratory;

(IV) Multi-functionality (MF) methods: SE: System expansion; Alloc: Allocation.

3.2 Sustainable Aviation (SA) systems

Sustainable Aviation systems for commercial aircraft are clustered into two main categories: (i) carbon-based, including biofuels and electrofuels, and (ii) carbon-free, including electric and hydrogen. These alternatives represent the predominant systems envisaged for future aviation. They are summarized here but are comprehensively detailed in **Chapter 2**.

3.2.1 Carbon-based systems

Carbon-based approaches, more specifically, hydrocarbon fuels, are compatible with existing infrastructure having similar properties to conventional (fossil-based) kerosene-type fuels, commonly referred to as Jet A-1 or Jet A.

3.2.1.1 Biofuels (alternative kerosene)

Biofuels can be produced from land-dependent biomass, e.g., palm and soybean oil (so-called 1st generation), residual biomass, e.g., primary forestry residues (so-called 2nd generation), or (farm)land-free biomass, e.g., algae (3rd generation). Several certified biofuel pathways have been introduced by the American Society for Testing and Materials (ASTM) International [733], namely Fischer–Tropsch (FT), HEFA, direct sugar to hydrocarbon, and alcohol intermediate pathways, including syngas- and sugar- fermentation to ethanol or more commonly to isobutanol for the latter, both requiring further upgrading to jet fuels (**Chapter 2**). Other pathways including a variation of the certified production pathways are also awaiting certification, these include: hydrodeoxygenation synthetic aromatic kerosene (HDO-SAK), high freeze point HEFA (HFP-HEFA), integrated hydropyrolysis (IH²) and alcohol-to-jet synthetic kerosene with aromatics (ATJ-SKA) [34].

3.2.1.2 Electrofuels (alternative kerosene)

Electrofuels are also liquid hydrocarbons; however, unlike biofuels, they rely on separate carbon (C) and hydrogen (H₂) sourcing. These fuels are also known as power-to-liquid, synthetic fuel, or E-fuels. The carbon source essentially stems from CO₂ that is either captured from point sources, e.g., fossil or biogenic CO₂ from power plants or industrial production sites (e.g., power generation plants, cement factories, steel industries) [141,734,735], or non-point sources

such as the atmosphere (so-called Direct Air Capture; DAC [85,483,736,737]). It could also stem from biomass, e.g., gasified to syngas [738]. Hydrogen can stem from conventional methane cracking from biomass (e.g., [739] or can be produced from water either through electrolysis [740–742], thermochemistry [67,743], or emerging techniques such as photo-electrochemistry [744,745] and bio-photolysis [746]. Water splitting represents the dominant vision of future renewable energy and low fossil carbon systems, electrolysis being the most discussed pathway [747,748]. Carbon and hydrogen are converted to aviation electrofuels through gas-to-liquid pathways either via FT or methanol conversion, the latter still awaiting certification [749].

3.2.2 Carbon-free systems

Carbon-free alternatives encompass electric- and hydrogen-based energy sources.

3.2.2.1 Electric (battery)

Electric aviation typically refers to aviation concepts involving electric motor(s), whether completely electric (also known as all-electric; here the electricity is either stored in batteries, or generated via fuel cells), or turboelectric (where there is an electric motor but no battery) configurations. Here, it is referred to electric aviation as systems involving batteries only, rather than all systems involving an electric engine; the term electric (battery) will be used henceforth. Electric (battery) planes have been demonstrated in test flights including the DHC-2 Beaver aircraft (8 passengers, 1,000 km; [750]), Cassio aircraft (4–10 passengers, 200–1,200 km; [751]), ES-19 aircraft (19 passengers, 400 km; [752]), and Eviation Alice aircraft (9 passengers, 1,046 km; [753]).

3.2.2.2 Hydrogen (H_2)

Hydrogen has a superior gravimetric energy density (120 MJ kg^{-1} ; [754]), whether in gaseous or cryogenic form, in comparison to conventional (fossil-based) kerosene (43 MJ kg^{-1} ; [149]). Hydrogen can propel planes via direct combustion, electricity supplied via a fuel cell, or a combination of the two. In the former case, additional developments regarding engines along with changes in specific components, e.g., high-pressure pump, injector, and cryogenic heat exchanger [755,756], are required. For the latter case, high-power fuel cells are mandatory for the purpose of propulsion; an increase from 0.75 kW kg^{-1} to 2 kW kg^{-1} is expected to make fuel cells feasible as an energy source on-board commercial aircrafts [754,755,757]. Another issue is the mass of hydrogen storage systems, particularly for aircraft, because H_2 has a volumetric energy density four times lower than conventional kerosene. Of the hydrogen-storage methods, cryogenic tanks are the most attractive, given their reasonable mass and volume, more so than gaseous and hydride storage methods [757]. Therefore, they are considered in this analysis [758]. A hydrogen-storage tank needs to be insulated to ensure the desired form of hydrogen, either gaseous or liquid, and the necessary amount for the flight. Developments of H_2 GIs approaching that of a $0.30\text{--}0.63 \text{ kg } H_2 \text{ kg}^{-1}$ fuel system are expected [756,757], making hydrogen systems competitive with current conventional (fossil-based) kerosene systems (ca. $0.75 \text{ kg kerosene kg}^{-1}$ fuel system; [521]). Cryogenic tanks can be positioned inside (integral) or outside (non-integral) the fuselage [754]. The former option is an efficient method to reduce drag, independent of the fuselage design, making it a realistic and feasible approach [505,754]. However, this feature may affect the carrying volume of the passenger cabin [758] and may only be applicable to short-to-medium-range flights. Meanwhile, the overall propulsion efficiency may be negatively affected in the latter case [505,759]. Alternatively, a blended wing body (BWB) may accommodate hydrogen tanks in addition to significantly improving the lift-to-drag ratio [760,761].

3.2.3 Need for blending/hybridization

Carbon-based SA systems have, up to now, been applied in a hybrid fashion with conventional (fossil-based) aviation fuels. This is because their use is currently limited to that of a drop-in fuel (from 10% up to 50%, depending on the type) on the basis of existing standards applied to aviation fuels, namely, ASTM D1655 and DEF STAN 91-091. Even though aviation fuels can be clustered into kerosene (i.e., Jet A, Jet A-1, TS-1, Jet Fuel No. 3, and JP-5), gasoline (known as aviation gasoline; Avgas), and a mixture of the two (i.e., Jet B and JP-4) [762], the Jet A and Jet A-1 kerosene fuel types are considered as reference systems because they are predominantly deployed for commercial aviation [762,763]. Furthermore, the blending limit is set based on a variety of parameters, including the minimum aromatics content (8% by volume) in the final fuel, set to avoid engine seal shrinkage. Yet, a variety of existing carbon-based SA fuels have negligible aromatics contents, including the widely produced HEFA-synthetic paraffinic kerosene (SPK) [510,764]. In addition, note that the SPK maximum blending quota set by ASTM (or even beyond that) needs to be achieved based on the characteristics of fossil-based kerosene, as detailed in [765]. However, the technical and safety aspects of using 100% alternative carbon-based SA fuels are being intensively investigated to overcome this limitation. Recently, aircraft and engine equipment manufacturers tested 100% HEFA-SPK on one engine for

comparison with other engines run on standard jet fuel in commercial aircraft, e.g., Airbus [766]; Boeing [767]; Rolls-Royce [768]. No difference was observed in the engine behavior. As a result, unblended alternative fuels have been announced as being compatible with state-of-the-art engines by Airbus [766], Boeing [767], and Deutsche Aircraft [769].

Based on current technological developments and demonstrations, electric (battery) aviation can already be used for short flights (limited to approximately 1,000 km) with a limited number of passengers (carrying less than 20 passengers), as in the case of the Eviation Alice [753] and Heart Aerospace ES-19 [752], without the need of hybridization with fossil kerosene or alternative SA fuels [731,770]. However, insufficient energy density and mass penalties are vital challenges for flying with electric (battery) aviation, in particular for commercial aircraft (e.g., A320, Boeing 747) [731,771]. Accordingly, this SA energy source is, in the near-term, applicable to long-range flights, e.g., >1,000 km for the A320 model [731], only in hybridization with either conventional (fossil-based) kerosene (short-term), hydrocarbon-based (medium-term), or hydrogen-based fuel cell or combustion (longer-term) SA systems.

From a theoretical point of view, a hydrogen-based SA system does not require hybridization. In other words, there are no significant technical constraints that would require its hybridization with another SA system for longer-range flights with reasonable carrying capacities. Even though announcements of 100% hydrogen-powered planes have been made for the near-term future, e.g., ZeroAvia announced planes carrying 100–200 passengers with a flight range of up to approximately 4,000 km in 2030 [626], no 100% hydrogen demonstration flights have yet been made.

3.2.4 Clustering into short- and long-term perspectives

To synthesize, Fig. 3.1 presents an overview of the SA systems that ought to facilitate comprehensive and complete LCAs for future aviation systems. Additional considerations between short- and long-term perspectives are further addressed (some are not shown in Fig. 3.1). (i) The improvement of overall propulsion efficiency (OPE_i), implying less fuel consumption in long-term scope, depending on the representative aircraft's models (Table 3.3). (ii) The marginal heat reacting to the demand is differently considered in the near- and long-term future. Low (LT) and high (HT) temperatures are defined with a border of 100°C. For example, natural gas is considered the heat source in the near-term for both LT and HT. On the other hand, in the long-term, (renewable) electricity is one of the relevant candidates, the level of generated temperatures varying with the applied equipment. The heat pump and electric furnace/boiler are considered as examples to provide LT and HT, respectively. (iii) The novel blended wing body (BWB) configuration was considered only in the long-term international segment regarding the ongoing ZEROe project [772].

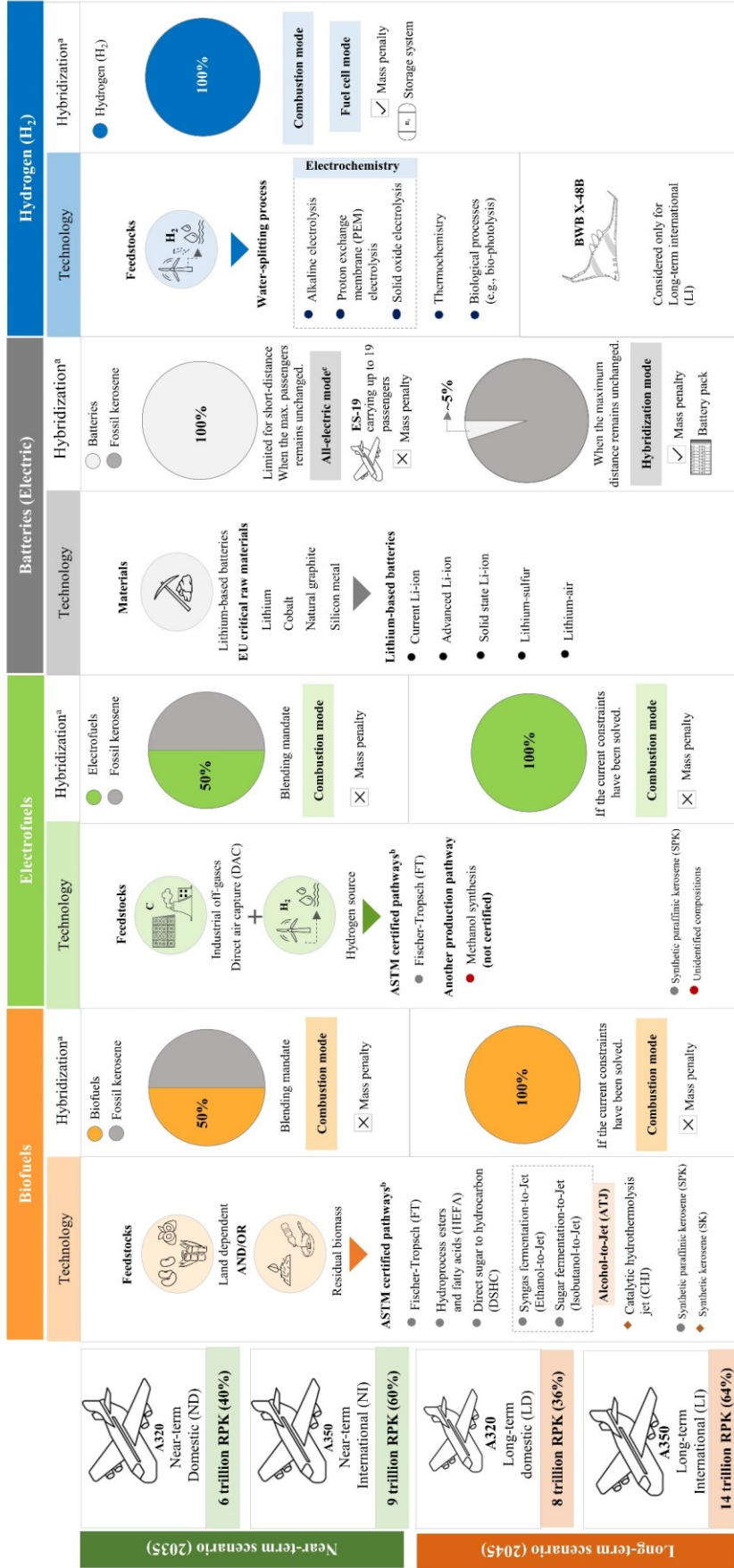


Fig. 3.1 The systematized SA systems with two time horizons: near- and long-term futures. This framework is further detailed in the SM 3.2.

Notes.

^aHybridization refers to the requirement of fossil kerosene in addition to the alternative energy sources, for aircraft operation.

This column also includes the mass penalties derived from using different energy sources.

^bThe ASTM-certified pathways are retrieved from [34]. Fuel variations from the same pathways are included, namely HEFA-SPK and Hydroprocessed hydrocarbon HEFA-SPK (HC HEFA-SPK), both considered as derived from the HEFA process.

^cThe distance is considered based on the different types of batteries (in the different short- and long-term scopes) (see details SM 3.2), while the number of passengers is assumed to be unchanged.

3.3 Functional unit selection

Table 3.1 highlights the fact that existing SA LCAs have essentially used the production and combustion of a fuel (in energy units) as a basis to define their functional units. While this may be useful when comparing liquid fuels for similar engines, it becomes limiting when introducing SA alternatives with adapted infrastructures and aircraft engines.

The key service supplied by the commercial aviation is the transport of a certain number of passengers over a certain distance in a given timeframe. Some types of SA may involve planes able to carry fewer passengers and/or be limited in the distance they can fly, e.g., electric (battery). This implies that a distinction between short- and long-range flights is necessary, often denoted as domestic and international travel, respectively [773,774]. Because the ‘domestic’ and ‘international’ flights are not defined based on the distance [775], all aircrafts capable of operating for short- and long-distance are considered in the scope of this framework (see SM 3.1 and SM 3.2).

Here, the revenue passenger kilometer (RPK) unit is the proposed functional unit, a transportation industry metric widely used by airline industries, aviation organizations (e.g., ICAO and IATA), and life cycle inventory (LCI) databases (e.g., ecoinvent and GREET), as a basis to set functional units for SA LCAs. In essence, this unit is expressed in boarded passenger kilometers and reflects the number of passengers carried and the number of kilometers traveled in a given flight for a given period during which a certain number of flights is taking place [773].

In Table 3.2, an additional level of granularity for the RPK functional unit by distinguishing the type of segment (domestic or international) and the time scope (near-term or long-term) are proposed. This is done by considering projected RPKs worldwide [638]. However, a different geographical scope could be considered (e.g., flights departing from a specific country or flights from a given airline), provided data are available. Several airlines (e.g., Air France-KLM, Lufthansa Group, Qatar Airways, and Singapore Airlines) publish such information, albeit typically for historical data, such that there is a need to extrapolate these data into the future. Based on Table 3.2, an adequate functional unit to compare the broadly available SA types could be, for the time scope of 2035, “Ensuring the annual global supply of 6 trillion RPK of domestic flights and 9 trillion RPK of international flights.”

Table 3.2 Global revenue passenger kilometers (RPK) by segment for 2035 and 2045, as forecasted by the International Civil Aviation Organization (ICAO).

Projected demand in trillion ^a RPK		
Service segment	2035	2045
Domestic	6	8
International	9	14
Total	15	22

^a 10¹²; ^b As defined in ICAO (2018). ICAO’s official definitions for domestic and international flights are provided in the Supplementary Material 3.2 (SM 3.2).

Moreover, in addition to carrying passengers, commercial airlines typically simultaneously carry merchandise, i.e., freight [776,777]. This is typically associated with the type of aircraft and the segment travelled.

To facilitate a comparison of different technologies, translating the functional unit in terms of the energy flow has been proposed, as further detailed in Sections 3.4.3 and 3.4.4. The freight service (if any) can then be incorporated at this stage.

3.4 Life cycle modeling issues

3.4.1 System boundaries

In LCA, the system boundaries define which activities are included in the analysis. As prescribed by the ISO standards for LCA (ISO 14040 2006 and ISO 14044 2006; [778,779]), an approach via system expansion with substitution, i.e., an attempt to reflect the uses of all possible products generated to supply the selected functional unit by the studied alternative is applied. Distinguishing five types of SA systems are further proposed including three carbon-based and two carbon-free, namely, (a) biofuel from residual biomass; (b) biofuel from land-dependent biomass; (c) electrofuel; (d) electric (battery) aviation; and (e) hydrogen aviation. The system boundaries involved for these five systems are represented in Fig. 3.2.

If compared with one another, existing and emerging SA systems involve a large number of differences. For LCA of one or another system, all processes included in the product system must be considered, as LCA by its nature encompasses all cradle-to-grave processes. However, by sake of simplicity and clarity, herein only the processes which

are different in the compared SA are highlighted. Any activity that would be involved in all systems but is unaffected by the type of SA system can therefore be excluded, namely the additional infrastructure required (e.g., fuel storage facilities) for biofuels/electrofuels that is identical to the one used for the conventional kerosene.

Seven categories of activities in the five SA systems are identified illustrated in Fig. 3.2 (represented by a color code).

The first is the “conventional (fossil-based) kerosene system” (in yellow). This encompasses all processes related to the need for blending with kerosene, as detailed in Section 3.2.3 (from the extraction of the resource to its production). According to the SA system, the amount of fossil kerosene involved will differ and may even be zero depending on the time horizon and/or the flight segment considered in the definition of the functional unit.

The second category is the “feedstock system”; this covers all processes related to the production of the feedstock involved prior to the operation of the aircraft (in green). This includes the conversion of the biomass or carbon plus hydrogen into bio-based kerosene in the biofuel systems and the harvest and/or collection of the residual biomass or the cultivation of the land-dependent biomass. It also includes the capture of carbon (C) in the electrofuel system and the hydrogen production in the electrofuel and hydrogen systems. Finally, it covers all processes related to battery manufacture in the electric aviation system.

The third category, labeled “counterfactual and displacement” (in blue), reflects several effects. This category reflects the uses of the different co-products generated in the production chain. These co-products are sold to the most competitive market segment and, accordingly, will supply a service that, in turn, will no longer need to be supplied in the way it was in a world without the additional production of the SA under study. This chain of displacement–replacement events is typically referred to as substitution [780–782]. The other effect of this category reflects the fact that some feedstock-related resources are constrained, whether as a result of the economic system, i.e., the production of residual biomass will not increase as a result of a demand change for bio-based kerosene, or because of a biophysical constraint, e.g., land. This effect is often referred to as the “counterfactual” (e.g., [127,783,784] and reflects the foregone use of a limited resource, here induced by using it for aviation biofuel. However, the mineral resources needed for batteries are not considered as being biophysically constrained resources because their long-term availability is determined primarily according to geopolitical and economic constraints rather than biophysical ones [785].

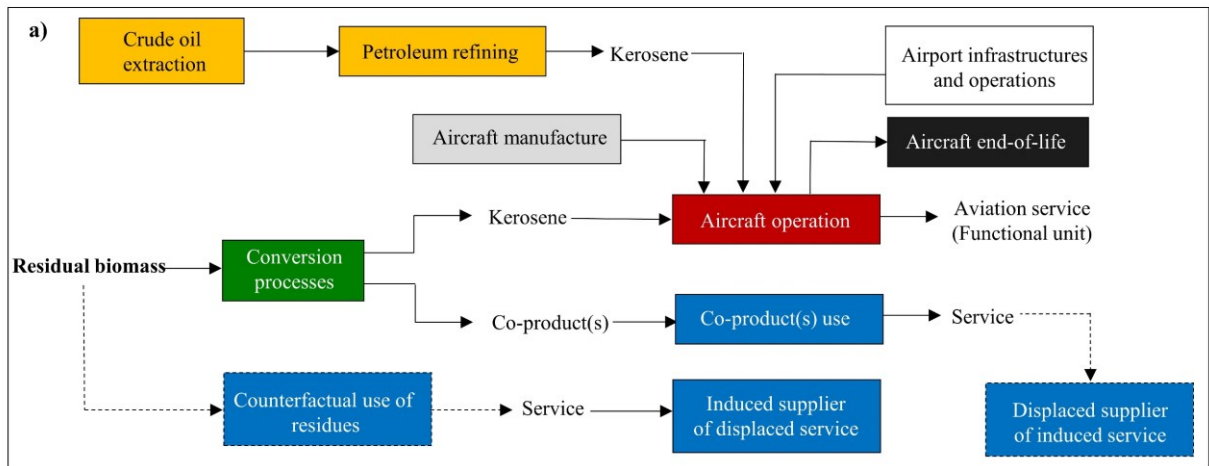
The fourth category, “aircraft manufacture” (in grey), relates to the very production of the aircrafts needed to supply the services defined by the functional unit. This is included as a category on its own to reflect two main points: (i) that not all SA systems will require the same number of aircraft and, more importantly, (ii) that the different SA systems may involve different aircraft designs, e.g., BWB for H₂ long-haul flights [761].

The fifth category, here called “operation” (in red), represents the energy consumption during the aircraft use to supply the aviation service, considering the different lifetimes of the different types of aircraft involved. While some authors argue that the differences are negligible when comparing conventional (fossil-based) kerosene to biofuels use (e.g., [336,786,787] or even electrofuels [336], other studies claim that there is a difference in terms of emissions like soot and particulate matter [500,788], as discussed in Section 3.5. However, the operation of the battery and hydrogen systems differ significantly because they do not involve the combustion of hydrocarbons, as further detailed in Section 3.5. This also has implications during the life cycle impact assessment phase. Therefore, here having the aircraft operation as a category in its own right is proposed.

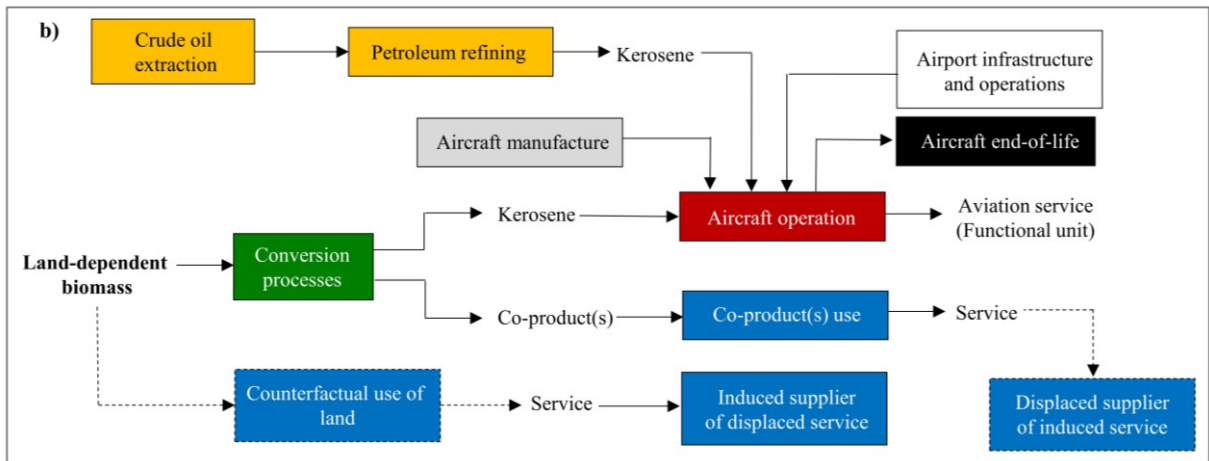
The sixth category, “infrastructure” (white box) reflects the required infrastructure and operation of the airport, which will depend on the type of energy source. For example, an electric system will require charging infrastructure that is not needed in other systems, while hydrogen and electrofuels will imply a certain storage infrastructure for hydrogen, as further detailed in Section 3.4.5.

The “end-of-life” (black box) management of the aircraft involved in the different SA systems will also vary as a result of the differences between the aircrafts themselves and the fact that the electric SA system may involve the recycling of batteries, as discussed in Section 3.4.5.

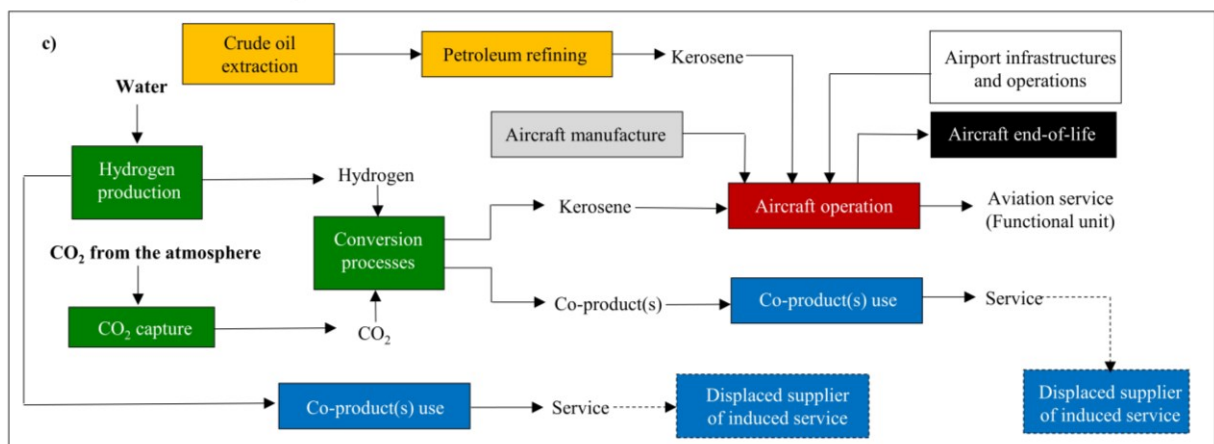
Aviation biofuel boundary (from residual biomass)



Aviation biofuel boundary (from land-dependent biomass)



Aviation electrofuel boundary (CO₂ from the atmosphere)



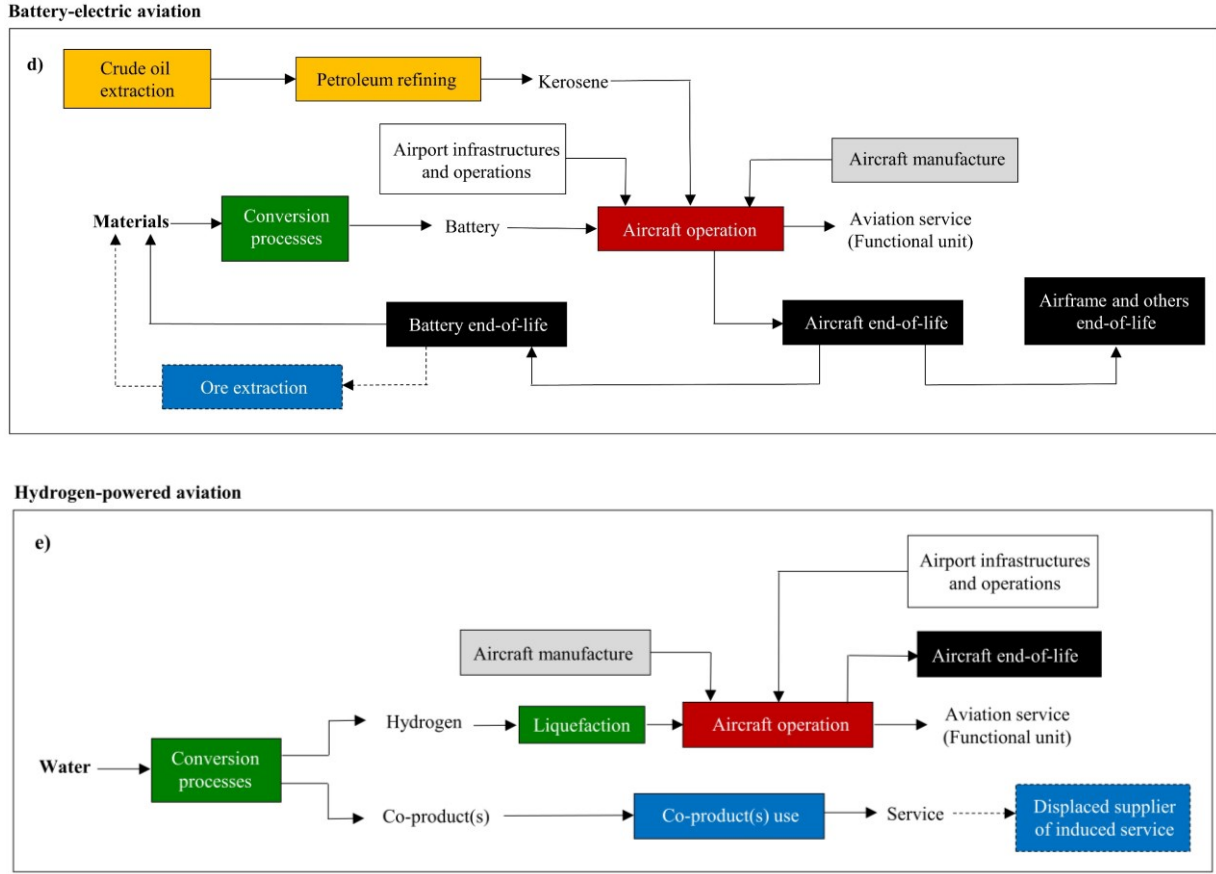


Fig. 3.2 System boundaries covered in the proposed framework

(a) biofuel from residual biomass; (b) biofuel from land-dependent biomass; (c) electrofuel (CO₂ from the atmosphere); (d) electric (battery) aviation; and (e) hydrogen aviation. Categories include the following: fossil kerosene system; feedstock system, any processes prior to aircraft operation; counterfactual and displacement; aircraft manufacture; aircraft operation; airport-related infrastructures and operations; and end-of-life management (whether for batteries or aircraft). Hybridization is shown here with conventional (fossil-based) kerosene only, representing the short-term vision in the case of biofuels and electrofuels.

3.4.2 Translating RPK demands into energy flows

Functional units based on the global RPK projections shown in Table 3.2 (according to time scope and segment type) can be translated into propelling energy requirements [EJ] over a certain period of interest on the basis of a few parameters, as detailed in Eq. (3.1). Because these projections are based on fossil kerosene, they are translated here into energy terms based on fossil kerosene (or more specifically, Jet A/Jet A-1) as a propellant for a given couple segment (j)–aircraft (i) ($E_{RPK,ij}$).

$$E_{RPK,ij} = EC_{ref,i} \times (1 + (1 - OPE_i)) \times M_{TK,ij} \times 10^{-12} \quad (3.1)$$

$$EC_{ref,i} = \frac{E_{F,ref,i}}{D_{max,ref,i} \times M_{PL,max,ref,i}} \quad (3.1.1)$$

$$E_{F,ref,i} = ED_{ref} \times M_{F,max,ref,i} \times 10^3 \quad (3.1.2)$$

$$M_{TK,ij} = [RPK_j \times c] + [(RPK_j \times c) \times F_i] \quad (3.1.3)$$

$$M_{F,max,ref,i} = M_{TF,max,ref,i} (\text{Trip fuel}) + M_{RF,max,ref,i} (\text{Reserve fuel}) \quad (3.1.4)$$

Here, $EC_{ref,i}$, the reference energy consumption rate based on conventional (fossil-based) kerosene or a full-electric battery, is the energy consumed per payload mass per kilometer for a given aircraft (i), with the payload mass being the mass of the passengers plus its share in terms of the freight and baggage mass. $EC_{ref,i}$, in turn, depends on $E_{F,ref,i}$

(Eq. (3.1.1)), i.e., the energy corresponding to the kerosene fuel needed to supply the maximal distance a given aircraft can ensure at full capacity ($M_{F,max,ref,i}$). $EC_{ref,i}$ also depends on the total payload mass of a given aircraft ($M_{PL,max,ref,i}$), including the overall passenger, baggage, and freight mass, and on the maximal achievable distance of an aircraft (i) with the reference fuel ($D_{max,ref,i}$). The eventual freight service is, in this way, included in the functional unit. $E_{F,ref,i}$ is calculated based on the reference kerosene gravimetric energy density ED_{ref} , and the maximum total mass of the fuel ($M_{F,max,ref,i}$) or the mass of the battery pack. These figures are often directly provided by aircraft manufacturers.

$M_{TK,ij}$ stems from the original functional unit (the RPK projection) for a given segment (j) and connects the passengers to the payload mass of the aircraft. The constant (c) defines the mass of the passengers and their luggage; this is herein invariably taken to be 100 kg [789]. The variable F_i represents the proportion of freight mass out of c (passenger plus luggage mass) for a given aircraft (i), which varies from 7% to 70% (SM 3.2)). Finally, $M_{F,max,ref,i}$ (used to calculate $EC_{ref,i}$) includes both the trip fuel needed for the maximal achievable distance ($M_{TF,max,ref,i}$), which is aircraft model dependent, and the reserve fuel ($M_{RF,max,ref,i}$), which is determined as a share of $M_{TF,max,ref,i}$; further details are given in SM 3.2. $M_{TF,max,ref,i}$ corresponds to the difference between the aircraft takeoff mass and its landing mass. The calculation of $ER_{PK,ij}$ also involves OPE_i , the overall propulsion efficiency of a given aircraft (i), defined as the achievable engine performance [790,791].

Table 3.3 summarizes the specific values considered for each parameter and presents a translation of the ICAO projections [638] (a basis for defining the functional unit) from the original RPK to EJ y^{-1} (defined as $ER_{PK,ij}$) based on the reference fossil kerosene considered (Jet A/Jet A-1).

Table 3.3 Translating global RPK demands into energy flows [EJ y^{-1}] ($ER_{PK,ij}$) based on a fossil kerosene or all electric system.

Service segment (j)	Plane configurations (i)	F_i	$M_{F,max,ref,i}$ [tonne]	Maximum distance ($D_{max,ref,i}$) [km]	Share of M_{TF} to calculate $M_{RF,ref,i}$	OPE_i		$ER_{PK,ij}$ [EJ y^{-1} demand]	
						2035	2045	2035	2045
Domestic route	TW (A320 neo)	7%	14.70	6300	21%	58%	65%	4.41	5.61
	TW (ES-19)	-	3.00	452	-	78%	87%	2.31	2.84
International route	TW (A350)	69%	88.65	15550	14%	58%	65%	7.12	10.57
	BWB (X-48B)	54%	134.74	15742	9%	73%	81%		16.71

Notes. For tube and wing (TW) models, A320 and A350 XWB were determined to be representative planes for domestic and international services, respectively. Heart Aerospace ES-19 is considered to be a representative all-electric aircraft for domestic ranges carrying up to 20 passengers per flight mission. The Boeing X-48B is considered for a blended wing body (BWB) aircraft. Calculation details and data sources are available in SM 3.2.

3.4.3 Hybridization

For LCAs of commercial aircraft, the need for hybridization, in light of Section 3.2.3, needs to be considered both as a function of the studied SA technology and in light of the studied time scope and type of transport segment to be covered, as defined by the functional unit. This implies a variety of possibilities regarding hybridization that are summarized in Table 3.4. This section is considered in the ‘‘Aircraft operation’’ box, as shown in the system boundaries (Fig. 3.2).

Table 3.4 Hybridization requirements foreseen for commercial aircraft according to type as per the SA approach and segment type.

Time scope	Short-term horizon (2035)		Long-term horizon (2045)	
	Domestic route	International route	Domestic route	International route
Biofuels	Hybridization	Hybridization	No hybridization (Unblended biofuels)	No hybridization (Unblended biofuels)
Electrofuels	Hybridization	Hybridization	No hybridization (Unblended electrofuels)	No hybridization (Unblended electrofuels)
Electric (battery)	Hybridization	Hybridization	Hybridization	Hybridization
All-electric	No hybridization	No hybridization	No hybridization	No hybridization
Hydrogen (H ₂) [*]	No hybridization	No hybridization	No hybridization	No hybridization

Notes: The definitions for domestic and international routes shown in Supplementary Material 3.1 (SM 3.1) are derived from the ICAO Glossary [775]. It is assumed that the expected ranges, whether domestic or international, are unchanged, meaning that the amounts of energy required are unchanged. The changeable parameter is expressed in the number of carried passengers corresponding to a hybridization mode. * In H₂ combustion mode or in H₂ fuel cell mode.

3.4.3.1 Biofuels/Electrofuels

Here, the degree of energy hybridization ($H_{E,alt}$) has been introduced to represent the energy distribution between the alternatives (whether biofuels or electrofuels) and the reference fuels (here conventional fossil-based kerosene), as illustrated in Eq. (3.2). $H_{E,alt,ij}$ depends on the allowable (maximum) blending ratio ($B_{max,ij}$, expressed in terms of the volume) for a given segment (j) and type of aircraft i and the alternative fuel characteristics, including the fuel density (ρ_{alt}) and the gravimetric energy density expressed in units of kg L⁻¹ and MJ kg⁻¹, respectively; details are given in SM 3.2.

$$H_{E,alt,ij} = \frac{E_{F,alt,ij}}{E_{F,alt,ij} + E_{F,ref,ij}} \quad (3.2)$$

$$E_{F,alt,ij} = B_{max,ij} \times \rho_{alt} \times ED_{alt} \quad (3.2.1)$$

Here, $E_{F,alt,ij}$ and $E_{F,ref,ij}$ express the energy consumption for alternatives and conventional (fossil-based) kerosene, respectively, depending of the type of aircraft and segment.

Alternative biofuels (including electrofuels) are currently considered as blending components with conventional kerosene, with varying quotas ($B_{max,ij}$) from 10% to 50%, as illustrated in SM 3.2. As the most commonly used types of kerosene-based aviation fuels, Jet A and Jet A-1 serve as the reference fuel required to meet the corresponding standards, e.g., ASTM D1655 [667]. Therefore, the maximum blending ratio of each certified fuel is considered to indicate the maximum fuel allowed, whether from biofuels or electrofuels; details are provided in SM 3.2. Here, this is defined as the short-term solution for the time horizon in the year 2035.

Unblended SPK has been announced for a new generation of engines, as explained in Section 3.2.3. It is therefore considered that 100% SPK ($B_{max,ij}$) can be applied as the long-term solution defined for the year 2045 in this framework. The detailed calculation is provided in SM 3.2.

3.4.3.2 Electric (battery) SA

The degree of energy hybridization (H_E) is introduced to represent the energy distribution between the battery and the liquid fuel, either kerosene or an alternative liquid fuel providing technical issues such as the lack of aromatics are resolved, as shown in Eq. (3.3).

$$H_{E,bat,ij} = \frac{E_{bat,ij}}{E_{bat,ij} + E_{F,ref,ij}} \quad (3.3)$$

The battery (electrical) and reference fuel, denoted as conventional kerosene energy, are represented by $E_{bat,ij}$ and $E_{F,ref,ij}$, respectively [792]. However, E_F could be alternative kerosene (biofuels or electrofuels; $E_{F,alt,ij}$), when the issues concerning the aromatic content will be resolved.

$H_{E,bat,i}$ ranges between 0 and 1, where $H_{E,bat} = 1$ would represent an aircraft solely supplied by battery energy. Several H_E values have been examined; detailed calculations are provided in SM 3.2. The choice of $H_{E,bat}$ is also based on the accepted mass penalty, as described in Section 3.4.4. Thus, the known value of H_E allows to calculate the E_{bat} value.

Although no hybridization for all-electric is considered, the limited distances are addressed in respect of the different types of batteries (see SM 3.2).

3.4.4 Mass penalty

Both electric (battery) and hydrogen SA systems involve an overall mass that is greater than that of the reference conventional kerosene system for specific aircrafts and segments. To overcome this, the number of seats available on-board can be reduced (which affects the number of passengers transported per aircraft and therefore $M_{PL,ref}$).

Here, the seat numbers should be reduced by a maximum of 40% of full capacity (i.e., a passenger load factor above 60%) has been hypothesized to ensure a certain level of economic activity. This assumption is approximate and can be changed; yet, it corresponds to the drop that was observed in aircraft worldwide between 2019 and 2020 as a result of the COVID-19 pandemic [793].

The payload mass of the distinguished system, either electric (battery) or hydrogen SA, can be determined based on the maximum landing mass ($M_{L,max}$), information that is generally provided by aircraft manufacturers (SM 3.2). Then, taking the mass of the reserve fuel to be $M_{RF,max,ref}$ (liquid hydrogen (LH₂) or kerosene), the overall additional mass related to the batteries (e.g., the mass of the batteries and the electrically driven components) or the LH₂ storage system including the fuel cell in the case of the LH₂ fuel cell scheme (Sections 3.4.1 and 3.4.3) to be M_{system} , and the operating empty mass of the aircraft to be M_{OE} , the number of allowable payloads can be calculated accordingly for a given aircraft (i).

$$M_{PL,max,system} = M_{L,max} - M_{RF,max,ref} - M_{system} - M_{OE} \quad (3.4)$$

$$N_{seat,max,system} = \frac{M_{PL,max,system} \times (1 - F)}{c} \quad (3.5)$$

The number of maximum seats available ($N_{seat,max,system}$) depends on $M_{PL,max,system}$, where F and c represent the proportion of the freight mass and the mass of the passengers and their luggage (invariably taken to be 100 kg, as noted in Section 3.4.2).

Accordingly, the seat changing capacity ($SC_{seat,system,i}$) can be calculated as

$$SC_{seat,system} [\%] = \frac{N_{seat,max,ref} - N_{seat,max,system}}{N_{seat,max,ref}}, \quad (3.6)$$

where $N_{seat,max,ref}$ is the maximum number of seats available depending on the aircraft (i) model, as illustrated in SM 3.2. This section is linked to the ‘‘aircraft manufacture’’ system boundary (Fig. 3.2), providing the estimated number of aircraft needed to serve the projected number of passengers during different periods (2035 and 2045). $N_{seat,max,system}$ and the maximum distance travelled ($D_{max,ref}$) are subsequently used to calculate the expected number of aircraft needed to reach the projected RPK; calculations are detailed in SM 3.2.

The maximum distance traveled ($D_{max,system}$) in the case of a all-electric aircraft in which different types of Li-based batteries are considered, can be calculated according to the Breguet range equation [794].

3.4.4.1 Electric (battery) SA

The key parameter defining the mass penalty of the electric (battery)/kerosene hybrid system is the mass of the batteries required to supply E_{bat} for a given aircraft (i) model, as defined in Eq. (3.3). This parameter is referred to as $M_{F,bat}$ and is defined as

$$M_{F,bat} = \frac{E_{bat}}{c_{bat} \times n_{eff}}, \quad (3.7)$$

where c_{bat} is the specific energy density of the battery [Wh kg⁻¹] and n_{eff} is its efficiency [%], that is, out of the total battery capacity, the amount of useful energy that is supplied. The latter parameter is fixed to 95% based on [795], and a compilation of data from the literature concerning the energy density of a variety of Li-based batteries is available in SM 3.2.

M_{bat} (Eq. (3.8)) only relates to the mass of the battery prior to its insertion in the aircraft. The mass of other components including all the accompanying required infrastructure, e.g., the battery management and cooling systems, is referred to here as $M_{bat, others}$. According to [796], approximately 60% of the overall battery system mass ($M_{F, bat}$) is due to $M_{bat,i}$, the remaining 40% being here attributed to $M_{bat,others}$.

$$M_{F,bat} = M_{bat} + M_{bat,others} \quad (3.8)$$

Theoretically, improvements regarding kerosene savings or batteries that are more performant (greater than $n_{eff} \times c_{bat}$) could lead to a greater proportion of E_{bat} (or $H_{E,bat}$) than calculated here with limited reductions in the carrying passenger capacity, as shown in the study of [731]. The present framework can therefore be regarded as conservative.

3.4.4.2 Hydrogen SA

The mass penalty for the hydrogen SA system relates to the mass of the required cryogenic storage tank infrastructure (M_{tank}). To represent this, the concept of the gravimetric index (GI; sometimes known as the system gravimetric capacity) defined by [521,755], expressing the mass of LH₂ ($M_{F, LH2}$) with respect to the system’s mass ($M_{F, LH2} + M_{tank}$) is used:

$$GI = \frac{M_{F,LH_2}}{M_{F,LH_2} + M_{\text{tank}}} \quad (3.9)$$

GI values range from 0 to 1 [521,755]. Here, on the basis of the aircraft (i) models presented in [755] is proposed, a GI value of 0.5 for the short-term horizon (2035), which can be increased for longer-term (2050), considering technical improvements that will likely allow a decrease in M_{tank} . For batteries, the total energy required is assumed to correspond to $E_{F,\text{ref}}$ (Eq. (3.1.2)), which defines, based on a gravimetric energy density of LH_2 of 120 MJ kg^{-1} , the value of M_{F,LH_2} .

In addition, M_{F,LH_2} is composed of useable LH_2 and vented H_2 , both associated only with the flight stage.

$$M_{F,LH_2} = M_{F,\text{useable } LH_2} + M_{F,\text{vented } H_2} \quad (3.10)$$

The recent study of [755] suggests considering a ratio of 90% useable LH_2 ($X_{\text{useable } LH_2}$) and 10% vented H_2 .

3.4.5 Required infrastructure and end of life (EoL)

3.4.5.1 Needs of novel fueling/charging infrastructure and operation

The transition period from fossil-based kerosene, or alternative liquid fuels, to emerging energy systems needs to be handled gradually because all aircraft will not change overnight; this is considered in the sixth category of the proposed inventory system. Substantial changes to existing airport infrastructure and investments would need to adapt to a ramp-up/down implementation corresponding to the demand shares of these future systems.

Importantly, in the case of battery plug-in charging (BPC) infrastructure, improvements in high-power fast-charging infrastructure ($>20 \text{ kW}$; [797]) are crucial to ensure turnaround time requirements. The Pipistrel SkyCharge station with its maximum power 80-kW model, for example, is an available BPC facility dedicated to an electric aircraft at the Compton/Woodley Airport [798]. However, considering the feasibility of hybrid-electric propulsion in the B737-800, 3.5 MWh of electrical energy from the batteries, approximately 6% of the total energy consumed, is required during takeoff [799], resulting in an unacceptably long recharging time using current charging stations, even with the aforementioned fast-charging equipment. Therefore, charging options, i.e., alternating current (AC) and direct current (DC), may be developed for electric (battery) airplanes. Furthermore, an on-board AC-to-DC converter is mandatory for AC chargers because DC is required for batteries. As abovementioned, charging times depend on several parameters, e.g., the power level, charging efficiency, charge-point/aircraft plugs and sockets, and battery size. However, battery performance and lifespan have been demonstrated to decrease with fast-charging stations as a result of the greater amounts of heat generated [800].

Battery-swapping stations (BSSs) have been proposed as an alternative to eliminate waiting periods [801]. However, short-time battery exchange systems and high investment costs are major challenges [802,803]. A plug-in charging station, which facilitates terrestrial transport modes, is the most practical method at an airport via the application of flexible cables and chargers for different aircraft models. However, there is large room for improvement with respect to BSS, particularly for fixed scheduled flights. Using BPCs or BSSs, providing a high-power electricity supply would require substantial changes to existing airport infrastructure [755,791].

Hydrogen aviation concepts can be adopted via either combustion engines or fuel cells. LH_2 has a higher physical energy density (70.8 kg m^{-3} at 1 bar, 20.3 K; [804]) relative to the compressed gaseous form (39 kg m^{-3} at 700 bar, 293 K; [805]), both being possible in aviation and aerospace applications [754,757]. Liquid boil-off (also referred to as evaporation loss) is relevant, especially when the liquefaction plant and storage system are disconnected (designated as off-site production plants). The stored hydrogen lost per day varies from 0.03% to 5% depending on the storage capacity, shape, and insulation materials [805,806]. Off-site hydrogen sources could be derived either from hydrogen production plants or as a by-product, e.g., styrene production, production of chlorine, or caustic soda via chlor-alkali electrolysis [807], imported from other proximate sources. In addition, hydrogen transportation to airports and refueling infrastructure need to be considered. A liquefaction plant is an additional on-site requirement at airports in the case of imported/produced gaseous hydrogen.

Currently, most hydrogen is produced and consumed in close proximity, i.e., at on-site production plants [807,808]. Various schemes have been considered corresponding to several parameters such as the availability of resources, e.g., water and electricity for on-site hydrogen production [755], space limitations at airports, and the overall forecasted fuel demand related to the airport profile [809]. Whether from off-site or on-site production plants, a liquid hydrogen-storage system with a double-walled vessel with insulation is required [758,810]. Stationary storage applications and

fueling infrastructure adjacent to or at an airport vary depending on the demand and the boil-off rate, especially for the off-site scenario, because the re-liquefaction process can be achieved with low additional cost in other cases [804]. Liquid hydrogen delivery to an aircraft can be achieved via insulated refueling vehicles [758] or an alternative method such as a hydrant system [754,755]. The former approach appears to be the most flexible and viable fueling technology for the near-term horizon [755,809] because a cryogenic hydrant refueling system is technically and economically infeasible, with costs five times higher than that of conventional hydrant systems [755].

3.4.5.2 EoL management for used airframes and batteries

EoL management approaches for airframes and battery packs are summarized in Table 3.5.

Table 3.5 End-of-life management

Parameters	Lifespan	EoL approach, current and announced
Airframes	Average 25 years for passenger-carrying aircraft [811,812]	<ul style="list-style-type: none"> • Conversion from passenger-carrying aircraft to air freighter, expanding the in-service time by 10–20 years [811–813] Once an aircraft is no longer being operated, either as a passenger craft or a freighter, and is disassembled, three significant EoL options are possible. <ul style="list-style-type: none"> i) Reuse of components, e.g., engines and door handles, in aircraft still being operated, under the supervision of the authorized/certified sector [811,812,814] ii) Recycling applications for recyclable materials <ul style="list-style-type: none"> • Aerospace applications for aircraft creation [811,815] • Non-aerospace applications of recycled composites, e.g., in automotive or sporting goods [816,817] iii) Land-filling as the last option for non-recyclable components [814]
Battery pack ^a	Battery degradation rates are roughly estimated in terms of calendar ageing (years) and/or cycle ageing (charge–discharge cycles) by manufacturers. This data gap is usually solved via assumptions based on the reported cycles, state-of-charge, and estimated years for environmental impact analyses.	<ul style="list-style-type: none"> • Life expectancies of batteries depend on numerous factors, including environmental conditions, such as outranged temperature [818–820], battery utilization [796,819,821], and charging speed [800]. Lifetime of batteries significantly on the battery composition [800]. • When the batteries reach 70%–80% of the initial battery capacity (defined as the first-life EoL) and are certified for second-use standard^b [585,819,822], batteries can be: <ul style="list-style-type: none"> Directly reused (repacking^c might be performed) for automotive purposes in electric vehicles [823,824] Re-purposed (repacking^c is required) as stationary energy storage, e.g., in households, industrial sites, or electricity production sites [822,824,825] • When the end-of-second use retained capacity is reduced to 60% of the initial capacity, recovery of valuable metallic components such as cobalt nickel [824,826,827] for uses either in battery manufacturing or other industries is possible.

Notes: ^a The battery management system, the cooling system, and the battery packaging are not considered.

^b The certification process involves dismantling at the pack or module level and inspecting the hardware of the modules [824].

^c The repacking process is the stage following certification and involves inserting new materials and/or components [824].

3.5 Life cycle inventory and impact assessment for tailpipe emissions

3.5.1 Overall approach

Herein, dividing the tailpipe aircraft pollutant emissions into two well-acknowledged flight phases is proposed, namely, taxi, takeoff, and landing (LTO) and climb, cruise, and descent (CCD) for flight activities above 915 m altitude [714] in order to account for the difference in their emissions with respect to the flight phases. Herein, CCD emissions are equivalent to the term “cruise emissions” presented in the studies by [7,715,828,829], where the majority of flight take place. The scope of subsonic aircraft with cruise altitudes of 8–12 km [7,16,830] is considered in this framework.

CO₂ drives the climate impact of aviation particularly important for fossil-based or alternative fuels (bio/electro-fuels). Non-CO₂ emissions (SM 3.1), e.g., water vapor and NO_x from the combustion with air of hydrocarbon-based fuels or H₂, also generate a significant climate impact [715]. However, currently these emissions are not addressed in official

targets, e.g., European Union Emission Trading Scheme, the CORSIA initiative [831], the Kyoto Protocol [832], because they can vary depending on the background atmospheric conditions, flight range, and cruise altitude and latitude [832–834].

In general, the tailpipe emissions of a given aircraft (i) model and segment (j) can be obtained using the following equation:

$$TPE_{\text{pollutant,phase}} = \sum(EF_{\text{pollutant,phase}} \times M_{TF, \text{phase}}) \quad (3.11)$$

Here, $TPE_{\text{pollutant,phase}}$ indicates the tailpipe emission for a given pollutant for the phase LTO or CCD. The emission factor of the pollutant in phase ($EF_{\text{pollutant,phase}}$) depends on the energy source. Unless specific data are available, the emissions from the reserve fuel (RF) can be assumed to be negligible because such fuel is not consumed during the flight.

The maximum trip fuel consumption can be estimated by:

$$M_{TF,\text{max,phase}} = \frac{(1-X_{RF,\text{ref}}) \times E_{RPK,ij} \times X_{TF,\text{phase}}}{ED_{\text{ref}}} \quad (3.11.1)$$

The energy proportion of the RF for conventional kerosene is defined as $X_{RF,\text{ref}}$ depending on the aircraft model (i); details are given in SM 3.2. $X_{TF,\text{phase}}$ is the proportion of fuel consumption in the phase (LTO or CCD), and ED_F the gravimetric energy density of the energy sourcing whether the reference fuel (conventional kerosene) or alternative kerosene (biofuels/electrofuels) (see SM 3.2).

In Fig. 3.3, the overall energy consumption (E) for the projected RPK can be evaluated in terms of $E_{RPK,ij}$ for the alternative energy (Case a) corresponding to Eq. (3.1) and for the reference kerosene (Case b).

In this framework, the overall tailpipe emissions are estimated according to the SA type, except for all-electric (battery) aviation for which it is considered that no emissions are generated during the flight. The climate impact is further expressed in terms of CO₂ equivalent by multiplying $TPE_{\text{pollutant,phase}}$ by the characterization factor, $CF_{\text{pollutant,phase}}$, including global warming potential (GWP) and the global temperature change potential (GTP). In addition, the climate impact could be declined according to the flight phase (LTO and CCD).

$$\text{Impact, CO}_2\text{-equivalent} = \sum_{\text{pollutant}} (TPE_{\text{pollutant,LTO}} \times CF_{\text{pollutant,LTO}}) + \sum_{\text{pollutant}} (TPE_{\text{pollutant,CCD}} \times CF_{\text{pollutant,CCD}}) \quad (3.12)$$

where the amounts of emitted pollutants can be calculated using Eq. (3.11), and CF is the characterization factor used to convert the $TPE_{\text{pollutant,phase}}$ value of interest to its CO₂ equivalent in mass units.

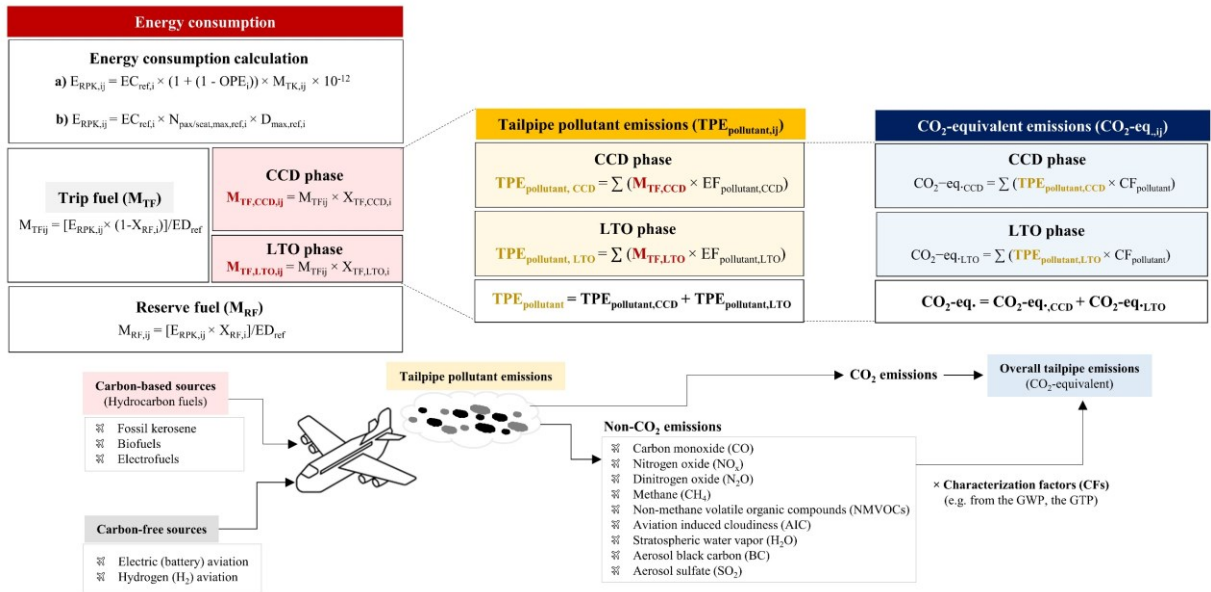


Fig. 3.3. Overall tailpipe emissions calculation based on the fuel consumption data applied in this framework.

The energy requirement can be calculated with two different formulas (as expressed in a) and b)) regarding the data availability.

3.5.2 Estimating tailpipe emissions per SA type

In the proposed framework, CO₂ along with non-CO₂ emissions are covered, as demonstrated in Table 3.6; these emissions contribute to one- up to two-thirds of the climate impact of aviation [715,831,833,835,836]. However, as no best-fit approach has been approved to reveal the overall tailpipe emissions and impacts, the conventional LCA approach is recommended to be used, as expressed in Eq. (3.12) and Fig. 3.3. In this section, the EF_{pollutant,phase} of each emitted pollutant by phase is defined according to the type of fuel. They are considered to apply for the pollutant's amount computation (TPE_{pollutant,phase}) (yellow in Fig. 3.3).

In this methodology, the default EF_{pollutant,phase} value for fossil-based kerosene, biofuels/electrofuels (alternative kerosene), and hydrogen (H₂) is applied, as indicated in Table 3.6. These values represent the amounts per fuel consumption in the distinguished phase of flight if available. The available values from IPCC for the cases of fossil kerosene are prioritized when available, namely CO₂, CO, non-methane volatile organic compounds (NMVOC). Otherwise, applying the values (e.g., soot, water vapor, SO₂) cited in the literature [714,715,837] is recommended.

Even though biofuels/electrofuels (alternative kerosene) follow similar trends to fossil-based kerosene in terms of hydrocarbons, the differences in their chemical compositions, such as the aromatic constituents, the hydrogen-to-carbon (H/C) ratios, result in differences in the combustion properties [500,838,839]. For example, the emission factors for CO₂ in case of lower carbon-content fuels (mainly in SPK fuel category), are quantitatively reported as being lower [493,787,840,841]. Similarly, soot emissions are reduced for fuels with lower level of aromatic content [500,839,842]. The reduction of NO_x emissions has also been investigated [788,843]. However, this phenomenon cannot be interpreted from the chemical composition of the fuels only, because it also depends on the operating conditions [187,838,839].

Because some EF_{pollutant,phase} are unavailable for alternative kerosene (biofuels and electrofuels), the EF_{pollutant, phase} values of fossil-based kerosene are used as proxy, including CH₄, N₂O, NMVOC, water vapor, soot, and SO₂. If the EF_{pollutant,phase} of each flight phase, such as H₂O and soot, are not available, the available value is used as a proxy for both phases. The EF_{pollutant} of each fuel have been reviewed and are summarized in Table 3.6. The median/average values are provided with the minimum and maximum ranges, and the sources of references, in SM 3.3.

Flight emission calculations for carbon-free aviation have focused on hydrogen aviation since electric (battery) aviation has been proposed as being zero-emission during flight operations, for all-electric schemes.

In the case of hydrogen, two main climate forcers are considered owing to the available data: water vapor and NO_x emissions. The latter results from the combustion with air (di-nitrogen) as a result of high-temperature flame generation [519,757]. Hydrogen fuel leads to higher water emissions per energy content of the fuel, e.g., approximately 2.6 fold more water than hydrocarbon fuels.

Table 3.6 Emission factors (EF_{pollutant,phase}) proposed in the proposed framework depending on the type of energy source (in g pollutant kg⁻¹ fuel used). Detailed data (with the min/max ranges) can be found in SM 3.3.

Pollutants ^a	Phase	Fossil kerosene		Alternative kerosene (Biofuels/Electrofuels)		Hydrogen (H ₂)		Notable impact on the environment (Climate change impact: +warming/- cooling)
		per phase	Overall ^b	per phase	Overall ^b	per phase	Overall ^b	
Well-mixed greenhouse gases (GHGs)								
CO ₂	LTO	3155.00 ¹	3152.50	3016.00 ₂₋₅	3000.00			• Greenhouse gas (+) ²⁰
	CCD	3150.00 ¹		2984.00 _{2-3,5-6}				• Greenhouse gas (+) ²⁰ • Stratospheric CO ₂ from CH ₄ oxidation ²⁷
CH ₄	LTO	0.48 ¹	0.24	0.48 ¹	0.24			• Greenhouse gas (+) ²⁰ • Precursor for photochemical O ₃ formation (+) ¹⁷
	CCD	0.00 ¹		0.00 ¹				• Greenhouse gas (+) ²⁰ • Precursor for photochemical O ₃ formation (+) ¹⁷ • Enhancement of stratospheric H ₂ O (+) ¹⁷

N ₂ O	LTO	0.10 ¹	0.10	0.10 ¹	0.10			• Greenhouse gas (+) ²⁰
	CCD	0.10 ²		0.10 ¹				• Greenhouse gas (+) ²⁰ • Depletion of stratospheric O ₃ ¹⁷
Other aviation forcers								
CO	LTO	14.77 ¹	10.38	11.67 ⁷	10.34			• Harmful gas for living organisms (e.g., respiratory problems) ¹⁶⁻¹⁷ • Acceleration/contribution to the photochemical smog formation (+) ¹⁷ • Precursor for photochemical O ₃ formation (+) ¹⁸⁻¹⁹
	CCD	6.00 ¹		9.00 ⁷				• Precursor for photochemical O ₃ formation (+) ¹⁸⁻¹⁹
NMVOC	LTO	10.35 ¹	6.03	10.35 ¹	6.03			• Contribution to tropospheric O ₃ formation (+) ¹⁷ • Destruction of ambient methane concentration (-) ^{17,19}
	CCD	1.70 ¹		1.70 ¹				• Contribution to tropospheric O ₃ formation (+) ¹⁷ • Destruction of ambient methane concentration (-) ^{17,19}
NO _x ^c	LTO	14.20 ¹	14.10	1.71 ³⁻⁴	2.10		7.87	• Contribution to photochemical smog formation ^{18,21} • Particulate emissions (e.g., respiratory morbidity) ²⁰ • Induce the tropospheric O ₃ formation (+) ^{16,18,21} • Destruction of ambient methane concentration (-) ^{16,18,21}
	CCD	14.00 ¹		2.50 ^{2,5}				• Destruction of ambient methane concentration (-) (associated with the reduction of stratospheric H ₂ O (-)) ^{16,18} • Increase stratospheric O ₃ formation as a protective layer ²⁷
AIC ^{d,e}	LTO	3155.00 ¹	3152.50	3016.00 _{2,5}	3000.00			• Absorption of longwave radiation (+) ^{22,23} • Influence the cirrus cloud formation (+) ^{22,23}
	CCD	3150.00 ¹		2984.00 _{2-3,5-6}				• Absorption of longwave radiation (+) ^{22,23} • Influence the cirrus cloud formation (+) ^{22,23}
H ₂ O	LTO	1199.50 ₉₋₁₂	1199.50	1199.50 ₉₋₁₂	1199.50		8575.00	• Absorption of shortwave radiation (+) ²²⁻²⁴ • Removed through the hydrological cycle within a few weeks ²²⁻²⁴ • Contribution to contrail formation (as condensation nuclei) (+) ²²⁻²⁴
	CCD	1199.50 ₉₋₁₂		1199.50 ₉₋₁₂				• Absorption of shortwave radiation (+) ²²⁻²⁴ • Persist up to 0.5-1 year in the stratosphere ²²⁻²⁴ • Contribution to contrail formation (as condensation nuclei) (+) ²²⁻²⁴

Soot	LTO	0.03 ¹³	0.03	0.02 ⁴⁻¹³	0.02			<ul style="list-style-type: none"> • Particulate emissions (e.g., respiratory morbidity)²⁰ • Absorption of longwave radiation (+)²⁵⁻²⁶ • Precursor for contrail and cirrus cloud formations (+)²⁵⁻²⁶
	CCD	0.03 ¹³		0.02 ⁴⁻¹³				<ul style="list-style-type: none"> • Absorption of longwave radiation (+)²⁵⁻²⁶ • Precursor for contrail and cirrus cloud formations (+)²⁵⁻²⁶
SO ₂	LTO	1.20 ¹⁴	1.20	1.20 ¹⁴	1.20			<ul style="list-style-type: none"> • Contribution to photochemical smog formation^{17,22,24} • Particulate emission (e.g., respiratory morbidity)²⁰ • Reflection of solar radiation (-)^{17,22,24}
	CCD	1.20 ¹⁴		1.20 ¹⁴				<ul style="list-style-type: none"> • Reflection of solar radiation (-)^{17,22,24}

■ No data available

Notes: ^a Emissions of NO_x are given in grams of NO₂, including the conversion of NO to NO₂ [831].

^b Overall AV. refers to the average EF_{pollutant} derived from LTO and CCD phases.

^c Contrail and cirrus cloud formations are included in AIC.

^d Only NO_x emissions are considered when hydrogen is combusted [758]. The EF_{NO_x} is computed from 80% NO_x emissions reduction relative to fossil kerosene [758]. The NO_x emissions from fossil kerosene retrieved from [501,844] are used as calculation baseline.

^e For the future scenario as applied in this framework, the CO₂ EF is applied as a proxy for AIC quantification when the actually traveled distances are used [715]. To ensure tractability, numbers are presented with a maximum of 2 significant digits after the point. This, however, is not to be seen as an indication of precision.

Acronyms: AIC (Aviation induced cloudiness); CCD (Climb, cruise, and descent flight phase); LTO (Landing and take-off flight phase); NMVOC (Non-methane volatile organic compounds)

Refs.: ¹ [844]; ² [500]; ³ [788]; ⁴ [845]; ⁵ [787]; ⁶ [846]; ⁷ [843]; ⁸ [758]; ⁹ [847]; ¹⁰ [848]; ¹¹ [849]; ¹² [714]; ¹³ [732]; ¹⁴ [837]; ¹⁵ [850]; ¹⁶ [835]; ¹⁷ [851]; ¹⁸ [852]; ¹⁹ [853]; ²⁰ [854]; ²¹ [855]; ²² [856]; ²³ [857]; ²⁴ [832]; ²⁵ [836]; ²⁶ [829]; ²⁷ [858].

3.5.3 Assessment of the climate impact of tailpipe emissions

In the conventional LCA approach, the climate characterization factors (CFs) are required in addition to emission factors (EF_{pollutant, phase}; in section 3.5.2) to calculate the impact (Eq. 3.12).

The most commonly used metric for global warming impact in LCA is the GWP which has primarily been defined and applied to well-mixed (long-lived and short-lived) GHG (e.g. CO₂, N₂O, CH₄). Extension of GWP to other short-lived, or indirect climate forcers, or high altitude emissions from aviation, is matter of current investigations [859]. The impacts of these non-CO₂ emissions have not been integrated into the available LCA literature, as illustrated in Table 3.1, because of the high uncertainties in the reported CF values; these uncertainties arise from numerous factors, such as the atmospheric conditions, latitudinal variations, and the distance traveled [832,833]. Moreover, these CFs, particularly for the aviation sector, were not presented in the most recent IPCC report (AR6) [852,853].

As an alternative to GWP, CFs were derived for the GTP metric, as shown in Table S3.6 [860–862]. . With the GTP metric, the additional inclusion of climate sensitivity, i.e., the change in the equilibrium surface temperature per unit RF, is required which introduces more uncertainty in the climate impact evaluation [835,860].

In order to alleviate the inconsistency of using GWP or GTP metrics for short-lived climate forcers, new metrics were recently proposed like GWP*/GTP* (primarily demonstrated for CH₄; [863,864], and CGTP [865]. Sustained (step) emission rates are used instead of pulse emission to define such metrics. These new metrics, applied to changes in the emission rate (in unit of mass per annum) rather than changes in the emission amount (in unit of mass), was demonstrated as more relevant to account for time dependent emissions of e.g. a country [865].

However, at present, there are no CFs available for these new metrics. In addition, the emission rate (instead of a quantity) is not always available/compatible with conventional (static) LCA. For these reasons, the conventional GWP/GTP is proposed in our framework.

In addition to using CFs, another approach to reveal the overall tailpipe emissions in CO₂-equivalent is using the CO₂ emission weighting factor (EWF). This factor is the ratio of warming effects (radiative forcing; RF; e.g., in [829,866,867]) or GWP in, e.g., [829,832]) of the overall emissions including CO₂ and non-CO₂) and those of CO₂ emission alone. The EWF can be directly multiplied with the known CO₂ emissions at the CCD phase to account for overall climate change effects (CO₂ and non-CO₂). This simple approach has been proposed to estimate non-CO₂ impacts in e.g., European Union Emission Trading Scheme (EU ETS) [831,868]. However, the EWF values are variously reported without gathering a global agreement at the time of this work was performed. On top of that, this factor is not applicable to the carbon-free approach (e.g., H₂). Further details are retrieved in SM 3.1 and elsewhere [828,832,857,866,867]. The existing CFs for aviation (e.g., in [715], [832]) are specific for high altitudes, implying that the use is adapted to the CCD phase. The LTO emissions should also be taken into account, especially for short flights (<1,500 km) because the proportion of fuel consumption is relatively important (for exampleecoinvent 3.8 indicates approx. 18-40% CO₂ emitted at low altitudes). Nevertheless, the CFs for LTO phase emissions have not been established. The common CFs are proposed to apply. In the LCA literature, it is not always clear to which phase the inventory and impact calculation is applied [829].

The available CFs for aviation emissions are summarized in Tables S3.5 and S3.6. There is no distinction between the tailpipe emissions of CO₂, CH₄, N₂O, and NMVOC and the surface (on-ground) emissions of these pollutants, so the common CFs apply for them.

To better understand the implications of using the different state-of-the-art approaches for calculating the global warming impact in LCA, an application case is presented hereafter for the four SA systems. The emission factors and impact calculation methods exposed in the previous sections are used. For the comparison of the methods, three key parameters are considered: i) the impact calculation method, ii) the emission factors (EFs), and iii) the share of fuel consumption between LTO and CCD phases. In addition, 16 scenarios (fossil kerosene and biofuels/electrofuels) and 8 scenarios (H₂) are further analysed. The different cases calculated are described in table 3.7. The detailed calculation can be accessed in SM 3.3.

Table 3.7 Defined parameters for comparative approaches in tailpipe emission calculation (with the calculation basis of GWP₁₀₀ metric). Further detailed calculations can be retrieved in SM 3.3.

Parameters	Description
i) Calculation approach	<p>Method 1 (M1): This method uses CFs for well-mixed GHGs and other aviation forcers independently from the phase of flight. It means the emissions from LTO or CCD are used with the same CFs:</p> <p>The CFs for well-mixed GHGs, CO, and NMVOC are those established for the surface emissions, no specific values are available for aviation (high altitude). All mentioned CFs are available in the IPCC assessment report [835,851,853].</p> <p>The CFs for aviation forcers are taken from ([715]) and are applied for both LTO and CCD phases. This is due to the lack of CFs for LTO emissions from aviation.</p>
	<p>Method 2 (M2): Similar to the M1, the CFs for well-mixed GHGs, CO, and NMVOC are the same whether LTO or CCD, as no specific values are addressed for aviation (high altitude). Whereas the other remaining emissions are considered depending on the phase.</p> <p>For the LTO emissions, the CFs for unspecified (any anthropogenic activities) NO_x, soot (as a mixture of organic carbons and black carbons; [715]), and SO₂ are retrieved from the IPCC assessment report [851]. The impacts derived from water vapor is excluded because it is considered that H₂O vapour is removed through the hydrological cycle in the troposphere [831]. The AIC impact is considered negligible as it is typically generated at high altitudes [869].</p> <p>For the other aviation emissions at the CCD phase, the CFs of [715] are used, similar to the M1.</p>
	<p>Method 3 (M3): Only the CFs of well-mixed GHGs, CO, and NMVOC are considered. This corresponds to the method applied in the conventional LCA approach.</p> <p>It is noted that for hydrogen SA, only NO_x and water vapor are considered in the tailpipe emissions because of the lack of information in this field. Besides, in conventional LCA there are no CFs for these substances.</p>
Emission weighting factor (EWF)	<p>Method 4 (M4): The EWF-based GWP₁₀₀ with the factor of “1.7” is selected to harmonize with the CFs GWP₁₀₀ obtained from [715]. This factor is multiplied by the known CO₂ emissions at the CCD phase to obtain the overall CCD emissions. This figure is further added to the CO₂ emissions in the LTO phase [828,859].</p> <p>As no carbon emissions are considered, the impacts from H₂ combustion are not compatible with this approach, therefore the hydrogen SA is excluded from the comparison.</p>

ii) Emission factors (EFs)	<p>E1: The reported EFs for LTO and CCD phases regarding the fuel types are used independently of the flight phase. They are referred to the values with the headline “overall” in Table 3.6.</p> <p>E2: The EFs depending on the flight phase, are employed as stated with the headline “per phase” in Table 3.6.</p>
iii) Fuel consumption	<p>F1: The fuel consumption at LTO is assumed to account for 10% (by mass or energy) of the total fuel demand [501,870].</p> <p>F2: Approximately 3% (by mass or energy) of fuel consumption is considered applicable during the LTO flight phase. This figure is retrieved from ecoinvent 3.8: transport, passenger aircraft, long-haul (>4,000 km) {GLO}. In addition, this is retrieved from the shares of CO₂ emissions at low and high altitudes (the direct relationship to the amount of fuel consumption is assumed; [355,828]).</p>

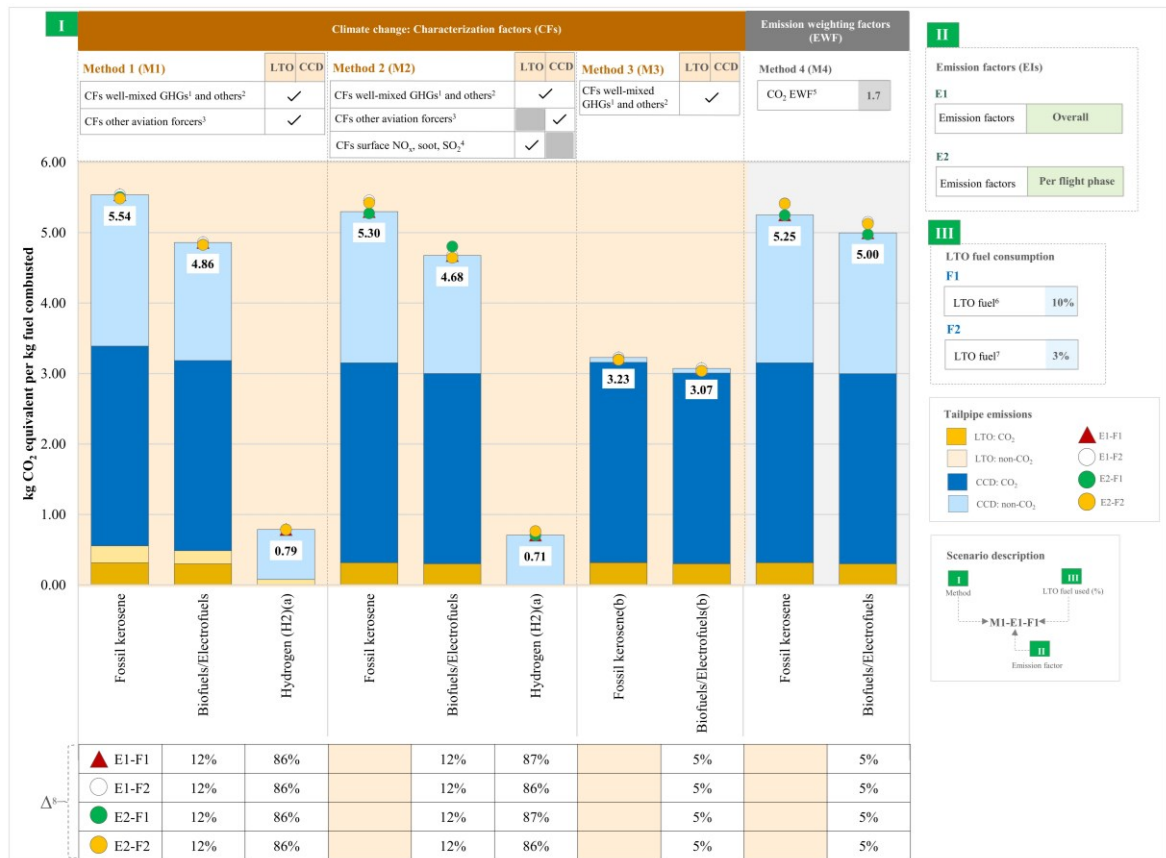


Fig. 3.4. Comparative CO₂ equivalent calculation approaches from the combustions of fossil kerosene, alternative kerosene (biofuels/electrofuels), and H₂. The M1/M2/M3/M4-E1-F1 scenarios are presented in a bar graph with their net values. The net results of other scenarios are displayed in the scatter plots.

Notes.

- ¹ GWP₁₀₀ of well-mixed GHGs, including CO₂, CH₄, and N₂O, is extracted from the IPCC assessment reports [853].
- ² GWP₁₀₀ for CO and non-methane volatile organic compounds (NMVOC) are retrieved from IPCC [851] and [835], respectively.
- ³ GWP₁₀₀ for aviation climate forcers, NO_x, soot, H₂O, SO₂, and AIC, are obtained from [715].
- ⁴ In method 2 (M2), GWP₁₀₀ of NO_x, soot, and SO₂ for unspecified (anthropogenic activities) applied for LTO emissions are available in the IPCC assessment report [851].
- ⁵ Emission weighting factor (EWF) are computed based on the GWP₁₀₀ metric, with the factor “1.7,” [715] in order to avoid the bias from the other sources..
- ⁶ LTO fuel consumption (% by mass) of 10% is assumed based on [501,870]
- ⁷ LTO fuel consumption (% by mass) of 3% is obtained from the CO₂ emissions shared between low and high altitudes (when the amounts of the CO₂ emissions are directly related to the amount of fuel consumed; [355,828]). Data are available in ecoinvent 3.8: transport, passenger aircraft, long-haul (>4,000 km) {GLO}.
- ⁸ The relative changes (Δ, %) have been calculated with respect to fossil-kerosene as reference.

In the graph:

- (a) The combustion of hydrogen is considered, in which NO_x and H₂O are the main climate forcers clustered as non-CO₂ in the displayed graph.
- (b) The non-CO₂ emissions in method 3 (M3) are referred to a CO, CH₄, N₂O, and NMVOC.

■ Not considered in that flight phase (as used in M2)

Acronyms: CCD (Climb, cruise, and descent flight phase); EWF (Emission weighting factor); LTO (Landing and take-off flight phase)

From Fig. 3.4, it is evident that M1, M2 and M4, with the inclusion of other aviation forcings along with CO₂ provide significantly higher impacts than M3, which considers only CO₂ (conventional approach). The other aviation climate forcings represent up to 40% of the total impacts (details in SM 3.3). The small variations between the results of M1, M2, and M4 are due to the choice of applied EFs as some pollutants are reported in different amounts in a particular phase, e.g., CH₄ and NMVOC are higher in LTO phase.

When compared to the fossil-kerosene, biofuels/electrofuels and hydrogen systems demonstrates a better performance, of up to 12% and 87%, respectively, and this for both M1 and M2 methods. This ranking is quantitatively conserved when variations in the fuel share between phases are considered (F1, F2) or when the EFs are global or detailed by phases (E1, E2).

Regarding the tailpipe emissions and impact integration in LCA framework, M1 and M2 are highlighted as the most complete approaches for conventional (static) LCA studies because these methods include all climate forcings and the flight phases. These approaches should be completed when specific CFs according to the altitude and latitude will be developed.

Unlike the EWF, this approach is not limited by energy source in which the total emissions are not computed relative to CO₂.

It should be noted that for a complete assessment of environmental performance in the aviation sector, not only climate impact but also other environmental impacts must be considered. For example, in Table 3.6, soot, NO_x, SO₂, and CO are all particulate pollutants associated with respiratory health hazards, acidification or eutrophication, mainly affecting the low altitude areas [850,854,854,871–873]. Some methods (e.g., on European Platform on Life Cycle Assessment; [874]), provide the CF for the upper troposphere and lower stratosphere (UTLS) sub-compartment for particulate matter, which should be applied if available. Those CFs are already provided by the LCIA methods, e.g., Environmental Footprint (EF; adopted by European Commission).

Noise impact should also be integrated in LCIA, especially for the airports' locations and their surroundings. The CFs for environmental noise from transportation have already been integrated into some LCIA methods, including the Swiss eco-factors [875] and the Environmental Priority Strategies (EPS) [876,877]. Additional CFs have been intensively studied (e.g., [878], [879]). They should further be expanded to the other LCIA and LCI database (e.g.,ecoinvent).

3.6 Conclusions

A comprehensive and complete framework is proposed for LCA, built on the consequential approach, for the field of commercial aviation for passenger transport, capable to ensure transparent and robust comparability when evaluating the overall environmental performances of emerging energy-sourcing for aviation, i.e., biofuels, electrofuels, electric, and hydrogen.

The aviation service unit is defined as the projected global RPK and is selected as the functional unit for two timeframes, i.e., 2035 (short-term) and 2045 (long-term), and for two segments namely domestic and international.

The system boundaries are defined with the key activities for five (three carbon-based and two carbon-free) systems: (i) biofuel from residual biomass, (ii) biofuel from land-dependent biomass, (iii) electrofuel, (iv) electric (battery) aviation, and (v) hydrogen aviation. The activities are grouped in seven categories: (i) conventional (fossil-based) kerosene activity, (ii) feedstock with the conversion process, (iii) counterfactual and displacement, (iv) aircraft manufacture, (v) aircraft operation, (vi) additional infrastructure needed, and (vii) end-of-life management (applied to aircraft or batteries).

According to the proposed functional unit, a model is proposed to translate it in energy requirements in each timeframe and for each service segment. The model also includes: (i) hybridization (the use of more than one source of energy to power an aircraft), (ii) the mass penalty affecting the number of carried passengers, and (iii) impacts stemming from non-CO₂ tailpipe emissions and effects. All these aspects are currently neglected in most LCA studies.

This work also provides a complete review of the tailpipe emissions by energy-sourcing category, including details by flight phase. A deep analysis of the existent methods for climate impact calculation and their utilization with LCI is

provided. Whichever approaches (M1, M2, and M4) are employed, their results are not far different (up to 6% difference between M1, M2, M4) relative to excluding non-CO₂ emissions (M3). Therefore, despite the uncertainties, the non-CO₂ impacts are recommended to be addressed rather than considering them negligible.

The proposed methodology includes the most recent knowledge in the field, however, some choices are indebted to current scientific advances concerning e.g., tailpipe emissions and their environmental impacts, and are subject to significant uncertainties. Overall, this framework provides a guideline for LCA practitioners when considering new energy sources in the future aviation sector.

3.7 Supplementary materials

Three supplementary materials are provided to provide all relevant datasets not presented in **Chapter 3**. SM 3.1 can be retrieved from this document. SM 3.2 and SM 3.3 can be accessed at <https://doi.org/10.48531/JBRU.CALMIP/N4TNMA>. The SM 3.2 consists of baseline calculations for sections 3.2-3.4. In addition, the calculation procedures to assess aviation tailpipe emissions can be found in SM 3.3.

Supplementary material 3.1 (SM 3.1)

This document presents additional and more detailed aspects not covered but referred to within **Chapter 3**.

1. ICAO's official definitions: Domestic and International flight [775]

International: A flight stage with one or both terminals in the territory of a State other than the State in which the air carrier has its principal place of business

Domestic: A flight stage not classifiable as international. Domestic flight stages include all flight stages flown between points within the domestic boundaries of a State by an air carrier whose principal place of business is in that State. Flight stages between a State and territories belonging to it, as well as any flight stages between two such territories, should be classified as domestic. This applies even though a stage may cross international waters or over the territory of another State.

2. Aircraft model characteristics used in this framework

The current commercial aircraft with a standard tube-and-wing (TW) configuration is considered to be used in all alternative energy systems except for hydrogen-powered aviation for international flight (in SM 3.2).

Representative aircraft variants have been determined to correspond to the different service segments. Therefore, Airbus A320 and A350 XWB models are considered for domestic and international services, respectively, as the projected dominant platform [813,880].

While a blended-wing-body (BWB) concept is assumed to be modelled for hydrogen-powered aviation [881,882], particularly for long-route distances as shown in SM 3.2, from Glenn Llewellyn's presentation, engineering from the Airbus working on the Zero-e aircraft project, the transformation in hydrogen propulsion system with novel airframe configuration cannot be reached within 2035. Therefore, the BWB concept is assumed to be available in service around 2045. The Boeing BWB X-48B model has been chosen as the representative BWB aircraft derived from [883] as the closest seat available relative to the Airbus A350 XWB model. The BWB's material breakdown is not available at the time of writing. Therefore, breakdown composition is estimated based on the long-haul A350 aircraft instead. Carbon composite materials have been considered the main composition of this airframe as the most advanced materials at the time of writing [884,885].

3. Emission components during flight operations

The airborne pollutants from aircraft operations are responsible for different impacts on the environment and human health. These pollutants can affect the quality of air from a sanitary point of view, for example, products from the (incomplete) combustion of liquid fuels: CO, VOC, SO₂, NO_x, and black carbon [832,885].

Hereafter we detail the effect on climate change of the pollutants emitted with direct and indirect induced radiative forcing.

3.1 Direct effects of aviation pollutants

3.1.1 Long-lived compounds

CO₂ is the main long-lived well-mixed gas emitted during the combustion of liquid fuels, either fossil- or sustainable liquid fuels [835]. Other direct GHG can result from the (incomplete) combustion of fuels. [832,885]. For these compounds, the standard metrics GWP and GTP can be used since their lifetime is of years (CH₄) and centuries (CO₂, N₂O) [832].

3.1.2 Short-lived compounds

The short-lived compounds have lifetimes in the atmosphere of hours to several months. Their climate impact depends on the latitude and altitude of the emission, some of them being particularly impacting at high altitudes (approximately 8-12 km for the subsonic aircraft) [832,886]. These substances are not covered by the metrics proposed by the Kyoto Protocol as used in policymaking [832]. Models are under development to estimate these climate impacts [836,886].

Nitrogen oxides

Nitrogen oxides (NO_x) are considered another abundant component of aviation operations [832,887]. NO_x can persist for several hours near the surface for around a few weeks in the upper troposphere [888]. However, its impact on radiation is insignificant [889]. Aviation NO_x emissions can be generated from the combustion of either liquid fuels or hydrogen [832]. Albeit, NO_x emissions can also lead to ozone destruction depending on the local quantities of NO_x [836,887,890]. NO_x aircraft emissions are more effective for ozone formation in the upper troposphere than the ground emissions [891].

Aviation aerosols

Sulfate and black carbon (sometimes denoted as soot, e.g., in [835]) are the most abundant aerosols from aircraft operations [835], resulting from liquid fuel combustion. Sulfate can directly reflect solar radiation and change cloud properties to reflect more sunlight resulting in a negative RF [832,835]. On the other hand, a positive effect for the emitted soot can be observed due to shortwave radiation absorption [832,892,893]. They can also act as condensation nuclei in cloud formations [832,835].

Water vapour

Water vapour is emitted from liquid fuels or hydrogen combustion. Water vapour released in the troposphere is removed by precipitation within a few weeks and considered without effect on the RF [836]. However, when emitted in the stratosphere, it remains up to 0.5-1 year [894] and plays a role in global warming, as described in the following section.

3.2 Indirect effects of aviation pollutants

Some emitted pollutants (CO, VOC, NO_x, black carbon) can react in the atmosphere to produce direct GHG or other perturbation effects.

3.2.1 Tropospheric ozone formation and methane destruction

Tropospheric ozone is a direct GHG formed by complex atmospheric reactions of the indirect GHG (NO_x, VOC) and CH₄. The generated tropospheric ozone is not linearly proportional to the amount of emitted precursors (e.g., NO_x depending considerably on location and season, VOC) [895], here mainly focused on aviation nitrogen oxides. The impact on tropospheric ozone formation seems to depend on the cruise altitude [836,896].

Hydroxyl (OH) radical is the dominant tropospheric oxidant [855] and an intermediate for tropospheric ozone formation and methane destruction [855]. The released nitrogen oxides can produce excited oxygen atoms by photolysis [897]. The excited oxygen atoms can react with oxygen molecules (O₂), resulting in tropospheric ozone formation, which decays with a lifetime of a few months [898]. The ozone produced also enhances the oxidative capacity of the atmosphere by increasing the hydroxyl level [898,899]. Additionally, they can react with the ambient methane leading to a decrease in its lifetime and concentration, associated with a negative RF response [855,898,900].

Other indirect GHG like CO and VOC are rapidly converted to CO₂ in the atmosphere [901].

3.2.2 Aviation-induced cloudiness (AIC)

Aviation-induced cloudiness as an emission-related effect can be divided into two phases: persistent linear contrails and cirrus clouds.

Linear contrails (or condensation trails) are directly generated from water vapour depending sensitively on ambient atmospheric conditions (e.g. humidity, latitude/altitude, temperature, pressure) [862,890,896]. Generally, the contrail

formation is likely to occur at higher altitudes in the upper atmosphere [890,902]. They can persist for many hours to several days based on the mentioned parameters [903]. For instance, persistent contrails are formed mainly in the supersaturated region, particularly in the tropopause as the interface between the troposphere and stratosphere [896]. Linear contrails can also transform into non-linear, natural-looking cirrus clouds [890,902,903]. They absorb longwave radiation rather than reflecting solar radiation, causing a strong warming potential [835].

Apart from triggering the formation of linear contrails, aircraft operation potentially induces cirrus cloud formation. They influence the chemical and particle microphysical properties in the upper atmosphere resulting in changes in the RF [886]. These effects are not well understood due to the natural variability and complex phenomena [862]. Cirrus clouds can be formed if the background atmosphere is sufficiently supersaturated for the ice phase and are indistinguishable from natural cirrus clouds from surface observation and satellite images [886,893,903]. On the other hand, the accumulation of emitted components containing black carbon (or soot), organic compounds, and sulfate constitute cloud condensation nuclei triggering the cirrus clouds generation [886]. The upper atmosphere's modifications, such as cloud composition, changes in cloud particle sizes and forms, etc., have been investigated from aircraft-induced aerosols. These cloudiness are potentially affected by natural climate variability and anthropogenic climate change [893].

To avoid these effects on climate, the contrail formation can generally be mitigated by lowering overall cruise altitude [886,887,890]. However, flying at lower altitudes increases fuel consumption and direct CO₂ emission [890].

4. CO₂ Emission weighting factors (EWF) for total tailpipe emissions calculation

A CO₂ equivalent-EWF can be applied to estimate the non-CO₂ climate impacts by directly multiplying with CO₂ emission at the CCD phase, referring to flight activities occurred at an altitude higher than ~915 m [501] in terms of CO₂-equivalent emissions [892,904]).

For instance, the CO₂ emissions at the CCD phase are assumed for one particular flight as one tonne (the EWF factor of “3” is assumed). The CO₂ emissions are multiplied by three. The overall climate effects (from CO₂ and non-CO₂) are equivalent to 3 tonnes CO₂eq. are revealed for the CCD phase instead of just the 1 tonne of actual CO₂ emitted. This obtained figure is then added to the actual CO₂ emissions in the other phases of flight to reveal the total tailpipe emissions [892,905]. EWFs from several studies have compiled, as shown in Tables S3.1-S3.3.

These factors are sometimes referred to as non-CO₂ multipliers [861] and aviation multipliers [715]. EWFs can be calculated using the potential warming ratio of the CO₂ and non-CO₂ emissions divided by CO₂ emissions as explained by [833,892,906]. Those warming potentials are retrieved from radiative forcing (RF) and GWP, as commonly proposed concepts are reviewed as follows. Meanwhile, these metrics' details can be found elsewhere [886,892,905].

4.1 Radiative Forcing (RF)

The stratospheric adjusted RF concept is a good approximation for homogenous climate forcers such as CO₂ [907]. However, the ERF has been introduced as a better indicator, particularly for heterogeneous climate forcers contributing to aviation pollutants, namely aviation-induced ozone and contrail cirrus [715,907,908]. The ERF includes tropospheric adjustment and climate sensitivity at the top of the atmosphere (TOA), whereas the adjusted temperature change in the stratosphere is only included in the adjusted RF concept [909,910].

The Radiative Forcing Index (RFI) concept was introduced by [911]. RFI value is calculated based on the RF (whether adjusted RF or ERF) of emitted pollutants from burning aviation fuels at a given time horizon compared to the RF induced by CO₂ [892]. However, this concept is a backwards-looking perspective depending on the RF at a particular period (e.g., by 2020). Therefore, it may not be applicable to demonstrate aviation's non-CO₂ effects on future emissions (taking into account the current and future impact) [832,833,860,886,887,912], which is not preferable as an emissions-equivalent concept for policy purposes [886,892].

Several researchers have calculated the RFIs, as shown in Tables S3.1-S3.3.

Table S3.1 Aviation radiative forcing (RFs) and radiative forcing index (RFI) (excluding AIC)^a

Year	RF (mW m ⁻²)					Total RFs	RFI ^g	References
	CO ₂	NO _x ^b	H ₂ O	Contrails	SO ₄ ²⁻			
1992	18.0	9.0	1.5	20.0	-3.0	3.0	48.5	2.69 [891]

2000^c	25.0	10.4	2.0	33.9	-4.0	4.0	71.3	2.85	[893]
2000^d	25.3	11.5	2.0	10.0	-3.5	2.5	47.8	1.89	[893]
2005^e	23.0	11.0	2.0	10.0	-4.0	2.5	44.5	1.93	[906]
2005	28.0	13.8	2.8	11.8	-4.8	3.5	55.1	1.97	[886]
2005^f	25.0	12.9	1.4	34.8	-5.3	0.7	69.5	2.78	[715])
2011^f	29.0	13.6	1.5	44.1	-5.6	0.7	83.3	2.87	[715]
2018^f	34.3	17.5	2.0	57.4	-7.4	0.9	104.7	3.05	[715]
2020	40.8	21.4	4.0	20.2	-7.0	5.0	84.4	2.07	[886]

Notes.

^a AIC stands for aviation-induced cloudiness (including linear contrails and the formation of cirrus cloudiness). Due to the poor understanding of AIC, RF and RFI of this factor are not presented.

^b Nitrogen oxide (NO_x) emission results, including the formation of tropospheric ozone (O₃), a reduction of the ambient methane (CH₄), and a further slight decrease in tropospheric O₃.

^c RFs are scaled from data in [891] to the year 2000 as reported by [893] using linear interpolation.

^d RFs data are derived from the TRADEOFF project.

^e [906] retrieved the original aviation RFs value derived from IPCC AR4 (2007), these RFs values relative to the start of the industrial era in the year 1750.

^f Effective radiative forcing (ERF) is used according to the study of [715].

^g RFI is calculated using the following equations: $RFI = (\text{total (effective) RF}) / (\text{effective) RF CO}_2$ as can be retrieved in [906].

Table S3.2 Radiative forcing (RF), including AIC factor

Year	RF			References
	Lower limit	Best estimate	Upper limit	
1992	0		40	[891])
2000	10	30	80	[893]
2005	11	33	87	[886]
2020	16	47	125	[886]

Table S3.3 Radiative forcing index (RFI), including AIC factor

Year	RFI			References
	Lower limit	Best estimate	Upper limit	
1992	2.69		4.92	[891]
2000	2.28	3.08	5.05	[893]
2005^a	2.41	3.37	5.72	[906]
2005	2.36	3.15	5.08	[886]
2020	2.46	3.22	5.13	[886]

Note.

^a Due to the RF value of AIC is not provided [906]. The RFs used in this calculation for 2005 are derived from [886].

4.2 Global warming potentials (GWP)

EWFs can also be calculated from the relative emission metrics, for instance, the GWP metric calculating the climate impact of a pulse emission of pollutant against the references such as the CO₂ in specific time horizons. EWF-based GWP values have been calculated using either emissions data (with GWP₁₀₀ factor; kg CO_{2eq} kg⁻¹ emission) [715,905,913], the absolute GWP (AGWPs) at different time horizons (in Table S3.4). The shorter time horizons demonstrated, the higher EWF-based GWP, as shown in Table S3.4, mainly corresponds to short-lived compound emissions.

However, the GWP metric is still the subject of scientific debate since it was initially developed for long-lived, well-mixed GHGs (e.g., CO₂, CH₄), which is less accurate for short-lived gases (e.g., aerosols, NO_x, soot) [835,914] as mainly emitted during flight operations. The global temperature change potential (GTP) was introduced by [860] Shine (2005) (see also [861,862]) and also included in the Fourth Assessment Report (AR4) of the Intergovernmental Panel on Climate [835]. The effect of short-lived species on long climate time scales (e.g., 100 years) retain less in the GTP metric (concerned with the temperature responses at a particular point in time) relative to the GWP [907,914]. Though EWF-based GTPs have not been demonstrated, they could be calculated similarly to the mentioned EWF-based GWPs.

Table S3.4 AGWP and EWF-based GWP of aircraft emissions

Time horizon	AGWP ($\times 10^{-14} \text{ W m}^{-2} \text{ kg CO}_2^{-1} \text{ yr}$)				EWF ^b	References
	CO ₂	NO _x ^a	AIC	Water vapour		
1	0.25	2.00	6.70		35.80	[833]
20	2.47	0.34	5.50		3.36	[833,904]
	2.47		7.26	1.70	4.63	[832]
	2.49		7.70		4.09	[717]
100	8.69	-0.04	5.50		1.63	[833,904]
	9.15	0.01	6.70		1.73	[833]
	8.69		7.30	1.74	2.04	[832]
	9.17		7.70		1.84	[717]
	9.17		7.70	1.83	2.04	[905]
500	28.60	-0.01	6.70		1.23	[833]
	28.60	-0.04	5.50		1.19	[904]
	28.60		7.26	1.69	1.31	[832]

Notes.

^a AGWP of NO_x is derived from their indirect emission effects, including tropospheric ozone and methane formations.

^b AGWP in the table is the average value from each reference used for EWF-based GWP calculation.

Albeit, the international agreement has not been met yet at the time of writing about which metrics (e.g., RFI, EWF-based GWP) and values should be applied. They have coincidentally indicated similar figures (Tables S3.1 and S3.4) but differ in concept. The relative emission metrics (e.g., integrated-based GWP, endpoint-based GTP) are the preferable EWF-based values as a forward-looking metric for aviation projections on the climate [887]. On the contrary, a backward RFI metric is applicable when the current non-CO₂ emissions need to be accessed at a given time [832,833]. The most current EWF value is recommended as an appropriate criterion for selection, implying that the obtained results are generated from the most up-to-date information/models [892].

Though these EWF factors are meaningful, non-CO₂ impacts only depend on the CO₂ emission (, which may not be practical for a carbon-free approach (mainly interested in H₂). Therefore, characterization factors (CFs) are further introduced to compare carbon-based and carbon-free categories, as explained in section 3.5.3.

5. Comparative approaches: CO₂ equivalent emission calculations

This section demonstrates the comparative approaches for the approximate non-CO₂ emission. Three parameters include i) the different CO₂ equivalent calculation methods, ii) the applications of emission factors (EFs), and iii) the fuel consumption at distinguished phases of flight. The aim is to provide a clear picture of the obtained results with the different approaches to support decision-making. The overall tailpipe emissions from the combustion of 1 kg fuel (fossil kerosene, biofuel/electrofuel) have therefore been investigated. The descriptions of analyzed parameters can be found as follow.

I) The CO₂ equivalent calculation methods

Two main approaches are presented in this framework with the uses of climate characterization factors (CFs) (see section 3.5.3) and emission weighting factors (EWFs) (in the SM 3.1 section 4). In addition, the time horizon of 100 years is defined in this analysis.

The GWP climate metric has been considered the representative approach for using CF, commonly used in the LCA. Aviation emissions are clustered into two groups (as shown in Table 3.6): Greenhouse gases (GHGs) and the warming forcers induced mainly by aviation. As the CFs of the former groups are well established by the IPCC assessment report [715,835,914], they are considered. While the CFs retrieved from the study of [715], have been applied for five main climate forcers, including NO_x, aviation-induced cloudiness (AIC), water vapour, soot, and SO₂, as one of the most updated publications in this issue. The lists of applied CFs can be retrieved in SM 3.3.

While the EWF factor of 1.7 retrieved from GWP₁₀₀ is also retrieved from the study of [715] to avoid the uncertainty derived from the source of calculation basis.

II) Emission factors (EFs)

The emission factors (EFs) are one parameter that potentially influences the overall emissions. For fossil kerosene, the EFs are well-established in the IPCC emission database (2006). However, the applied EFs for biofuels/electrofuels (alternative kerosene) are gathered from the literature (see SM 3.3). The EFs of fossil kerosene combustion are considered a proximation if the data are unavailable for the biofuels/electrofuels such as CH₄ and non-methane volatile organic compounds (NMVOC). While the EFs for hydrogen combustion are computed in terms of NO_x and water vapour as two dominant pollutants. Only water vapour is considered when H₂ fuel cell mode is applied (not included in this comparison). The sensitiveness of EIs has been carried out using the averaged EFs (derived from the EIs of LTO and CCD phases), and the standalone EFs reported in particular for each phase (whether LTO or CCD). The influences of EFs' choices are addressed.

III) Fuel consumption

Fuel combustion is a critical generating source of emissions. However, the consumption rate varies depending on, for example, the distance travelled, aircraft models, etc. Herein, two proportions of fuel are considered for the comparison. First, 10% of fuel consumption used during the LTO is applied regarding the unavailable data of air operation for H₂ aviation [501,870].

Additionally, 3% (by mass) of total fuel consumption is used during the LTO phase. This figure is obtained from theecoinvent database of the CO₂ emissions shared between the troposphere, upper, and lower stratosphere (UTLS). This comes along with the assumption that CO₂ emissions are directly related to the amount of fuel consumed. This proportion of 3% occurred when the travelled distance was >4,000 km implying the long duration of fuel spent during the CCD phase rather than the LTO. The detail can be found in the ecoinvent database.

Overall, sixteen scenarios (with three considered parameters) are carried out for fossil kerosene and biofuels/electrofuels (alternative kerosene). Hydrogen aviation is analyzed with eight scenarios. The M3 is not considered owing to no data for GHG emissions from H₂ combustions. Meanwhile, the carbon-free emissions from the use of H₂ are not compatible with the M4, as they are computed based on the warming potential of total emission impacts relative to CO₂.

From Figs. S3.1-S3.3, the overall climate impacts from the use of GWP₁₀₀ (M1 and M2) are up to 5% perturbation in the case of fossil kerosene and biofuels/electrofuels (see SM 3.3). In comparison, a 10% perturbation is detected in H₂. The difference in fuel consumption (F1/F2) is the key driver for all cases. This can be highly varied regarding the aircraft models, distance travelled, and flight routes [355,858]. Albeit the CCD emissions are crucial, M1 is highlighted to include the impacts of LTO emissions and the downward transportation of the CCD emissions into the troposphere (at mid and high latitudes) [836,915]. Meanwhile, CCD emissions influenced by the Hadley circulation [836] are considered at lower latitudes to address the global tailpipe emissions.

When the overall methods (including aviation non-CO₂ in M1, M2, and M4) are compared, the lower CO₂eq. emissions are shown for the fossil kerosene case when the EWF is employed. On the contrary, a higher trend is found in the case of biofuels/electrofuels. This is due to the inclusion of other GHGs considered in M1 (such as CH₄, N₂O, CO, NMVOC) relative to M4 for fossil kerosene. The difference in using EFs is additional drivers (e.g., CO₂, NO_x). Therefore, while EWF is computed upon the fossil kerosene-based EFs [715], the biofuels/electrofuels applied herein show lower amounts of some pollutants, namely CO₂ and NO_x, resulting in the higher CO₂eq. emissions are obtained.

For the H₂ (Fig. S3.3), the generated results have significantly relied on the proportion of fuel consumption (F1/F2), whichever methods (M1 and M2) are employed. While excluding aviation, non-CO₂ impacts (in M2) result in approximately a 3-10% decrease compared to M1.

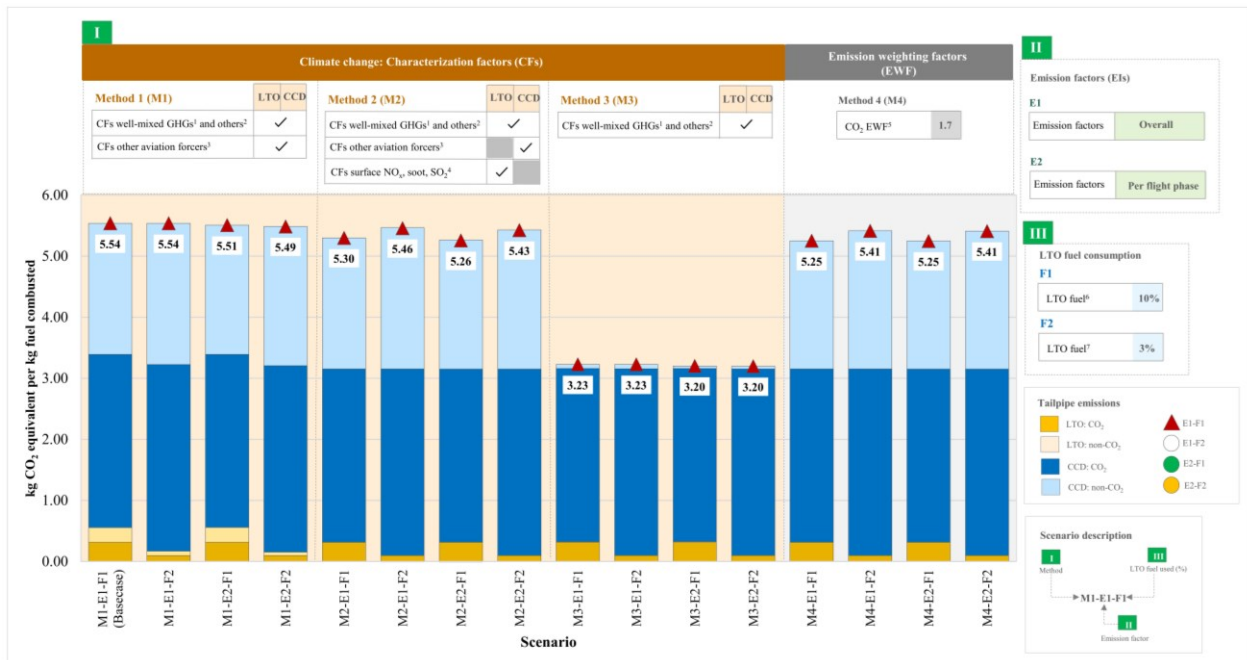


Fig S3.1. Overall climate impacts from fossil kerosene combustion, representing in terms of CO₂ equivalent with the different scenarios

Notes.

¹ GWP₁₀₀ of well-mixed GHGs, including CO₂, CH₄, and N₂O, is extracted from the IPCC assessment reports (CO₂, CH₄, and N₂O [853].

² While GWP₁₀₀ for CO and non-methane volatile organic compounds (NMVOC) are also retrieved from the IPCC assessment by [851] and [835], respectively.

³ GWP₁₀₀ for aviation climate forcer, including NO_x, soot, H₂O, SO₂, and AIC, are obtained from the study [715].

⁴ In method 2 (M2), GWP₁₀₀ of NO_x, soot, and SO₂ for unspecified (anthropogenic activities) applied for LTO emissions are available in the IPCC assessment report [851].

⁵ Emission weighting factor (EWF), computed based on the GWP₁₀₀ metric, with the factor “1.7,” has also been considered [715] in order to avoid the subjective derived from the source of references.

⁶ LTO fuel consumption (% by mass) of 10% is assumed based on [501,870]

⁷ LTO fuel consumption (% by mass) of 3% is obtained from the CO₂ emissions shared between low and high altitudes (when the amounts of the CO₂ emissions are directly related to the amount of fuel consumed; [355,905]). Data are available in ecoinvent 3.8: transport, passenger aircraft, long-haul (>4,000 km) {GLO}.

Acronyms: Characterization factors (CFs); Emission Weighting Factor (EWF); Landing & Take-off (LTO) flight phase; Climb, Cruise & Descent (CCD) flight phase

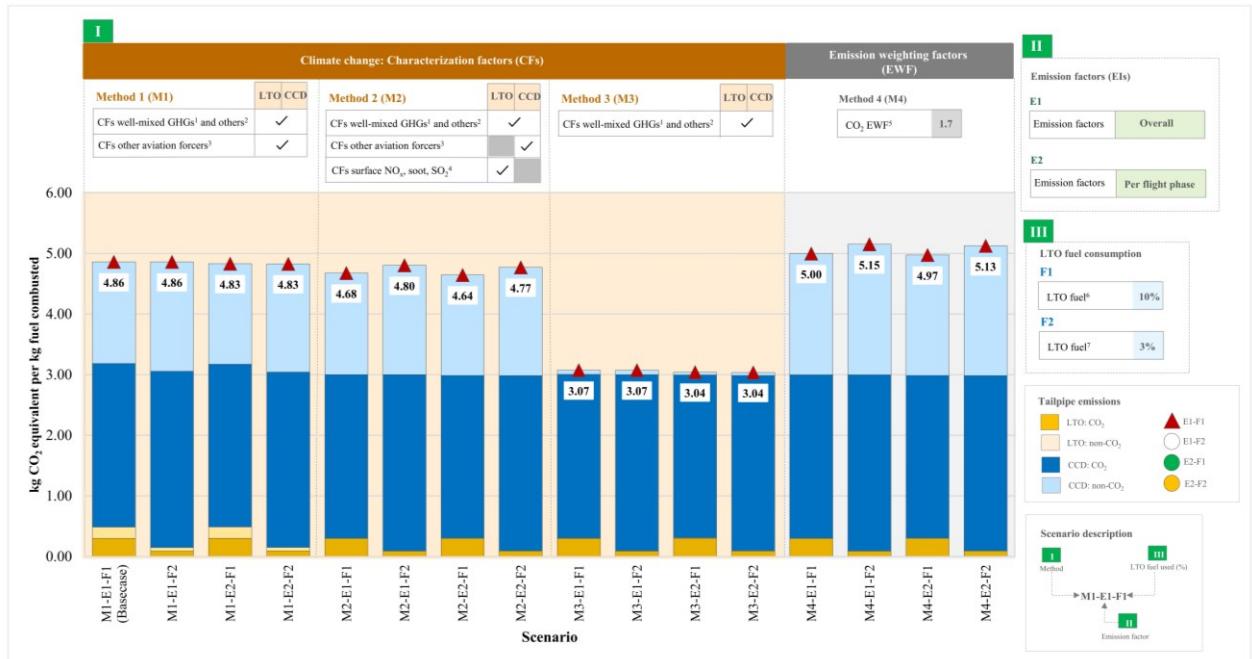


Fig S3.2. Overall climate impacts from **biofuels/electrofuels combustion**, representing in terms of CO₂ equivalent with the different scenarios

Notes.

¹ GWP₁₀₀ of well-mixed GHGs, including CO₂, CH₄, and N₂O, is extracted from the IPCC assessment reports (CO₂, CH₄, and N₂O [853]).

² While GWP₁₀₀ for CO and non-methane volatile organic compounds (NMVOC) are also retrieved from the IPCC assessment by [851] and [835], respectively.

³ GWP₁₀₀ for aviation climate forcer, including NO_x, soot, H₂O, SO₂, and AIC, are obtained from the study [715].

⁴ In method 2 (M2), GWP₁₀₀ of NO_x, soot, and SO₂ for unspecified (anthropogenic activities) applied for LTO emissions are available in the IPCC assessment report [851].

⁵ Emission weighting factor (EWF), computed based on the GWP₁₀₀ metric, with the factor “1.7,” has also been considered [715] in order to avoid the subjective derived from the source of references.

⁶ LTO fuel consumption (% by mass) of 10% is assumed based on [501,870]

⁷ LTO fuel consumption (% by mass) of 3% is obtained from the CO₂ emissions shared between low and high altitudes (when the amounts of the CO₂ emissions are directly related to the amount of fuel consumed; [355,905]). Data are available in ecoinvent 3.8: transport, passenger aircraft, long-haul (>4,000 km) {GLO}.

Acronyms: Characterization factors (CFs); Emission Weighting Factor (EWF); Landing & Take-off (LTO) flight phase; Climb, Cruise & Descent (CCD) flight phase

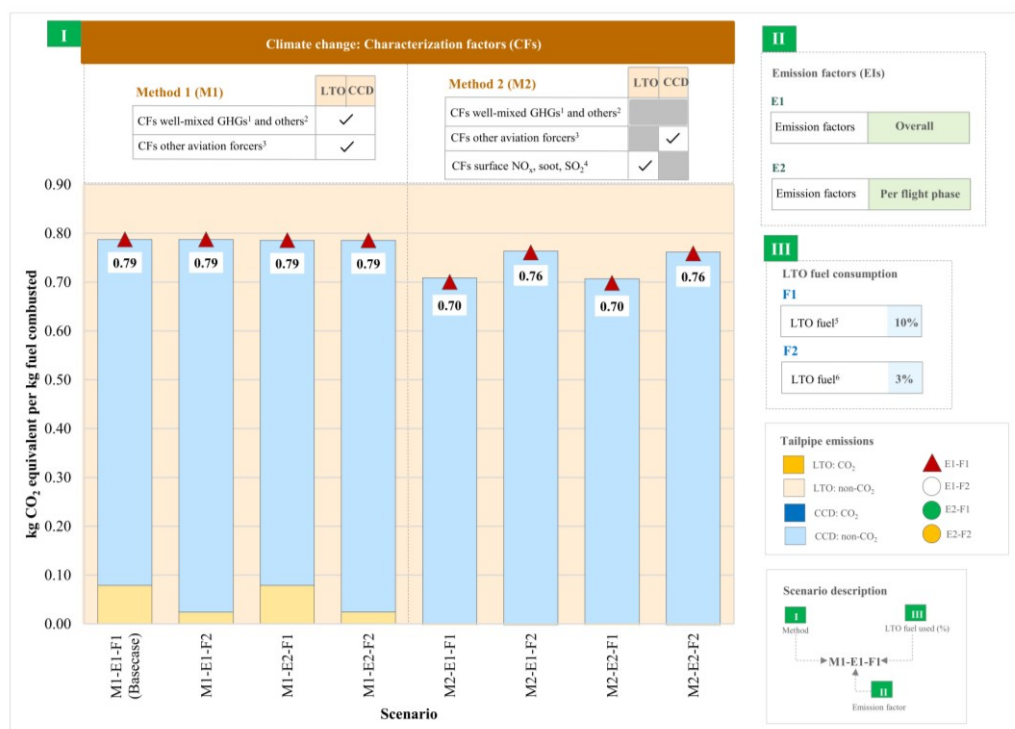


Fig S3.3. Overall climate impacts from **hydrogen combustion** represent CO₂ equivalent to the different scenarios. The non-CO₂ emissions in M1 and M2 are referred to as NO_x and H₂O from H₂ combustion.

Notes.

- ¹ GWP₁₀₀ of GHGs, including CO₂, CH₄, and N₂O, are not considered from H₂ combustion.
- ² While GWP₁₀₀ for other emissions, including CO and NMVOC, are not also considered from H₂ combustion.
- ³ GWP₁₀₀ of NO_x, AIC, H₂O, SO₂, and soot are applied, according to [715].
- ⁴ In method 2 (M2) for LTO emissions, GWP₁₀₀ of unspecified sources for NO_x, soot, and SO₂ are derived [851].
- ⁵ 10% fuel consumption during the LTO phase is assumed according to [501,870]
- ⁶ 3% fuel consumption during the LTO phase is applied from ecoinvent 3.8: transport, passenger aircraft, long-haul (>4,000 km) {GLO}.

Acronyms: Characterization factors (CFs); Landing & Take-off (LTO) flight phase; Climb, Cruise & Descent (CCD) flight phase

6. Supplementary tables: Characterization factors (CFs) for the GWP and GTP metrics

The available characterization factors (CFs) are gathered and listed in Tables S3.5-S3.6. Some (GWP₁₀₀) apply to aviation tailpipe emissions (from the previous section). However, they are not limited to use with the other approaches, depending on the choice of practitioners.

Table S3.5 Characterization factors (CFs) derived from the global warming potential (GWP) metric of aviation pollutants. The aviation NO_x and sulfate aerosol are given in terms of N and SO₂, respectively.

Climate forcers	Applied flight phase		GWP [kg CO ₂ -eq kg ⁻¹ forcer] for different time horizons (years)				References
	LTO	CCD	20	50	100	500	
Well-mixed greenhouse gases (GHGs)							
Carbon monoxide (CO)	/		5.90	3.20	1.90		[851]
Methane (CH ₄), fossil	/		82.50		29.80	10.00	[853]
Methane (CH ₄), non-fossil	/		79.70		27.00	7.20	[853]
Dinitrogen oxide (N ₂ O)	/		273.00		273.00	130.00	[853]
Other aviation forcers							
Carbon monoxide (CO)	/		5.90	3.20	1.90		[851]

Non-methane volatile organic compounds (NMVOC)	/			3.40		[835]
Unspecified NO _x	/ ^d	16.70	-15.60	-10.80		[851]
Aviation NO _x ^b		410.00		6.90	2.00	[832] ^a
		177.00		2.70	0.80	[916]
		415.00		75.00	23.00	[917]
	d /	247.50		34.50	10.50	[855]
		322.00		59.00	17.00	[918]
		411.00		77.00		[717]
		619.00	205.00	114.00		[715]
Aviation induced cloudiness (AIC) (including contrail and cirrus clouds)	d /	2.94		0.84	0.25	[832] ^a
		3.10		0.84		[717]
		2.32	1.09	0.63		[715]
Water vapour	d /	0.49		0.14		[836]
		0.22	0.10	0.06		[715]
Unspecified soot ^c	/ ^d	2177.00	1024.40	592.20		[851]
Aviation aerosol (soot) ^c		1600.00		460.00		[836]
	d /	3628.00		983.00		[717]
		4288.00	2019.00	1166.00		[715]
Unspecified (source) SO ₂	/ ^d	-141.10	-66.40	-38.40		[851]
Aviation aerosol (SO ₂) ^c		-140.00		-40.00		[836]
	d /	-559.00		-152.00		[717]
		-832.00	-392.00	-226.00		[715]

Notes:

^a The median value of each GWP is presented if the upper, median and lower values have been reported [832].

^b The net NO_x was derived from short-lived O₃, long-lived O₃, and methane-induced O₃ [855]. Emissions of NO_x are given in terms of NO₂, including the conversion of NO to NO₂ [831].

^c Soot is a mixture of organic carbons and black carbon [715,717].

^d The emissions generated at the upper troposphere and lower stratosphere (UTLS) can also have impacted the LTO phase. This is because of downward circulation into the troposphere (only at mid and high latitudes) [836]. However, the LTO emissions are not specified which CFs should be used. Therefore, we analyzed the comparative approaches by using either the similar CFs (in the CCD phase; see method 1; M1) or CFs of NO_x, soot, and SO₂ from unspecified (anthropogenic activities) in method 2 (M2).

^e The emission of aviation aerosols (sulfate) is given in terms of SO₂ as emitted initially from fuel combustion, which is further oxidized to sulfate (SO₄²⁻) [715].

To ensure tractability, figures are expressed with a maximum of three significant digits. This, however, is not to be seen as an indication of precision.

Table S3.6 Characterization factors (CFs) derived from the global temperature change potential (GTP) metric of aviation pollutants. The aviation NO_x and sulfate aerosol are given in terms of N and SO₂, respectively.

Climate forcors	Applied flight phase	GTP [kg CO ₂ -eq kg ⁻¹ forcer] for different time horizons (years)				References
		20	50	100	500	
Well-mixed greenhouse gases (GHGs)						
Methane (CH ₄), fossil	/		13.20	7.50		[853]
Methane (CH ₄), non-fossil	/		10.40	4.70		[853]
Dinitrogen oxide (N ₂ O)	/		290.00	233.00		[853]
Aviation tailpipe pollutants						
Carbon monoxide (CO)	/ /	3.70	0.70	0.30		[851]
Unspecified (source) NO _x	/ ^d	-86.30	-27.40	-2.80		[851]
Aviation NO _x ^b	d /	-240.00	-60.00	-2.20		[832] ^a
		-292.00	-79.00	-4.10		[916]

			-239.00	-56.00	8.60	[917]
			-138.00		9.00	[717]
			-222.00	-69.00	13.00	[715]
Aviation induced cloudiness (AIC) (including contrail and cirrus clouds)	d	/	0.74		0.21	0.06 [919]
			0.93		0.12	[717]
			0.67	0.11	0.09	[715]
Water vapour	d	/	3.15	0.49	0.40	[832] ^a
Unspecified (source) soot ^c	/ ^d		631.90	98.90	81.60	[851]
Aviation aerosol (soot) ^c	d	/	1140.00		147.00	[717]
			1245.00	195.00	161.00	[715]
Unspecified (source) SO ₂	/ ^d		-40.90	-11.10	-9.10	[851]
Aviation aerosol (SO ₂) ^e	d	/	-162.00		-21.00	[717]
			-241.00	-38.00	-31.00	[715]

Notes:

^a The median value of each GWP is presented if the upper, median and lower values have been reported [832].

^b The net NO_x was derived from short-lived O₃, long-lived O₃, and methane-induced O₃ [855]. Emissions of NO_x are given in terms of NO₂, including the conversion of NO to NO₂ [831].

^c Soot is a mixture of organic and black carbons [715,717].

^d The emissions generated at the upper troposphere and lower stratosphere (UTLS) can also have impacted the LTO phase. This is because of downward circulation into the troposphere (only at mid and high latitudes) [836]. However, the LTO emissions are not specified which CFs should be used. Therefore, we analyzed the comparative approaches by using either the similar CFs (in the CCD phase; see method 1; M1) or CFs of NO_x, soot, and SO₂ from unspecified (anthropogenic activities) in method 2 (M2).

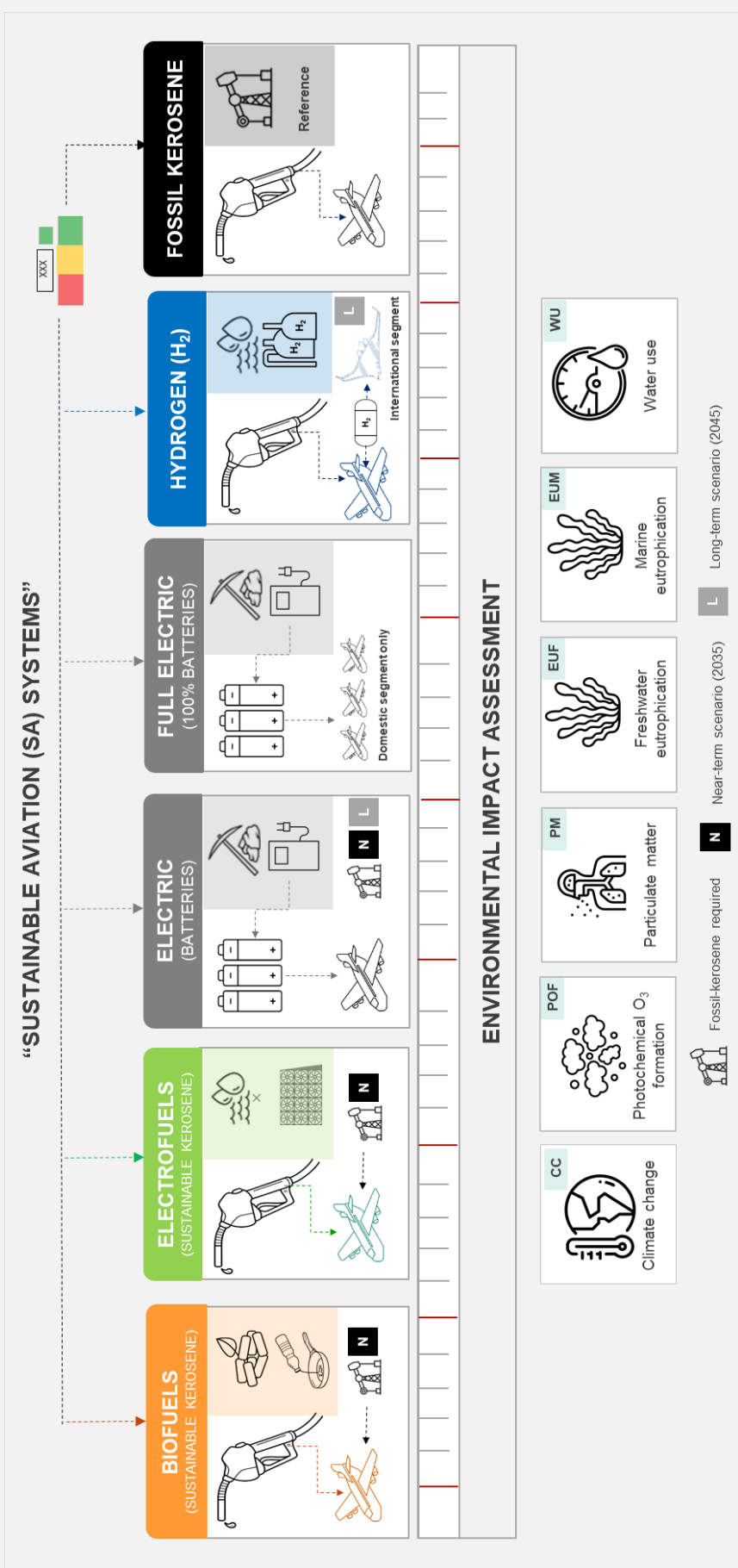
^e The emission of aviation aerosols (sulfate) is given in terms of SO₂ as emitted initially from the fuel combustion, which is further oxidized to sulfate (SO₄²⁻) [715].

To ensure tractability, figures are expressed with a maximum of three significant digits. This, however, is not to be seen as an indication of precision.

4

Uncovering the environmental performances of emerging candidates for Sustainable Aviation





ABSTRACT

Biofuels, Electrofuels, Electric (batteries), and hydrogen are key Sustainable Aviation (SA) systems to mitigate the environmental impacts of aviation. Here, the environmental performance of the most promising alternatives for each of these systems was compared and quantified through consequential Life Cycle Assessment (LCA) and takes into account issues of hybridization requirements, mass penalty, and the impacts of non-CO₂ tailpipe emissions. Two-time scopes, namely 2035 and 2045, are considered, in which different technological advancements are hypothesized. Results revealed the biomass gasification and the Fischer-Tropsch (FT) biofuel systems as the most promising approaches, specifically in the climate change and particulate matter impacts. This was true for both time scopes, for both domestic and international segments. Full electric systems were also shown to have relatively small impacts for most categories, though these only apply to the domestic segment. Electricity for H₂ production is a key driver in electrofuels and H₂ systems. In comparison, H₂ systems benefit from their non-carbon tailpipe emissions (H₂O and/or NO_x).

Keywords: Electric (batteries), Hydrogen, Life Cycle Assessment (LCA); Sustainable Aviation Fuels (SAF)

4.1 Introduction

Aviation was globally responsible for approximately 920 Mt CO₂ emissions in 2019 [1], ca. 88% generated by commercial aviation (whether passengers or cargo carrying) [13]. This amount represents 2.5% of CO₂ derived from anthropogenic activities [2]. The terminology Sustainable Aviation (SA) is used in this manuscript to designate aviation systems based on four emerging energy sources to mitigate the environmental impacts of commercial aviation. The focus is on four systems: i) Biofuels, ii) Electrofuels, iii) Electric (batteries), and iv) H₂ (Fig. 4.1).

One of the most feasible solutions launched is the employment of Sustainable Aviation Fuels (SAF) as defined in, e.g., the European ReFuelEU initiative [18], or the global CORSIA scheme [78]. SAF are drop-in fuels with identical and replaceable characteristics to the conventional (fossil) kerosene [920], commonly referred to as Jet A-1 or Jet A [30]. This comforts their advantages owing to their compatibility with the existing infrastructures (e.g., fuel storage facilities) and the few modifications required for the aircraft. Six SAF production technologies have complied with the American Society of Testing and Material (ASTM) International D7566 [733] for use in commercial aviation. However, the sustainability of their feedstocks must be scrutinized to ensure their environmental benefits. The eligible feedstocks are mentioned in the European Recast Renewable Energy Directive (RED II) [19] (considered in this study), or in the US Renewable Fuel Standard (RFS) [921]. The terms “biofuel” and “electrofuel” represent both kerosene type fuels, belonging to SAF, derived from different feedstock origins: i) biofuels are produced from bio-based materials in agreement with RED II; ii) electrofuels (equivalent to power-to-liquid) are synthetic kerosene produced from carbon and H₂ sources like industrial off-gas/air and water, respectively. In these processes, the (alkaline) electrolysis was found to be significant the most significant impact contributor when compared to the direct air capture (DAC) and other processes in general despite the use of renewable electricity sources [207,922]. Fischer-Tropsch (FT) and methanol synthesis are two relevant electrofuel production pathways; however, only the former has been approved [18].

iii) Batteries are another promising energy source (reaching zero tailpipe emissions); however, this seems harder to happen relative to terrestrial mobility because of the mass penalties induced on the aircraft. Moreover, albeit developed, the (current) lithium batteries representing 300-400 Wh kg⁻¹ cell [57] cannot compete with fossil kerosene (approx. 12,000 Wh kg⁻¹ cell [30]), particularly for the aeroplanes covered by, e.g., the European Certification Specification 25; CS-25, in which hybridization systems (for both energy source and propulsion) are needed [64]. Nevertheless, the full-electric (smaller) aircraft, namely the Eviation Alice [385] and the Heart Aerospace ES-19 [923], are expected to be certified, e.g., under the European CS-23 or the US Federal Aviation Administration's (FAA) Part 23.

iv) Another non-CO₂-based fuel is hydrogen (H₂), with its superior energy density (120 MJ kg⁻¹ [66], almost three times those of fossil kerosene). Water electrolysis is a promising technology for H₂ production when renewable energy sources (such as wind and solar) are used, as this is an energy-intensive process ranging from 0.39-0.48 kWh MJ⁻¹ of H₂ produced [225,740,742,765,924,925] according to the technology used. This represents 13-16 times the energy needed for fossil kerosene production (~0.03 kWh MJ⁻¹ fuel produced [14,334]). In addition, hydrogen aviation requires novel infrastructures and aircraft models to be developed. The aircraft can potentially operate with the fuel cell (electric) [393,394], combustion [323,324], or hybridization mode, as proposed in the Airbus ZEROe project [772].

Although relevant, other emerging systems based on ammonia (NH₃) [351–353], liquefied petroleum gas (LNG) [926], and direct use of alcohols (e.g., methanol [371], ethanol [373]) are not included in this work either due to resource limitation or public data accessibility. However, further descriptions for those systems can be retrieved in **Chapter 2**.

However, the sustainability of the emerging systems still needs to be proven, and, in this sense, Life Cycle Assessment (LCA) could be used to evaluate a panel of environmental impacts and compare the systems from the environmental point of view [927,928].

Regarding the literature, the existent available studies do not allow a fair comparison of the environmental performances of different technical solutions due to methodological differences, as previously demonstrated in **Chapter 3**. Moreover, some critical issues, like i) non-CO₂ tailpipe emissions, ii) SAF blending mandate, and iii)

mass penalty consideration in electric (batterie) and H₂ aviation systems, are not entirely included in the published aviation LCA studies [336,489,929]. Therefore, the established LCA framework is further applied to bridge existing gaps and quantify and compare the environmental consequences of implementing the emerging aviation systems (see Chapter 3).

The scope covers commercial aviation with a passenger carrying capacity of at least 19 passengers. Cradle-to-Grave approach is considered, from feedstock/materials origin, aircraft operation, to end-of-life (EoL) management (Figs. 4.1 and 4.2). The functional unit is the projected revenue passenger kilometres (RPK) applied for near- and long-term and domestic and international flights. The system expansion approach is applied to handle the multifunctionality of the co-product generations [927,928]. France is set as the representative geographical scope implying the use of its electricity mix for fuel production and battery manufacturing. Further details can be found in the methods section.

4.2 Methods

4.2.1 Selected SA systems

The selection of the most promising SA systems within each of the four categories was conducted with a semi-quantitative prioritization matrix established for two timescales, i.e., near-term future (2035) and long-term future (2045) (details in Chapter 2). These time scopes were judged representative to reflect the time elapsed between two generations of technologies to be implemented [332]. This matrix proposes three key criteria: technology status, market prospects, and environmental aspects. Fourteen biofuels (from land-use dependent and independent feedstock), nine possible approaches for electrofuels (with different DAC and liquid fuel production processes), five lithium-based batteries, and five water-splitting technologies for H₂ production have been scored.

The selected SA systems and the technological specificities are presented in Fig. 4.1 and summarized in Table 4.1. Further details can be retrieved in Chapter 2.

Table 4.1 Summarized key processes for fuel production and battery manufacturing

Systems	Technology (Feedstocks)	Description
Biofuels	HEFA (Waste cooking oils; WCO)	In Fig. 4.2a, WCO is applied as biofuel's feedstock rather than fuel for heat production in which induced heat is needed (depending upon the assessed time scopes). To do this, the WCO is first transferred to the pretreatment stage, where the food particles and suspended solid matter are filtered, and oils are further dewatered through the commercial boiler [930–932]. Subsequently, water degumming is conducted to remove phospholipids (gums) as they can interfere with the activity of hydrotreatment catalysts [933]. Next, centrifugation separates gums from purified oils fraction [934]. Gums herein are considered to be potentially replaced with the marginal lipid source (palm oil). Then, the purified oils (triglycerides-rich fractions) are converted to paraffinic compounds through three primary reactions: hydrogenation, propane cleavage and hydroprocessing. The operation conditions are 300–400°C and 30–100 bar in the presence of Pt/Al ₂ O ₃ , NiMo/Al ₂ O ₃ [652,654,935]. Finally, the paraffinic compounds perform hydrocracking and isomerization to improve fuel quality at 355°C and 40 bar [654,655,936]. Renewable propane, naphtha, and diesel are co-products considered to replace the production of fossil-based fuels. Detailed Life cycle inventory (LCI) can be retrieved in the SM 4.2 LCI folder.
	FT (Primary forestry residues; PFR)	PFR is used for fuel production instead of leaving it on the ground (in Fig. S4.2). For the FT system, the PFR is primarily shredded and dried before feeding to the gasification process. This pretreatment is required to improve the gasification's energy efficiency and producer gas quality [132]. The operating gasification has been considered 800–900°C the most commonly applied for biomass feedstock [937–939]. Regarding the economically feasible and readily available, the air is used as the oxidizing agent [132]. Recovered heat and char are co-products to be avoided heat production and natural gravel (construction materials), respectively. The producer gas is conditioned via the catalytic

		<p>reforming process, 800°C 25 bar, to improve the H₂/CO ratio (by volume) of 2.0 [150]. The reformed gas is cleaned using pressure swing adsorption (PSA) to remove CO₂ and H₂S before feeding in the FT reactor. The clean syngas is converted to paraffinic compounds at 200-230°C, 20-30 bar in the presence of a catalyst (typically cobalt, iron) [150,940,941]. Gasoline, propane, naphtha, and wax can avoid generating conventional products. While the fuel gas (mainly ethane) is considered internally burned for heat production. This is further avoided the external heat demands. Further detailed LCI can be found in the SM 4.2 LCI folder.</p>
	<p>Ethanol-to-Jet, via syngas fermentation (Primary forestry residues; PFR)</p>	<p>As shown in Fig. S4.3, PFR is converted to cleaned syngas, similar to the FT system, as explained above. However, the conditioning and cleaning stages are required to sufficiently remove fermentation inhibitors (e.g., sulfur), ensuring constant ethanol production [942,943]. The ethanol (as the main product) is obtained from the proprietary microbes operating at ambient temperatures. In addition, the 2,3-butanediol is generated alongside ethanol [738], potentially replacing fossil-based butanediol production. Ethanol is further recovered from the broth using the distillation unit. Finally, they are upgraded into kerosene through a series of reactions, including dehydration, oligomerization, and hydrogenation. During this stage, diesel is generated as a co-product [738,944,945]; a further explanation is in the SM 4.2 LCI folder.</p>
	<p>Isobutanol-to-Jet, via direct conventional sugar fermentation (Primary forestry residues; PFR)</p>	<p>In the isobutanol-to-jet system (Fig. S4.4), the PFR is first chopped into an appropriate size (e.g., 20-100 mm) to increase its surface area. Then, chopped biomass is further treated with the sulfite pretreatment to overcome the recalcitrance lignocellulose (SPORL) process with calcium bisulfite and sulfuric acid (140-190°C for 30-45 min) [489,946]. This method is chosen as it potentially recovers biomass carbohydrate fractions (such as cellulose and hemicellulose) for biofuel precursor productions [947]. Two stream outputs are generated: pretreated pulp and spent sulfite liquor, separated by filtration. The spent sulfite liquor is further filtrated to recover the lignosulfonate [948,949] and used as the water-reducing material. It can further avoid the production of naphthalene sulfonate production. The pretreated pulp is hydrolyzed over cellulase and hemicellulase complex to generate hydrolysate streams (consisting of xylose and glucose). The solid (lignin) and hydrolysate fractions are separated by centrifugation [947]. Lignin is considered a solid fuel for heat production [947,950,951], in which external heat production is avoided. The hydrolyzed sugars are sent to the fermentor in the presence of modified yeast (operating at 33°C [278]) for isobutanol production. Isobutanol is recovered through distillation, while the microbial sludge fractions are further applied as high-protein animal feed after evaporation [952]. It is replaced with marginal feed sourcing (carbohydrate: maize, protein: soy meal, and lipid: palm oil). Dehydration, oligomerization, and hydrogenation are applied to upgrade isobutanol to kerosene with isooctane as a co-product [945,950,953], potentially replacing fossil-based gasoline production. Detail LCI can be found in the SM 4.2 LCI folder.</p>
<p style="writing-mode: vertical-rl; transform: rotate(180deg);">Electrofuels</p>	<p>Liquid sorbent (H₂O and CO₂)</p>	<p>For electrofuels production (Fig. 4.2b), alkaline water electricity is considered the hydrogen production technology for fossil fuel independence. It is operated at ambient pressure, 60-90°C [765].</p> <p>CO₂ from the atmosphere is considered as the carbon source through liquid or solid sorbent technologies. The liquid sorbent is modelled based on Carbon Engineering Inc. Technology [736,954]. The hydroxide solution (e.g., KOH, Ca(OH)₂) is used as the sorbent with the required high temperature for their regeneration (at 800-880°C for CaCO₃ calcination for Ca(OH)₂ recovery). H₂ produced and CO₂ captured are further compressed at 20-30 bar to facilitate the downstream processes, including syngas production and the FT processes [207,922,955]. They are transferred to the syngas production phase (through the reverse water gas shift reaction [207]) to adjust H₂/CO of 2.0 before feeding to the FT reactor. The clean syngas is converted to paraffinic compounds at 200-230°C, 20-30 bar in the presence of a catalyst (typically cobalt, iron)</p>

		[150,940,941]. Gasoline, propane, naphtha, and wax can avoid generating conventional products. While the fuel gas (mainly ethane) is considered internally burned for heat production. This is further avoided the external heat demands. Further detailed LCI can be found in the SM 4.2 LCI folder.
	Solid sorbent (H ₂ O and CO ₂)	In this system, the solid sorbent is applied to capture CO ₂ . Herein, the amine-modified solid sorbents are used as adsorbents comprising the N-(2-aminoethyl)-3-aminopropyltrimethoxysilane as the active phase grafted on the silica gel bead/alumina (2-5 mm diameter). However, polyethyleneimine (PEI) production is used as a proxy amine instead of the N-(2-aminoethyl)-3-aminopropyltrimethoxysilane as there is no available data [737,956]. Moreover, the sorbent regeneration occurs at 80-100°C, which could be available as waste heat from some industrial plants [957,958]. As explained above, the other processes are carried out similarly to the liquid sorbent system.
Batteries	Current Li-ion (CB)	Lithium-ion batteries work with the intercalation process, in which lithium ions are reversibly incorporated into the structure of the electrode materials, such as graphite [308,959]. Therefore, different electrode materials have influences on the overall Li-ion cell capacity. For the current Li-ion batteries, in this analysis, lithium manganese oxide (LiMn ₂ O ₄) and graphite serve as the active cathode (+) and anode (-), respectively [58,960]. The expected energy density of 400 Wh kg ⁻¹ cell is considered [57,64]. Further details for the manufacturing process can be found in the SM 4.2 LCI folder.
	Advanced. Li-ion (AB)	Nickel-Manganese-Cobalt (NMC811) is served as the active cathode side [57,961,962], while silicon-coated graphite is applied for the anode side [963]. 500 Wh kg ⁻¹ cell is considered [57]. Further details can be found in the SM 4.2 LCI folder.
	Lithium-sulfur (LS)	Unlike the Li-ion battery mechanism, the operation of the Li-S battery is based on multiple redox reactions between elemental sulfur (S ₈) and lithium metals as cathode and anode active compounds [58,289,290,960], respectively. The cell energy density of 900 Wh kg ⁻¹ is considered [64,964]. However, the formation of dissoluble polysulfide (Li ₂ S ₂ and Li ₂ S) results in the reduction of active sulfur materials leading to a short cycle life [965,966]. Further details on the manufacturing stage can be found in the SM 4.2 LCI folder.
	Lithium-air (LA)	Lithium-air battery works based on the oxidation of lithium at the anode and the reduction of oxygen (commonly from the air) at the cathode electrode. Graphite is used as the mesoporous material to facilitate the airflow at the cathode site [967]. On the one hand, the pore size and volume should be maximized to accommodate a large amount of discharge product, Li ₂ O ₂ [290,968]. On the other hand, it should not be too large, which may further inhibit recharging. Air electrodes with high porosity and electrical conductivity are crucial for achieving a high energy density of Li-air batteries [290,960,968]. While lithium metals are applied as active anode material [960,967]. 1,300 Wh kg ⁻¹ cell is considered [57,64,967]. Further details can be found in the SM 4.2 LCI folder.
Hydrogen	Alkaline electrolysis (Al) (H ₂ O)	Alkaline water electrolysis is operated at 60-90°C, 1-30 bar [765]. Hydroxide solution is served as an electrolyte [969]. Furthermore, it is considered that approx. 40% of heat can be recovered and avoided external heat production [970,971]. The gaseous hydrogen is further transferred to the liquefaction plant. Herein, it is assumed that the H ₂ production plant and liquefaction plant are nearby (on-site production). Therefore, the boil-off rate is less concerned as the re-liquefaction could be applied to recover lost H ₂ [972,973]. Detail can be retrieved in the SM 4.2 LCI folder.
	PEM electrolysis (PEM) (H ₂ O)	Proton exchange membrane (PEM) is used solid electrolyte operating at 50-80°C, 20-50 bar [765]. As a result, 40% of the heat generated is considered to be recovered and further avoided heat production [970,971]. In addition, the produced H ₂ is further transferred to the liquefaction process. Detail can be retrieved in the SM 4.2 LCI folder.

Acronyms: PEM: Proton/Polymer exchange membrane; PFR: Primary forestry residues; WCO: Waste cooking oils

Adapted propulsion systems were considered corresponding to the energy source: i) the combustion propulsion systems, where the propellers are driven by mechanical forces generated from fuel combustions in biofuels, electrofuels, H₂-combustion, ii) electric propulsions in case of full electric (100% batteries) and H₂ fuel cell scenarios, iii) hybrid mode in which the combustion ((fossil) kerosene) and electric systems are integrated. A maximum 50% blending quota for biofuels/electrofuels was considered in the near term based on safety standards (e.g., ASTM D7566 [733]), while blending was phased out in the long term. Furthermore, mass penalty issues (e.g., battery packs, H₂ storage tanks) are taken into consideration when the new (fuel) systems are studied, implying that fewer passengers can be carried in a plane relative to the (conventional) kerosene systems. End-of-Life management of aircraft and batteries is also considered. Further descriptions can be retrieved in **Chapter 3**.

4.2.2 Life cycle assessment

The displacement multifunctionality approach and the marginal data were implemented in line with ISO 14040/44 to track the potential environmental impacts of the emerging SA systems [974,975].

The chosen functional unit is “the aviation service per time scope and segment,” with globally projected revenue passenger kilometre (RPK) as a metric. In a nutshell, this unit is expressed in boarded passenger kilometres and reflects the number of passengers carried on the number of kilometres travelled [976]. The years 2035 and 2045 were considered two perspective time scopes for near- and long-term scenarios, respectively, with two service segments of domestic and international travel. The number of projected RPKs was retrieved from the ICAO forecasting air demands [458]. Four projected RPKs were thus defined: i) near-term domestic to supply 6 trillion (ND), ii) near-term international for 9 trillion (NI), iii) 8 trillion for long-term domestic (LD), and iv) 14 trillion RPK for long-term international (LI). These functional service units were subsequently translated to the amount of energy required to reach the defined RPKs (details in **Chapter 3**).

LCA was applied with the SimaPro software and the background data from the ecoinvent version 3.8 consequential database [14]. The biofuels, electrofuels, and H₂ production systems (foreground processes) were set in France, which mainly determined the marginal heat and electricity mix (the same mix is considered for both time scopes) consisting of 84% wind power and 13% biomass (wood) combustion [14], whether in the conversion or aircraft operation phase. The background data were primarily selected within the European scope if they existed for the required inputs. The French scope also applies to battery manufacturing; however, the raw materials (e.g., lithium, cobalt, natural graphite) [977] are imported depending on the geographical context. The global trading systems are applied in the context of the co-products to be avoided/substituted for both time scopes, particularly for fossil-based fuels (e.g., naphtha, propane, diesel, gasoline) to minimize the dependency on those products from the fossil-fuel exporting countries. The consequences of using constrained resources, namely waste cooking oil (WCO) and primary forestry residue (PFR), have been investigated, encompassing their avoided/induced associated effects. The LCI was derived from literature, scientific reports, company reports, and patents, as demonstrated in SM 4.2 and LCI folder.

Environmental impacts were calculated using the Environmental Footprint (EF) 3.0 method; six (out of) sixteen impacts are presented in this study. Climate change with a horizon time of 100 years (CC) was considered due to the climate urgency [978] in aviation, with particular attention paid to the tailpipe emissions as addressed in the “Climate change impact calculation for aviation tailpipe emissions” section. It should be noted that biogenic carbon accounted for zero in CC according to the EF LCIA method. Negative emissions are only considered when a process is avoided, but not for absorbed biogenic carbon nor captured atmospheric carbon. Photochemical ozone formation POF (due to CH₄, CO, non-methane volatile organic compounds (NMVOC)) and particulate matter PM (soot, NO_x, SO₂) impacts are considered to analyze owing to their associated substances from tailpipe emissions. Eutrophication due to nitrogen (in marine ecosystems, EUM) and phosphorus (in freshwater, EUF) emissions were analyzed, being identified as vulnerable planetary boundaries [364]. Water scarcity (WS) impact was also selected because of the critical feedstock for H₂ production, liquefaction, and DAC sorbent regeneration.

4.2.3 System boundaries

The life cycle system boundaries include all processes from raw materials acquisition to production processes and end-of-life of the assets (cradle-to-grave approach), including the utilities, waste management, and direct emissions associated with each life cycle stage (Figs. 4.1 and 4.2). The generic SA systems are illustrated in Fig. 4.2 (FT,

ethanol-to-jet, and isobutanol-to-jet can be found in SM 4.1) and are classified into ten categories of processes: Fuel production and battery manufacturing are categorized in green. The counterfactual use processes are displayed in blue. Blending mandate (near-term) and mass penalty are included whether in aircraft operation (red) or aircraft manufacturing (grey). If fossil kerosene is needed, the yellow box is indicated. Additional required infrastructures for the cases of electric (batteries) and H₂ systems are shown in white. End-of-Life management processes (aircraft and/or batteries) are presented in a black box. The avoided processes are shown in dotted boxes; heat (green), product/service (blue), and virgin metal production (red).

Key different elements between near- and long-term scopes (Fig. 4.1) are i) the number of projected RPK, ii) the decreasing fuel consumptions with the improved overall propulsion efficiency (OPE; details in the SM 4.2 LCI folder), iii) different conversion processes for the biofuels and batteries production Fig. 4.1, iv) the 100% use of biofuels/electrofuels in the long-term instead of the limited blending quota for the near-term scenarios; v) the novel design of blended wing body (BWB) for the H₂ aircraft for the international haul according to the ZEROe Airbus project [772]; vi) the natural gas and electricity were selected as the main source for heat production in the near- and long-term scenarios, respectively.

Concerning the heat sources, the range of temperatures needed was a criterion for choosing the heating source (either fuel-based or electricity-based) and the related technology (though they are expressed equally in terms of MJ as available inecoinvent). Therefore, two delivery ranges of temperature were defined: the low-temperature range (LH: <100°C with a recovery efficiency of 50-85% [970,971]) and the high-temperature range (HT: >100°C with a recovery efficiency of 35-50% [979,980]), which also complies with the European Union regulation. Natural gas was considered a fossil fuel for heat in the near term because it can provide a wide range of delivery temperatures compatible with all consumer processes and is already established through grid distribution. However, fossil-based fuels will be gradually phased out, including hard-to-decarbonize industries and transport (expected to be powered mainly by renewable hydrogen) [981]. This is performed by using renewable sources of electricity, as demonstrated by the foreseen investments in low-carbon technologies such as solar (thermal) power and wind farms [981]. Therefore, low-carbon heat derived from (renewable) electricity is considered in the long-term scope: i) the heat pump was selected to provide LH as an up-and-coming technology [982–984], ii) the electric furnaces/boilers were considered for the production of HT (necessary in, e.g., steam reforming and metal smelting), with delivery temperatures up to 2,000°C (according to type, design, and more [984,985]). Additional details about the heat use assumptions can be found in SM 4.1.

Hydrogen is another important flow used as a material or energy source, owing to its ability to replace fossil-based sources and to be scaled sufficiently [215]. Hydrogen from alkaline electrolysis of water was assumed to supply biofuel production. Other water electrolysis technologies were tested only in the case of H₂ SA systems (hydrogen as fuel).

4.2.4 Climate change impact calculation for aviation tailpipe emissions

The tailpipe emissions of conventional kerosene aviation, considered climate forcers, include well-mixed greenhouse gases, namely CO₂, methane (CH₄), dinitrogen oxide (N₂O), indirect forcers including nitrogen oxides (NO_x), carbon monoxide (CO), non-methane volatile organic compounds (NMVOC), and other specific aviation emissions, i.e., aviation-induced cloudiness (AIC) referred to as contrail and cirrus cloud formations, high altitude water vapour (H₂O), soot and sulfur dioxide (SO₂) [870]. H₂O is considered the only emission from the H₂ fuel cell, while NO_x is the additional pollutant when H₂ is combusted.

Global Warming Potential with 100 years time horizon (GWP₁₀₀) was used as a metric for climate change impact. The EF LCIA applied here was adjusted by i) the updated characterization factors (GWP₁₀₀) from the IPCC AR6 (details in the SM 4.2 LCI folder) and ii) the inclusion of the GWP₁₀₀ of non-CO₂ emissions listed above. The CC impact (in kg CO₂ equivalent) was calculated by multiplication of GWP₁₀₀ (kg CO₂eq. per kg pollutant) with the emission factors (EF; g pollutant per kg fuel used). The GWP₁₀₀ of five non-CO₂ pollutants (NO_x, AIC, water vapour, soot, and SO₂) was retrieved from Lee et al. (2021) [354], the most updated study in the field. The EFs of each system are extracted from the available literature (SM 4.2 LCI folder).

The selected GWP₁₀₀ and EF values were considered to apply for both LTO (Landing and Taking off phase) and CCD (Climb, Cruise, and Descent) flight phases, irrespective of the time scopes. Therefore, the averaged EFs derived from the averaged data for each flight phase were employed (see SM 4.2 LCI folder).

4.2.5 Uncertainty analysis

Global sensitivity analysis was performed according to the procedure introduced in the study of Bisinella et al. (2016) [986]. This includes contribution analysis (step 0), perturbation analysis (step 1), and uncertainty propagation (step 2). In the contribution analysis, detailed in the LCIA folder (SM 4.2), the parameters contributing at least 3% to the impact result were investigated and subsequently selected if their contribution affected 5 out of the 16 categories. Next, the list of influent parameters for each scenario within near- and long-term scopes was addressed (details in SM 4.2 GSA folder). The influence of parameters was investigated by changing them one at a time (OAT) in the first step of the analysis, the variation being fixed within the initial value and its -10%. The sensitivity ratio was subsequently calculated for each parameter on the LCA results. Two additional factors are required for the uncertainty analysis (step 2): sensitivity coefficient and standard deviation. The first can be obtained by dividing the change of the results and the change of the parameter value, while a probability distribution of data was defined to obtain the standard deviation.

4.2.6 Sensitivity analysis

This sensitivity analysis was conducted on modelling hypotheses by changing processes within the system's boundaries, as indicated in the SM 4.2 SA folder. The concerned processes are i) the use of WCO for the biodiesel production instead of heat production for the HEFA scenario; ii) the oxygen recovered as the valuable co-product for all hydrogen (H₂) required scenarios; iii) the substitution of the French marginal electricity mix (as the default provider) by the United State (US) and China electricity mix as the source variation with the geographical scope was reported as one of the most influential parameters [68,69,737,987]; iv) the co-products use in long-term including propane (as a refrigerant) [988], naphtha (as a solvent) [989], fuel sources for diesel and gasoline (e.g., for heat and electricity productions); v) the heat source assumption in different time scopes. As a result, the heat sources for near- and long-term scopes differed. On the one hand, the district natural gas production process {Europe without Switzerland} (background data from the ecoinvent) was considered to be replaced with the market process as mainly derived from the co-generation plants in the European Union. On the other hand, the electrified heat was supposed to be substituted by the solar thermal system in the long run, which shows an increased installed capacity worldwide [990]. This was assumed because the geographical scope meets the requirements of solar radiation (e.g., low altitude and dry climate). Therefore, the existent ecoinvent process for heat production from the flat plate collector was selected as it can provide the requested temperature (<100°C [991]). In comparison, concentrated solar power (CSP) was selected to provide high-temperature heat as it can ensure sufficient high temperatures for most industrial processes due to the thermal energy storage equipment [985,992]. Finally, (vi) the choice of excluding the non-CO₂ tailpipe emissions (in the flight phase) in CC impact calculation was investigated versus including these aviation-specific climate forcers.

4.3 Results

Environmental performances of the SA systems are presented by time scope and for the considered service segments. The applied system boundaries are displayed in Figs. 4.1 and 4.2. The LCA results for six impacts (climate change; CC, photochemical O₃ formation; POF, particulate matter; PM, freshwater eutrophication; EUF, marine eutrophication; EUM, and water scarcity; WS) are presented in Fig 4.3 for the domestic segment and in Fig. S4.5 for the international segment, expressed in impact units per functional unit. Fossil kerosene aviation is considered the reference system for comparison. Primary forestry residue (PFR) is considered the biofuel feedstock for biomass gasification and the Fischer-Tropsch (FT), ethanol-to-jet (near-term), and isobutanol-to-jet (long-term). The waste cooking oil (WCO) is used as the feedstock for the hydroprocessed esters and fatty acids (HEFA) process.

In Figs. 4.3 and S4.5, the negative results mean avoided impacts (environmental benefits), while the positive results are induced impacts. Net results are displayed by the triangle symbol, while the dotted lines indicate the impact of fossil kerosene.

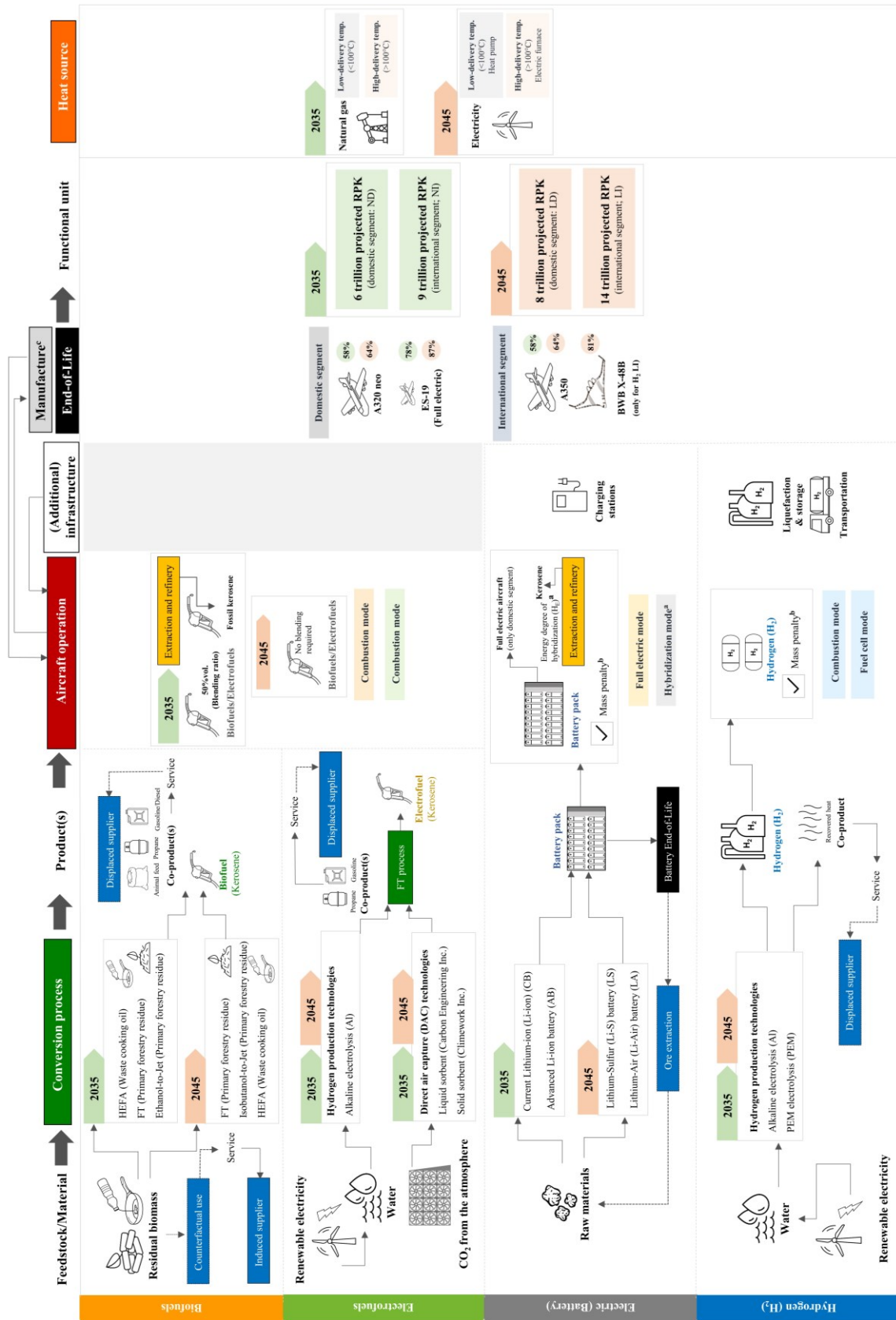


Fig. 4.1 System boundaries considered in this analysis for four SA systems: Biofuels, Electrofuels, Electric (Batteries) and Hydrogen (H₂)

Fig. 4.1 (continued) Near-term (2035) and long-term (2045) time scopes are represented in the light green and light orange, respectively. Seven color codes indicate (yellow) fossil kerosene production, (green) conversion system corresponding to the type of energy source, (blue) counterfactual & displacement, (grey) manufacture of the aircraft, (red) aircraft operation whether in the modes of combustion, hybridization (battery and fossil kerosene), full electric

battery, or hydrogen fuel cell, (white) other (additional) infrastructure required, and (black) end-of-life management whether recycling or any other uses. The dotted line indicates the substituted/avoided services/products of the origin. Natural gas and electricity are applied as the source of heat production for the near- and long-term scopes, respectively. Electrified heat derived from the heat pump and the electric furnace are considered in this analysis.

Notes.

^a Hybridization mode is referred to as the hybrid propulsion system that combines combustion (from (fossil) kerosene combustion) and electric (from batteries) schemes.

^b Mass penalty indicates that less passengers can be carried in a plane compared to the (conventional) kerosene system due to the additional masses (e.g., battery packs, H₂ on-board storage tanks).

^c Overall propulsion systems (OPE) are considered to be improved from near- to long-term scopes, as represented in the circles near the type of corresponding aircraft (detailed in the SM 4.2 LCI folder).

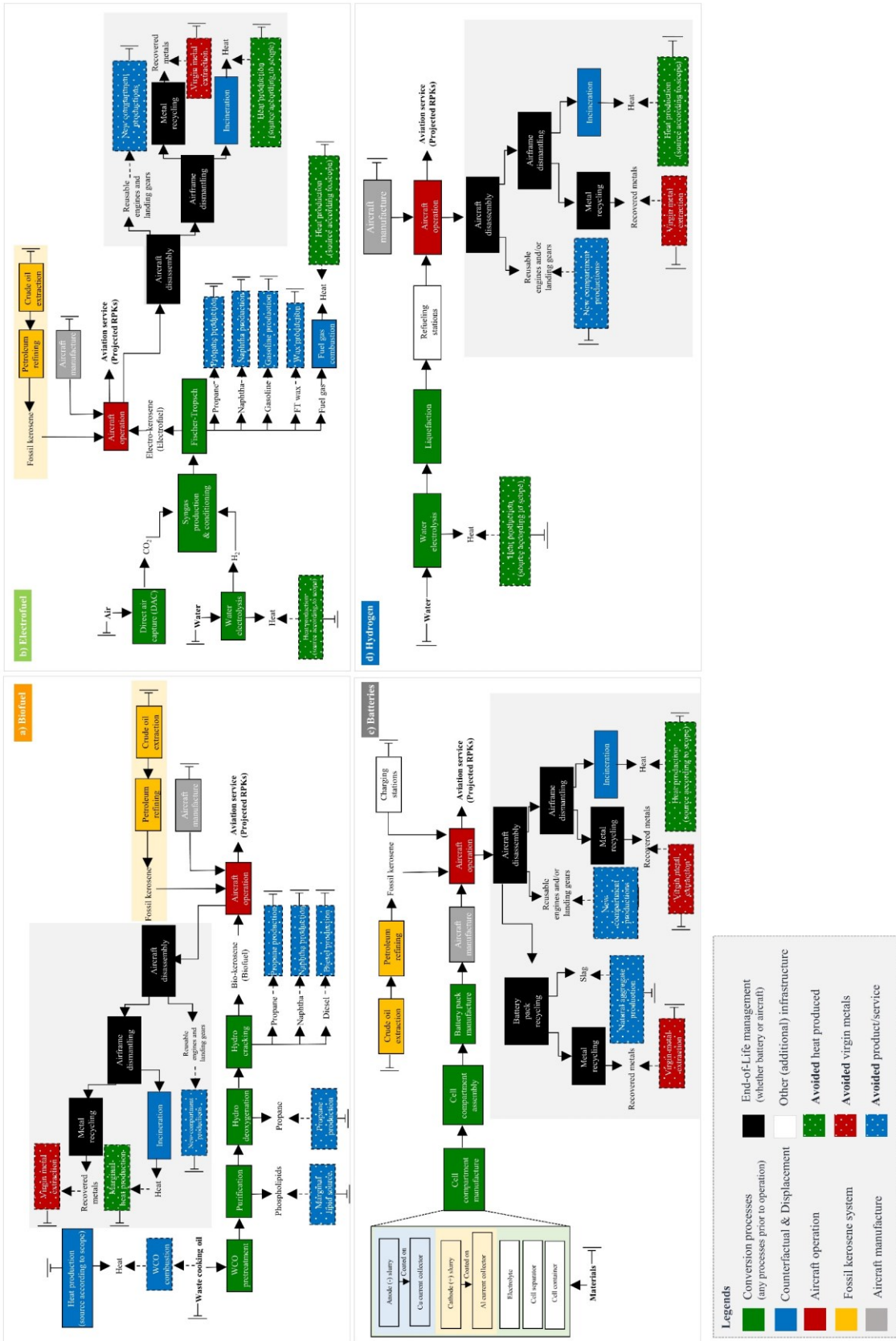


Fig. 4.2 The generic process considered in this analysis for the four aviation systems studied: a) Biofuels (HEFA based waste cooking oil; WCO as an example), b) Electrofuels (based on DAC and water electrolysis for H₂ production), c) Batteries, and d) Hydrogen (through water electrolysis). Additional biofuel pathways are illustrated in the supplementary information. Yellow background highlights activities related to fossil-kerosene production which is phased out for the long-term scope. The activities encompassed within end-of-life (EoL) management are highlighted in the gray background.

4.3.1 Near-term contribution analysis

Biofuels provide the most promising results irrespective of the service segments for three out of six impacts analyzed. Among the biofuels, FT and ethanol-to-jet (via syngas fermentation) are the most competing systems, providing they stem from primary forestry residues (PFR) that would have otherwise been left to degrade on forest

land. Another promising approach is the full electric for the domestic segment, with a net impact close to zero for all six impact analyzed, and H₂ for the international segment.

FT and ethanol-to-jet benefit from the PFR counterfactual use for the CC and PM impacts, with net negative impacts. This is essentially due to the avoided emissions of CH₄ (0.065 kg CH₄_{biogenic} kg⁻¹ PFR_{DM}) and NH₃ (0.0035 kg NH₃ kg⁻¹ PRF_{DM}) during on land degradation. However, there are quite some uncertainty related to the estimation of these emissions, as later discussed. It should also be noted that higher conversion yield in the ethanol-to-jet (0.17 kg biomass_{DM} MJ⁻¹ fuel produced; Fig. S4.8) results in worse performance relative to the FT (0.18 kg biomass_{DM} MJ⁻¹ fuel produced) for the assessed impacts.

For all impacts, the WCO is preferable to natural gas as heat source (0.0007 kg CO₂eq. MJ⁻¹ vs 0.07 kg CO₂eq. MJ⁻¹; HEFA scenario). Because of this counterfactual use for WCO, the overall CC impact is +77 to +87% higher for HEFA, in comparison to fossil kerosene. However, HEFA is also the only scenario with a net negative WS impact owing to the avoided co-products (e.g., diesel, propane).

The electricity for batteries recharge (Figs. 4.3 and S4.5, red bar) contributes significantly in all impacts (for the domestic segment). CC, EUF, and WS impacts are here due to the construction materials required for wind turbines (~84% French electricity mix [14]), while the wood chips harvesting for biomass-based electricity production (~13% shared [14]) contributes to the POF, PM, and EUM impacts (through the fossil diesel consumption). The additional infrastructure contributes to POF, EUF, and EUM impacts, mainly due to the copper mine operation and production. Battery manufacturing and end-of-life are insignificant contributors compared to the operation stage. Concerning the metal & mineral resources depletion (MRD) impact, battery manufacturing demonstrates a share of approximately 43-67% net (Hybrid modes) and 11-13% (full electric modes), attributing to the copper needed (for electronic components, current collector) and nickel (active cathode for AB scenarios). The hybrid modes show a more considerable MRD impact because electricity has a higher impact (6.14×10⁻⁷ kg Sb eq. kWh⁻¹ or 2.21×10⁻⁷ kg Sb eq. MJ⁻¹) than fossil kerosene production (4.27×10⁻⁹ kg Sb eq. MJ⁻¹), though higher kerosene content is required.

Electricity is also an important contributor (Figs. 4.3 and S4.5, green bar) in all impacts of the H₂ and electrofuels systems. This owes to the electricity-intensive processes in low-temperature (LT) H₂O electrolysis: 50-67 kWh_{elec.} kg⁻¹ H₂ [66,85,740,765,969,993]. For electrofuel production, electricity contributes to 79-81% of the overall energy requirement (33-34 kWh_{elec.} kg⁻¹ electrofuel). Heat requirement and sorbent production for DAC are other impact drivers, with contributions depending on the production pathway. In the liquid sorbent system, the water requirement for the sorbent regeneration leads to a WS impact of +5% of the solid sorbent system. The result is not in line with Schmidt et al. (2016) [45] because the water for sorbent regeneration is not included (accounting for 55% of water demand). Nevertheless, overall water consumption for H₂ production (approx. 5.14-6.30 kg H₂O per kg fuel produced) corresponds to Petitjean and Crespi (2022) [994] (about 4.50-5.52 kg H₂O per kg fuel produced, although CO₂ sources are not clarified). This results in higher water consumption than others due to the consideration of H₂ production and sorbent regeneration.

Recovered heat, whether from the gasification, FT (35-50% efficiency; >100°C [979,980]), or LT electrolysis (50-85% efficiency; <100°C [970,971]), significantly yields benefits in the CC. For the other impacts, however, the avoided co-products contribute more to the negative impacts than the avoided heat (though this does not apply to the H₂ systems).

Battery hybridization systems (H-CB and H-AB) perform similarly with fossil kerosene for all impacts. This is because the mass penalty caused by the battery (low energy content, 400-500 Wh kg⁻¹ pack [57]) accommodation requires comparable kerosene consumption with the fossil kerosene system (12,000 Wh kg⁻¹ fossil kerosene [30,150]). The fossil kerosene required by the H-CB and H-AB is the same for the fossil kerosene systems. For fossil kerosene systems, CO₂_{fossil} and aviation-induced cloudiness (AIC) are the main climate forcers in the CC. NO_x and non-methane volatile organic compounds (NMVOC) are responsible for 52 to 82% of the POF impact, adding CO and CH₄, while NO_x is responsible for the EUM impact. Hydrogen systems have an advantage from their non-CO₂ tailpipe emissions (mainly H₂O and NO_x) and show the best performance for POF impact for the international segment (reduction up to 27% in the fuel cell modes relative to the combustion modes).

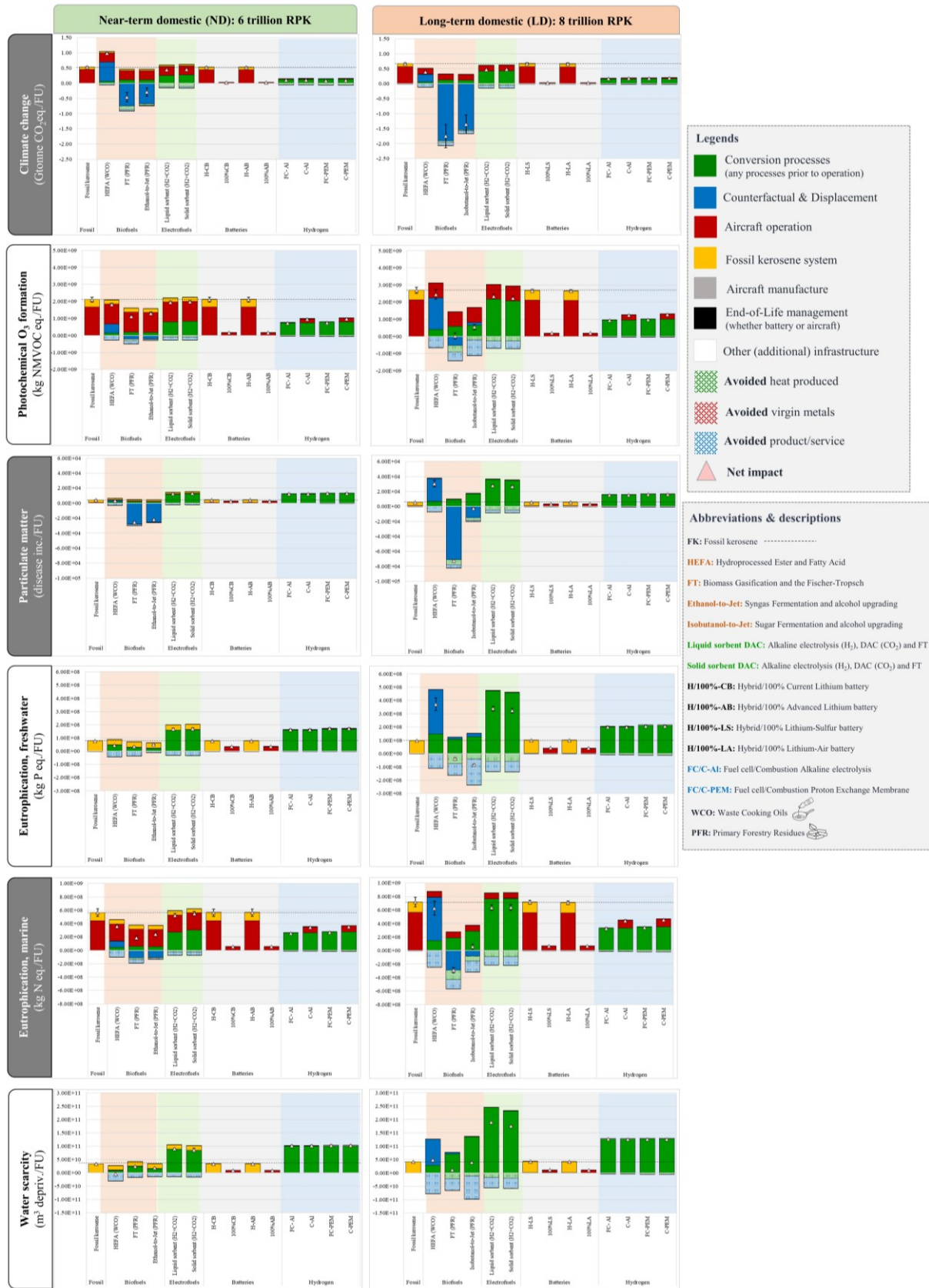


Fig. 4.3 Contribution analysis for near- and long-term time scopes for the domestic segment for the six assessed environmental impact categories for fossil kerosene (reference system), biofuels, electrofuels, electric (batteries), and H₂ systems. The contribution analysis for the international segment can be retrieved in SM 4.1, Fig. S4.5.

4.3.2 Long-term scenarios contribution analysis

Overall results indicate that the biofuel FT has the highest environmental savings for both service segments (Figs. 4.3 and S4.5) except in the EUF impact, where the isobutanol-to-jet approach yields the best saving irrespective of segments. Full electric systems are another promising approach for domestic segments with a 74-76% reduction of WS impact relative to fossil kerosene.

The FT shows lower performance in all impacts relative to the isobutanol-to-jet and irrespective of the segment, except the EUF (~185% reduction compared to fossil kerosene). This is due to the avoided impact from co-products (e.g., naphthalene sulfonate), contributing 48% of the net impact. Indeed, such substances are conventionally obtained from fossil raw materials and using fossil energy sources, and the greater functional unit (in comparison with the short-term) accentuates this effect. The other impacts are influenced by the higher conversion yield of the isobutanol-to-jet pathway (0.15 kg biomass_{DM} MJ⁻¹ fuel produced; Fig. S4.8), resulting in lower avoided impacts. The FT system has the best (net negative) EUM impact because of the avoided PFR decomposition (avoided NH₃ emission) and exhibits a reduction of 137-141% relative to full-electric systems (Fig. 4.4).

On the other hand, the HEFA provides a CC impact reduction of 43-45% relative to fossil kerosene, reflecting that the induced heat is here electrified heat rather than natural gas (17 times impact reduction relative to WCO-based heat), accounting for 51-54% of the total impact. Unlike the near-term, the impact of induced electrified heat is visible for other impacts in the HEFA case. However, in Fig. 4.4, this induced electrified heat production causes the HEFA to have the worst performances in PM (+450-461%) and EUF (+277-278%).

Due to a large amount of electricity required, H₂ and electrofuels perform even worse than fossil kerosene in the PM, EUF, and WS impacts. On the contrary, for electrofuels, POF and EUM impacts are also lower (with 13-20% and 10-18%, respectively) relative to fossil kerosene because of lesser NO_x emissions, as later discussed. Electrified heat consumption (about 0.68-0.75 MJ MJ⁻¹ electrofuel produced) is an important contributor to CC, PM, and EUM in the case of electrofuels. Albeit negative impacts are obtained from avoided co-products and heat (~23% for EUF and ~20% in EUM), they cannot compensate to provide an overall net negative result for the electrofuels. Using the liquid sorbent technology in DAC instead of a solid sorbent increases the WS impact by +2-7%. Other significant contributors to WS are the alkaline electrolysis with 68% and H₂ liquefaction with 21-22% of the net result in H₂ systems (see SM 4.2 LCIA folder).

Considering that, in the long-term, there is no more blending with fossil kerosene, the contribution of AIC to the CC impact becomes the dominant (around 92% of overall tailpipe emissions impacts with a small share of H₂O and NO_x) for biofuels and electrofuel operation phases (see SM 4.2 LCIA folder). This also generates lower POF and EUM impacts corresponding to the lower NO_x emissions (2.10 g NO_x kg⁻¹ biofuels/electrofuels combusted [47,49,500,846,995]) relative to fossil kerosene (6.03 g NO_x kg⁻¹ kerosene combusted [501,996]). H₂ fuel cell system (FC-AI and FC-PEM) has lower impacts than H₂ combustion (C-AI and C-PEM) in CC, POF, and EUM, due to less NO_x emission (Fig. 4.4 and details in SM 4.2 LCI folder). Avoided co-products (e.g., diesel, gasoline, naphtha) contribute more than avoided electrified heat in all impacts except FT (PM and WS) and PM electrofuels.

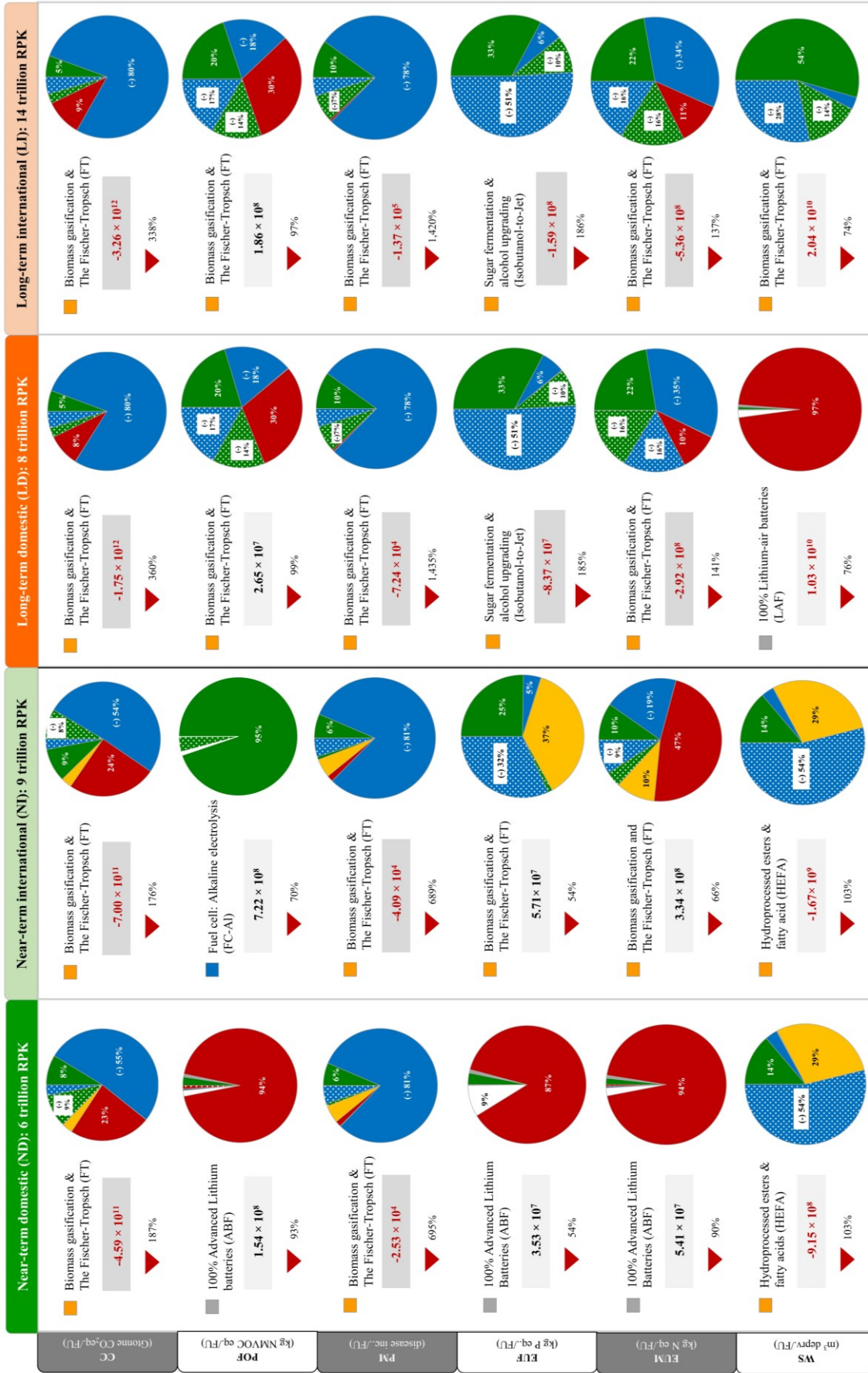


Fig. 4.4 Detailed contribution analysis for the most performant Sustainable Aviation system, for each impact category, service segment and time scope. The SA system families are identified by the colored squares: Biofuels (Orange), Electrofuels (Green), Electric (batteries) (Grey), and Hydrogen (Blue). The pie charts show the share of impact results between the main contributors; the negative results are indicated in parenthesis. The net impact result is indicated on grey background, and when negative is it highlighted in red. The impact reduction relative to fossil kerosene systems is represented with a red triangle, in %.

4.3.3 Synthesizing results in near- and long-term scenarios

Fig. 4.4 summarizes the best pathways identified for each impact, segment, and time scope, with their main impact contributors.

- The higher projected RPK in the long-term induced, for biofuel FT, higher impact savings (with respect to fossil kerosene) for CC, PM and EUM. However, FT exhibits a higher net impact (positive values) for EUF, POF and WS.
- Tailpipe emission impacts are mitigated when no blending mandate is considered for the biofuels/electrofuels systems. Furthermore, the impacts of fossil kerosene production are then not applied.
- Electrified heat (0.011-0.012 kgCO₂eq. MJ⁻¹ heat) is better than natural gas-based heat (0.07 kgCO₂eq. MJ⁻¹ heat) only for CC, so avoiding heat no longer leads to savings for this impact in the long-term. However, higher avoided impacts from heat recovery are observed in the long-term for POF and EUM impacts. This also applies to the induced electrified heat production (e.g., in the HEFA).
- The type of lithium batteries does not influence the LCA results; on the contrary, the aircraft construction for H₂ systems (blended wing body; BWB) in the case of LI segments do have an impact on the results, as it makes the plane heavier (Fig. S4.5), though it is based on prototype data. On top of that, the fact that the full-electric systems need ca. 4,000-10,000 planes depending on the lithium batteries' types to fulfil the FU (in comparison with up to 1,400 planes for other cases; calculation details in SM 3.2, sheet "aircraft number manufacturers") did not affect the results.

In summary, although all systems involve different contributors with negative impacts, the net impact results are positive for almost all scenarios. One notable exception is PFR-based biofuel systems with all impacts negative, except the POF (Fig. 4.4.; details in the SM 4.2 LCIA folder). Electricity used for water electrolysis is the critical impact contributor to H₂ and electrofuels systems. Electric systems are the most promising option only when batteries are considered the sole energy source in both domestic time scopes.

4.3.4 Sensitivity analysis to model choices

The sensitivity study (Figs. 4.5 and S4.6) conducted with other marginal electricity mixes (i.e., China and US) shows higher impacts (all categories) for all assessed scenarios and time scopes. This is flagrant for electricity-intensive pathways (electrofuels and H₂) and HEFA long-term with induced electrified heat.

The exclusion of non-CO₂ tailpipe impacts yields lower CC impact results. The net impacts of biofuels and electrofuels decreased by 12-77% and 33-35%, respectively. A 42-44% reduction was observed in the case of H₂ combustion concerning fuel cell scenarios. For H₂ systems, a decreased net impact was observed in the sensitivity analysis with high-temperature (HT) solid oxide electrolysis (SOE) owing to the lower electricity consumption (~54 kWh kg⁻¹ H₂; 4-7% reductions) relative to low-temperature (alkaline and PEM) electrolysis. However, this does not apply to the near-term CC impact, essentially due to the natural gas used as a heat source (+48-75% related to LT base case).

As discussed in sections 4.3.1-4.3.2, WCO is preferred as biofuel feedstock rather than a heat source when it competes with natural gas heat. Using electricity instead of natural gas for heat-induced use results in lower net CC (reduction of 82%). In contrast, the fossil diesel refinery process causes the other impacts to be increased, with different magnitudes. Relative important uncertainty ranges are observed only in the HEFA long-term scopes in all impacts (Figs. 4.3 and S4.5, details in SM 4.2 GSA folder), except the CC and EUM impacts, essentially due to the electricity consumption (0.31-0.46 kWh MJ⁻¹ heat [997]) in the induced heat process (representing ~98% parameter contribution).

The selected heat process influences the overall net results as observed using the market heat from co-generation {Europe without Switzerland} in the near term. Scenarios with avoided heat credits (e.g., the ethanol-to-jet, electrofuels) demonstrate lower net impacts for CC (2-27% concerning the base case) and POF (2-39%) owing to the simultaneous avoided electricity generation and vice versa. On the other hand, albeit insignificant, the solar heat systems generate higher CC (due to infrastructures, e.g., thermal storage systems, collector field) and WS (for mirrors cleaning 0.04-0.12 L kWh⁻¹ electricity produced [14]) in the long-term, in case of HEFA (induced heat) and electrofuels. The investigated aviation systems demonstrated low sensitivity to other process choices (e.g., recovered O₂ from electrolysis or different uses of co-products) (Figs. 4.5 and S4.6; see SM 4.2 SA folder).

4.3.5 Global sensitivity analysis (GSA) results

Thirty-nine parameters are selected for GSA (selected from the contribution analysis; Table S4.2). It should be noted that not all of these apply to all scenarios. GSA provides two answers; (i) it highlights to which parameters the results are the most sensitive and (ii) which parameter uncertainty contributes the most to the total systematic uncertainty. This is applied to all impacts.

The most sensitive parameters, i.e., those where a change of 10% induces the highest percentage change on a given impact result, vary from scenario to scenario (details in SM 4.1 (Table S4.2) and SM 4.2, GSA folder). Notably, the HEFA results are highly sensitive to the amount of induced heat (MJ per MJ heat produced) across all impact categories (Figs. 4.3 and S4.5). In the long-term, this is essentially due to the electricity consumption (0.31-0.46 kWh MJ⁻¹ heat) in the induced heat process [997]. The electricity used to produce a unit of hydrogen with low-temperature (LT) water electrolysis (including alkaline and PEM systems) (kWh per kg H₂) was also a particularly sensitive parameter for electrofuels and H₂ scenarios. For the latter, heat recovery (%) from electrolyzers was also found as a sensitive parameter affecting most impact categories. In addition, the overall propulsion efficiency (OPE %) and amount of aluminium used for plane production (%) were found as sensitive parameters for most impact categories of the electric (battery) scenarios. These results are presented and detailed in SM 4.2 (e.g. sheet ND GSA for the near-term, domestic segment results; values of sensitivity ratios within each scenario).

For uncertainty (Fig. S4.7), heat and electricity consumptions, the recovered heat, PFR generated emissions (degradation), and aircraft operation is parameters contributing the most to CC's near-term scenarios. The induced heat production accounts for ca. 80% uncertainty in the HEFA. The 55-60% uncertainty for H₂ systems is derived from electricity used in H₂O electrolysis, followed by their recovered heat. For operation, the uncertainty is explained by CO_{2fossil}, AIC, and NO_x for the hybrid scenarios (H-CB, H-AB). NO_x emissions are also observed as the POF and PM impact uncertainties for all scenarios except the solid sorbent and H₂ systems. Solid sorbent utilization affects all studied impacts uncertainty with varying contributions, e.g., 13% in the net CC and up to 91% for the EUF impact. From the PFR counterfactual uses, CH₄ emission is considered the sensitive parameter in the CC and POF impacts.

Electricity is the dominant driver for the uncertainty of H₂ systems (H₂O electrolysis) and the full-electric systems (during the operation) in all assessed impacts. Electricity is also a main PM impact contributor to the biofuel scenarios. Co-products uncertainties are important in the PM (i.e., contributing to 36% of uncertainty in HEFA, 18% in FT), EUF (i.e., 56% HEFA), and WS (i.e., 96% HEFA, 81% FT and 100% liquid sorbent) impacts. This is due to the propane and diesel in the HEFA scenario. In comparison, the FT is derived from gasoline and petroleum wax production.

Unlike the near-term HEFA scenario, induced electrified heat plays a key uncertainty role in all studied impacts. The solid sorbent, full-electric, hybrid batteries (H-LS and H-LA), and H₂ systems have similar behaviours. In the isobutanol-to-jet, the naphthalene sulfonate production provides the 54% uncertainty contribution in the POF and EUF impacts owing to the avoided (other than natural gas) heat production. Detailed results on the contribution of each of the 39 selected parameters to system uncertainty for each impact and each scenario are available in SM 4.2 (GSA folder), while a detailed example for the domestic segment (both time scopes) is presented in SM 4.1 (Fig. S4.7).

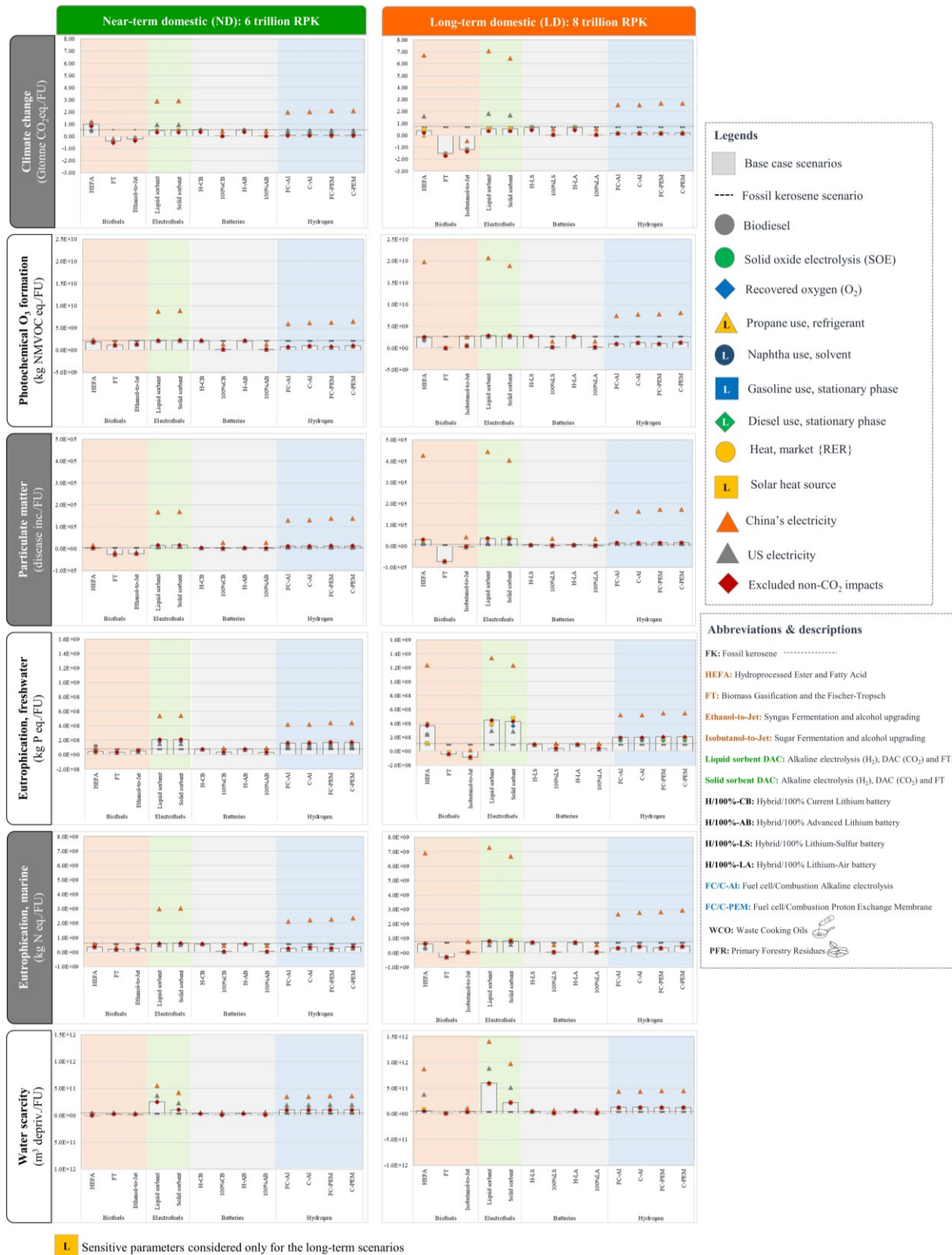


Fig. 4.5 Sensitivity analysis for near- and long-term time scopes for a domestic segment of the six assessed environmental impact categories for fossil kerosene (reference system), biofuels, electrofuels, electric (batteries) and H₂ systems.

4.4 Discussion

All considered SA systems perform better than fossil kerosene system with some exceptions (Figs. 4.3 and S4.5). These include i) HEFA because of the induced heat productions and ii) electrofuels & H₂ systems (irrespective of the assessed time scopes) for PM, EUM and WS impacts. Despite the variability in the reduction CC potential as

discussed in SM 4.1, this study confirms the environmental benefits regarding the mitigation goal (e.g., in the ReFuelEU proposal [18], in the international market-based basket CORSIA [78]). However, other impacts must be assessed in order to scrutinize their tradeoffs.

The counterfactual use processes significantly contribute to all biofuel's overall net (negative) impacts. PFR use as feedstock in biofuels systems (whether the FT, ethanol-to-jet or isobutanol-to-jet systems) instead of being left on the ground influences mainly the CC and PM impacts (with a conversion yield of 0.15-0.18 kg dry biomass MJ⁻¹ biofuel produced; detailed in the SM 4.2 and Fig. S4.8). However, this contribution should be relativized because the CH₄ emissions from PFR decay rely on relatively few and uncertain data, and are considered high (here estimated as 10% [998]; this is to be seen as a maximum). The counterfactual use of WCO and the induced heat sources (and their conversion yields) strongly influence the near- and long-term results. WCO is preferable as a heat source rather than biofuel feedstock at the mean term when it replaces natural gas for CC, PM, EUF and EUM impacts. Here, 0.11 kg of dry WCO MJ⁻¹ biofuel produced was applied, corresponding to the CORSIA methodology [78]. Conversely, in the long term, WCO is preferred as biofuel feedstock when electrified heat is induced (for PM and EUF).

Regarding the projected air demands (varying upon the functional unit; see Figs. S4.8 and S4.9), an estimated range of 327-1,939 Mt PFR (ca. 6.18-36.59 EJ) is required depending upon the biofuel conversion technologies. This amount corresponds to 18-105% of a maximal PFR potential (ca. 35 EJ) [999]. If only PFR (residual)-based biofuels are concerned, the existent biomass residues are potentially sufficient, at least on a global level (prior to considering imports/exports and actual access to these residues). However, the PFR demands from other sectors (e.g., bioplastics [1000], maritime [1001]) should not be negligible and raises the competition for (sustainable) feedstocks. Concerning WCO, ca. 230-1,105 Mt WCO (~8.95-42.95 EJ) would be needed for the HEFA system, which exceeds by far the available WCO amount (only 0.52 Mt WCO) in Europe [1002] and might be subject to frauding (e.g., palm oil slightly fried to quantify as WCO) [1003].

It should be highlighted that (renewable) electricity demand is evaluated at 642-790 TWh when the aviation full electric systems are in service (~34-42% of global wind power-based electricity generation in 2021 [1004]). For electrofuel production, 1,708-8,386 TWh electricity demand (excluding heat demands) represents ca. 7-37% of the current global electricity demand [484] or a 4 to 21 times increase of the nuclear-based electricity production in France [1005].

A lot of 293-1,404 Mt CO₂ (implying at least 293 DAC plants capturing the potential of 1 Mt CO₂ y⁻¹ [736]) and 424-2,033 Mt H₂ (about 3-13% of Australia's freshwater withdrawals in the year 2017 [481]) is estimated to reach the projected RPK demands. 405-1,825 Mt water and 2,356-9,107 TWh electricity (low-temperature electrolysis) are necessary for the H₂ system. Approximately 10-40% of today's global electricity consumption [484] would be needed.

At present, the existing production capacity of biofuels and electrofuels (around 0.26 EJ y⁻¹ [34,111,141,164,245,249,1006,1007]) represents roughly 12% (9% derived from the HEFA current production capacity) of projected fuel needs for the near-term domestic (ND; 50% blending quota), far from satisfying the demands. However, this is expected to be improved through technological advancements and financial support with policy incentives.

The presented analysis considered one SA system at a time. Actually, different SA systems could co-exist depending on the implementation dynamics of new technologies and infrastructures and should be investigated in their particular context (e.g., national, regional scale).

This very prospective analysis was based on a huge literature survey; however, only limited (public) information exists in the case of novel systems like electric and H₂, implying high-performance batteries, new aircraft development, and their end-of-life management. Furthermore, although the non-CO₂ impacts have been intensively studied [7,354,829,1008], their inclusion in the current LCA is challenging. Therefore, more accurate and precise results might be obtained when those issues are harmonized for the calculation basis (e.g., the applied climate metrics, particularly for short-lived forcers). Finally, albeit relevant, other emerging sources of energy, namely liquefied petroleum gas (LPG) [340] and ammonia (NH₃) [353], are increasing their attention, and further research is encouraged.

4.5 Supplementary materials

Two supplementary materials (SM) are provided for this chapter. SM 4.1 is presented below. It details several modelling assumptions, along with the impact assessment results. It also supplies the process flow diagrams for all individual biofuel pathways analyzed. SM 4.2 is a set of 101 files and can be accessed via <https://doi.org/10.48531/JBRU.CALMIP/D0PWA8>. It contains the unit The Life Cycle Inventory (LCI) of each individual processes considered within this chapter, the detailed Contribution analysis (impact assessment results), the uncertainty analysis (Global Sensitivity Analysis, GSA) and the sensitivity analysis.

Supplementary material 4.1 (SM 4.1)

1. Aircraft representative models: assumptions

Commercial aviation is the scope of this analysis; therefore, other purposes are excluded, such as air emergency, military, leisure, and business travel. It is assumed that the aircraft carrying at least 19 passengers belongs to this analysis.

Representative commercial aircraft variants were selected for the different service segments. Therefore, Airbus A320 and A350 XWB models are considered for domestic and international services, respectively, as the projected dominant platform [813,880]. Additionally, for the domestic segment, the Heart Aerospace ES-19 was chosen as the representative full-electric aircraft, which was announced to be ready for service within 2025 [1009].

While a blended-wing-body (BWB) concept is assumed for hydrogen-powered aviation [881,882], particularly for long-range distances, from Glenn Llewellyn's presentation, engineered within the Airbus Zero-e aircraft project, the transformation in hydrogen propulsion system with a novel airframe configuration cannot be reached by 2035. The BWB concept is assumed to be available for service around 2045. Therefore, the Boeing BWB X-48B model was chosen as the representative BWB aircraft, derived from [883] the closest seat available relative to the Airbus A350 XWB model.

The overall propulsion system efficiency (OPE_i) is defined by multiplying the propulsive and thermodynamic efficiencies [394]. The efficiency generated from the conversion of shaft power to propulsive power is referred to the propulsive efficiency [394]. On the other hand, thermodynamic efficiency derives from the conversions of fuel flow power to shaft power. As no fuel energy flow is detected in the full-electric propulsive system, only the propulsive efficiency is applied [1010].

2. Heat assumptions considered in this analysis

All assumptions about the heat processes applied in this analysis are provided in this section.

2.1 High-temperature required processes (>100°C)

The processes in which high temperatures are necessary are listed below. In the near term, the natural gas can still be used as source for a wide range of temperatures. In the long-term, the electrified heat can be used, with indifferent delivery temperatures depending on the heat production technology. Therefore, heat pumps and electric furnaces are possible long-term technologies. Heat pumps are potentially applied for industrial processes at temperatures from 90°C to 150-200°C in the future [982,984]. Furthermore, electric furnaces in e.g. metal processing, where temperatures can reach as high as 2,000°C, are considered [984], or for other industrial processes[985].

Table S4.1. High-temperature required processes to be considered in this study

Categories	Process	Operating temperature (°C)	Activities
HEFA	Hydrodeoxygenation	300-400 [654,1011]	Converting triglyceride-based feedstocks into the (straight) paraffinic compounds, including hydrogenation, propane cleavage, and hydroprocessing reactions [654,1011]
	Hydrocracking/Isomerization	355 [654,1012]	Performing the hydrocracking and isomerization of the obtained paraffinic compounds to improve

			fuel quality with the presence of a branched paraffinic compound.
FT and Ethanol-to-Jet	Steam reforming process	800-850 [937,1013]	Conditioning the syngas compositions, particularly for syngas prior to entering the FT reactors in which an H ₂ :CO ratio (by volume) of 2.0 is necessary
Isobutanol-to-Jet	Isobutanol upgrading process	250-350 [950,1014,1015]	Consisting of a series of reactions for the transformation of the isobutanol to kerosene; this includes hydrogenation, oligomerization, and dehydration
	Lignosulfonate filtrations	170-200 [1016]	Applying the spray dryer is considered an appropriate technology for the recovery of lignosulfonate from spent sulfite liquor during the pretreatment stage [948,949]
	Liquid sorbent regeneration	800-900 [736,1017]	For the regeneration of CaO to Ca(OH) ₂ , which is further recycled back to the precipitation stage [736,1017].
Electrofuels	Reverse water gas shift (RWGS) reaction	180-500 [207,1018] ^a	Converting CO ₂ to CO facilitates H ₂ :CO of 2.0 before accessing the FT process[149,207]. The temperatures are ranged regarding the used catalysts[1018].
End-of-Life	Composite incineration (degradation temperatures of 300-500 °C) ²¹	300-500 [1019] [*]	Combustion of aircraft composites (including carbon fiber reinforced polymer; CFRP, and glass fiber reinforced polymer; GFRP)
	Metal remelting process	Up to 2,000°C [984]	Remelting process of the metal scraps derived from the aircraft compartments comprising mainly aluminum, steel, and titanium

Notes.

^a The reverse water gas shift (RWGS) depends upon the used catalysts, including high-temperature shift at 300-510°C in the presence of a copper-promoted catalyst, low-temperature shift at 180-270°C compatible with copper-zinc-aluminum oxide-based catalyst [1018]. However, the reaction can independently occur without the catalysts above 950-1,000°C [1018].

^b The shown temperatures are the degradation temperatures of typical composite materials [1019,1020]; however, the temperatures vary by the material compositions and recycling technologies [1021].

Acronyms: Ethanol-to-Jet (Biomass gasification and Syngas fermentation & alcohol upgrading); FT (Biomass gasification and the Fischer-Tropsch process); HEFA (Hydroprocessed esters and fatty acids); Isobutanol-to-Jet (Sugar fermentation and alcohol upgrading)

2.2 Waste heat recovery (WHR) system

Waste heat recovery (WHR) systems, such as air preheaters, recuperators, plate heat exchangers, and thermal wheels [979], have been introduced in numerous technologies. Although different in technical principles, they have the same purpose for capturing and recovering the waste heat by increasing the overall energy efficiency in a process [1022]. However, they all have different advantages and disadvantages [1022–1024]; they also vary significantly following several factors: waste heat temperature, quality, compositions, design, and operations [980]. This section aims to scope the WHR-established technology selection and its efficiency according to the outlet temperature of waste heat [1024]. As shown in the main manuscript, two ranges of waste heat temperatures are defined: low-temperature waste heat (LWH: at <100°C, including heat derived from water electrolysis) and high-temperature waste heat (HWH: at >100°C, including heat provided from biomass gasification, the FT process).

The purpose for LWH recovery in this analysis is its upgrading by raising its temperature depending on the supplied process. This allows avoiding the demands of LH streams. Therefore, different heat pumps are proposed to lift the temperature with different enthalpic efficiency. For example, a vapor heat pump with around 35% efficiency is reported to increase the temperature from 140°C to 240°C [970]. Additionally, Keil et al. (2008) [971] estimated a maximum efficiency of approximately 50% by utilizing an absorption heat pump (based on water/lithium bromide) for rising LWH sources of 30–40°C to 82°C. Therefore, the enthalpic efficiencies ranging between 35% and 50% are used to determine the recovery ratio of LH in the base case scenario in our study.

Direct use of recoverable HWT improves the overall energy efficiency. Several technical approaches have been studied with varying efficiencies of 50-85% [979,980]. For example, the recovery of HWT ranging from 120-800°C has been investigated using plate heat exchangers with maximum efficiency of around 70-80% [979]. The rotating wheel and heat pipes are also applicable with the HWT limited up to around 315°C, with efficiencies of 50-85% and 60-80%, respectively [979,980]. As mentioned, the temperature limit is determined by numerous parameters such as construction materials, working fluid types, and so on [980]. Therefore, the average values of enthalpy efficiencies are applied for the base case scenarios.

The infrastructures related to the heat recovery are not included; only the % of recovered heat is applied regarding the heat outlet temperatures.

2.3 The selection of avoided/induced heat process

When the new production pathways are implemented, it is considered that the processes where heat is generated will impact the use of traditional heat sources. Herein, natural gas and electricity are considered as the primary sources for heat production for near- and long-term scopes. The avoided traditional heat processes are selected according to the time scope.

Heat generation from the combustion of co-products (such as biomass lost, composite) and recovered heat from gasification and the FT process are considered to avoid high-temperature (HT) heat production. It is because temperatures >500°C can be reached when solid fuels are combusted (e.g., up to 1,100°C wood chips [984]). With the high operating temperatures, the recovered HT heat is further considered for gasification and the FT process.

Notably, the avoided/induced heat processes are assumed to have similar properties (in terms of heat and temperature) as the traditional services and therefore, the substitution ratio of 1 is used. For example, heat derived from biomass combustion can avoid heat demands from natural gas (near-term). On the other hand, the high-temperature heat can be replaced with biomass combustion as the temperature reaches up to 750°C [984].

3. Comparison of climate impacts results of the fuel productions and battery manufacturing with the results from literature

In this section, the climate impacts from this analysis are quantitatively compared with the published studies with the chosen functional unit of 1 MJ fuel produced or 1 MJ battery production. Most previous studies have applied the allocation to deal with multifunctionality [308,337,489,1025,1026]. Whereas, in this analysis, the system expansion (displacement) method is used in which we investigated that the impacts derived from the counterfactual, avoided, and induced services/products are demonstrated as the major contributors in the cases of biofuels and electrofuels. Therefore, some assumptions and system boundaries have been adjusted in our cases or others to facilitate comparison purposes. However, it is essential to note that there are no precisely concrete answers as these studies used different perspectives in i) the assumptions (e.g., the modeled processes, the geographical scope) and ii) the multifunctionality approaches.

Another constraint to be mentioned is that the use phase of the battery and hydrogen are not included regarding the lacking sources of reference, particularly for aviation. The aim herein is to highlight the existent studies.

From the top view (Fig. S4.1), most of our results are close to the results from literature (whether the avoided/induced impacts are counted or not).

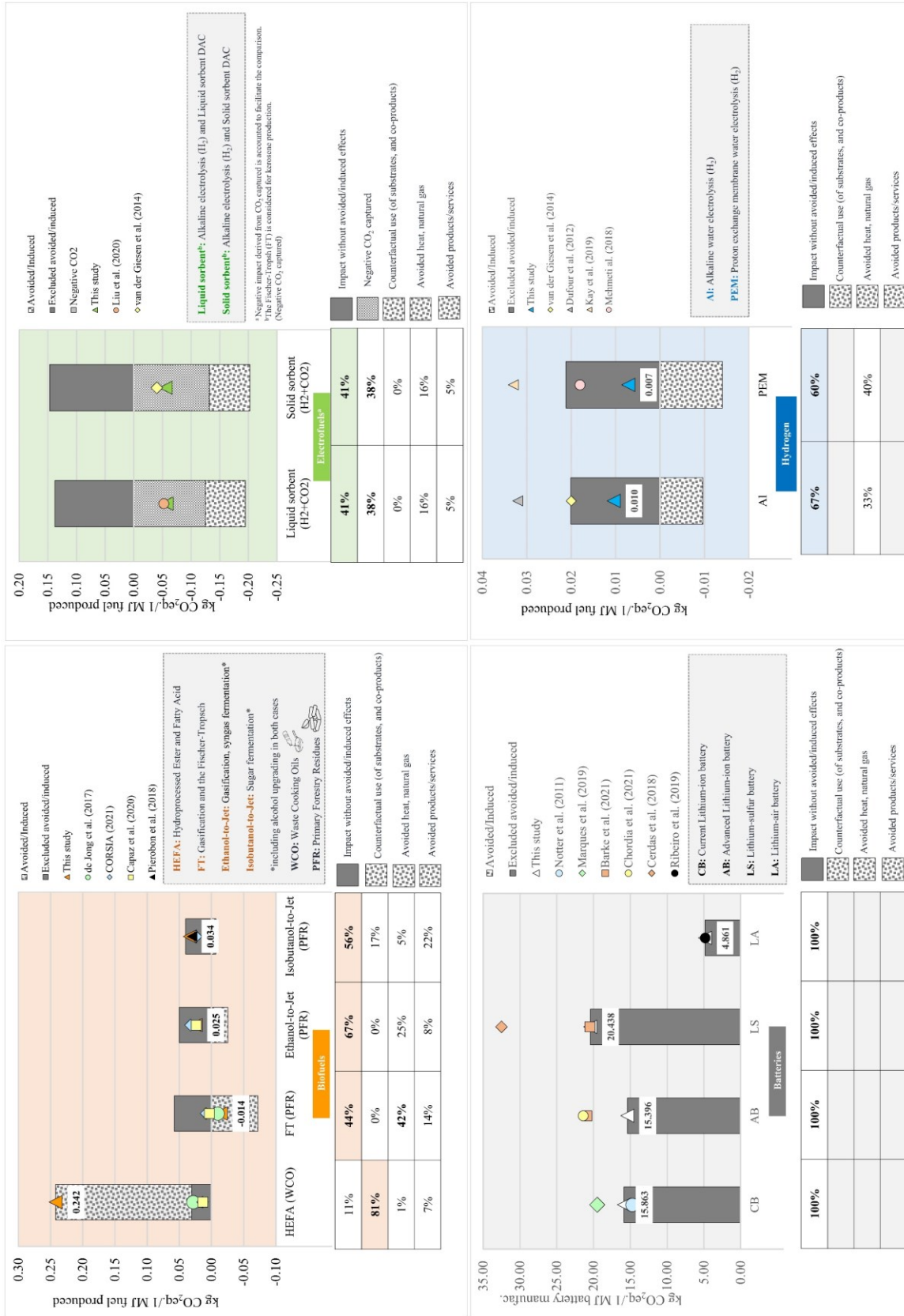


Fig. S4.1 Climate impact of the previous LCA studies “Cradle-to-Gate boundary with the functional unit of 1 MJ fuel production/battery manufacturing” relative to this analysis. However, some studies (e.g., Capaz et al., 2020 [1014]; Pierobon et al., 2018 [479]; Liu et al., 2020 [912]) have expanded the boundaries by including the use phase (and end-of-life phase). Therefore, herein only the results until the production phase (cradle to gate) are reported. On top of that, some assumptions in this analysis have also been modified to facilitate the comparison.

Biofuels

The impact result for HEFA-(based on WCO) are higher than the results from the other studies [336,337,1025], mainly due to the induced heat from natural gas, which occurs when WCO is used for the kerosene production instead for the generation of heat (which is one of its current use[193,1027]). However, when the impacts from induced/avoided are excluded, the obtained result of around 0.031 kg CO₂eq. MJ⁻¹ fuel combusted is in line with the study of de Jong et al. (2017) [336], where the 0.028 kg CO₂eq. MJ⁻¹ has been reported. Although consistent results are observed, the major parameters contributing to the overall impacts are different owing to the different modelling assumptions. In our case, excluding the induced heat effect, the heat consumptions (from natural gas) in the hydrodeoxygenation and the cracking processes show the highest shares, followed by the H₂-based alkaline electrolysis. In contrast, the impact of hydrogen produced through steam methane reforming (SMR) represents approximately 40-60% of the overall impact [336,1025], in which 5.58 kg CO₂ per kg H₂ is emitted during the production phase[1025]. This causes a high impact when the amount of hydrogen consumption is important. On the other hand, the alkaline water electrolysis applied in our study has a lower impact (2.96 kg CO₂eq. kg H₂ produced⁻¹ [67,969,987,1028,1029]) relative to the hydrogen derived from the reforming of natural gas (9.50-12.10 kg CO₂eq. kg H₂ produced⁻¹ [68,1030]). This makes the natural gas-based heat to have more significant influence than the H₂ needed in this case.

The negative climate impact for the case of FT based on forestry residue (-0.014 kg CO₂eq. MJ⁻¹) is shown to be similar to the result of de Jong et al. (2017) [336] (-0.010 kg CO₂eq. MJ⁻¹ fuel combusted). These close results can be explained by the deployment of system expansion as applied in our study.

However, the main contributors to the net negative impacts are not similar as we considered different displacement co-products/services. The negative impacts in this study (75% out of total avoided/induced effects) are mostly derived from the avoided heat (from natural gas), heat which can be recovered from both the gasification and the FT processes. The remaining negative impact is driven by the avoided productions of petroleum-based gasoline and waxes. While in the study of de Jong et al. (2017) [336], the avoided US grid electricity is considered as electricity is a co-product from the FT process, the avoided impact reaching about 62.5% of the overall climate impact.

For the pathway ethanol-to-jet based on forestry residues, the obtained climate change net impact is 0.025 kg CO₂eq. MJ⁻¹ fuel combusted. This is in agreement with other studies being in the range from 0.0234 kg CO₂eq. MJ⁻¹ [1025] to 0.040 kg CO₂eq. MJ⁻¹ [337] (although a different multifunctionality method is applied). In our study, the heat derived from natural gas required in syngas conditioning and ethanol upgrading is the main contributor (45% of the overall impact), while in Capaz et al. (2020) [1025], natural gas is also the major contributor but not for the same processes, the production of enzymes (further applied for ethanol synthesis) and of hydrogen (required for the jet fuel synthesis) are here incriminated.

In case of isobutanol-to-jet derived from forestry residue, our result of 0.0335 kg CO₂eq. MJ⁻¹ is close to the result of Pierobon et al. (2018) [489] (when the system expansion is considered), though the avoided products/services do not contribute with similar shares to the negative impact, 27% in this study and 41% of the net impact [489]. The avoided impacts from the production of conventional liginosulfonate are similarly provided as a significant negative contribution to the climate impact. Furthermore, the isobutanol-to-jet's climate impacts estimated through the allocation approaches ranges from 0.0238 kg CO₂eq. MJ⁻¹ to 0.0264 kg CO₂eq. MJ⁻¹. It highlights that the choice of multifunctionality significantly influences the overall impacts.

Electrofuels

Alkaline electrolysis coupling with two different direct air capture (DAC), including solvent- and solid-based sorbents, and the liquid fuel production through the FT process are considered for electrofuel productions. Net negative impacts can be observed in both electrofuel cases: -0.0571 kg CO₂eq. MJ⁻¹ for solvent-based DAC and -0.0559 kg CO₂eq. MJ⁻¹ for the solid-based DAC. This confirms the results from other studies in the range from -0.040 to -0.06 kg CO₂eq. MJ⁻¹ [207,922] when the negative carbon emissions are counted regarding the multifunctionality methods. For the positive impacts, the electricity requirement for alkaline electrolysis causes 67% out of the impacts without the negative and avoided/induced effects (as 41% of the overall impact), whichever solvent- or solid-based direct air capture (DAC) is employed (Fig. S4.1). Although the two approaches have similar

results, the latter provides a higher impact associated with the heat consumption of around $5.52 \text{ MJ kg}^{-1} \text{ CO}_2$ captured [736,1017,1031] relative to the former approach (approximate $4.98 \text{ MJ kg}^{-1} \text{ CO}_2$ captured [483,1032,1033]). The lower energy demands for the latter can be mitigated when the source of low-grade/waste heat (at a temperature of 100°C [1034]) is applied. This is also addressed in the studies of van der Giesen et al. (2014) [207] and Liu et al. (2020) [922]. Negative impacts in this study are mainly derived from the negative CO_2 emissions from the DAC operations contributing to approximately 50% (out of total negative impacts).

Additionally, with the consequential approach, the second main negative impact is derived from the avoided heat from natural gas that is considered to be recovered from alkaline electrolysis and the FT processes, followed by the avoided productions of the conventional approach (e.g., gasoline, naphtha). In contrast, approximately 40% of the overall impact is only due to the negative CO_2 uptake from the point of allocation approach [207,922]. Therefore, although the overall results are in the same line, the explanations may differ, as mentioned above.

Battery (Electric)

Climate impacts of all considered Li-based batteries have been closely characterized in the previous studies (as depicted in Fig. S4.1). There are no co-products from the battery manufacturing process (in the foreground). The avoided productions of co-products, namely molybdenite which is simultaneously extracted from sulfidic copper ores, during the mine operations are already integrated into the selected backgroundecoinvent, consequential. It is considered that the metals supplied are from the global suppliers, not defined explicitly from the EU sourcing countries such as aluminium and copper with 59% and 33% supply shared from China [977]). It implies that their climate impacts (e.g., the electricity mix source) vary based on where the metals are mined. In contrast, the battery cell manufacturing and pack final assembly are set out to be accomplished in France. Therefore, a French electricity mix is used.

The climate impact of the current Li-ion battery where the LiMn_2O_4 (LMO) is used as a cathode material is about $15.90 \text{ kg CO}_2\text{eq. MJ}^{-1}$ which agrees with the study of Notter et al. (2011) [1026] and Marques et al. (2019) [1035]. Approximately 80% of the climate impact derives from the production of battery pack, followed by cell assembling and LiMn_2O_4 cathode production. It is found that the energy requirements for aluminium production, namely electricity consumption in the metal electrolysis, are a significant cause of the climate impact in both pack manufacturing and current collector (in the assembling stage). They contribute with 59% and 26% of the impact of each process, respectively (with hard coal-based electricity in China). Similar results were found in Ellingsen et al. (2013) [1036] and Wu and Kong (2018) [1037].

It should be noted that the key contributor can differ in other studies given the variety of parameters (e.g., various anode/cathode chemistries and the configurations of cell containers). For instance, when steel is modeled for pack production instead of aluminium, the climate impacts are decreased, as applied in the study of Notter et al. (2011) [1026] ($14.70 \text{ kg CO}_2\text{eq. MJ}^{-1}$). While in the study of Marques et al. (2019) [1035], the sources of electricity influences the climate impact increasing from $19.21 \text{ kg CO}_2\text{eq. MJ}^{-1}$ (54% fossil) up to $19.80 \text{ kg CO}_2\text{eq. MJ}^{-1}$ (81% fossil). Respective to the French electricity mix, our result provides a lower value as wind power accounts for around 80% (retrieved from the backgroundecoinvent [14]).

From this study, the Adv. Li-ion (NMC 811) battery is observed to have an impact of $15.40 \text{ kg CO}_2\text{eq. MJ}^{-1}$. The battery pack production is the main contributor (65% out of the total impact). This is similar to the current Li-ion battery, as explained above. The second large contributor (25%) is the production of NMC 811. The productions of cobalt sulfate (CoSO_4), nickel sulfate (NiSO_4), and natural-based heat (applied during the NMC synthesis) contribute with 42%, 26%, and 29% of the impact derived from the NMC production. Similar observations were reported by Chordia et al. (2021) [308] and Barke et al. (2021) [1038]. A result of $28.89 \text{ kg CO}_2\text{eq. MJ}^{-1}$ was obtained by using the South Korean electricity mix, where the majority is generated from fossil fuels [1038]. A lower impact (approximately $13.89 \text{ kg CO}_2\text{eq. MJ}^{-1}$) was obtained when the Swedish electricity mix is used instead [1038]. It should be mentioned that the averaged results from the different electricity mixes are presented in Fig. S4.1.

Li-ion battery showed higher climate impact ($15.90 \text{ kg CO}_2\text{eq. MJ}^{-1}$) than Adv. Li-ion battery, due to its considered lowest gravimetric energy density (about 400 Wh kg^{-1} at cell level in our assumption) relative to Adv. Li-ion (NMC

811; 500 Wh kg⁻¹ cell). It means that more battery packs (cell mass accounting for 60% of the total pack's mass [1036,1037,1039]) are required to meet the energy requirement compared to the Adv. Li-ion.

In case of the Li-S battery, the energy requirements for the production of chemicals (1,4-butanediol and methylamine) required for the N-methyl-2-pyrrolidone (NMP) solvent production, account for 68% of the total impact. Our study result (20.48 kg CO₂eq. MJ⁻¹) is similar to those of Barke et al. (2021) [1038] and Cerdas et al. (2018)[58], being range from 20.48 to 32.50 kg CO₂eq. MJ⁻¹. On the other hand, battery module production was found as the second main contributor accounting for 28% of the total impact, similar to the two Li-ion batteries. Therefore, compared with the other Li-based batteries (in this study), the Li-S battery has the highest impact due to the high consumption of the solvent NMP (around 4 kg per kg of sulfur-electrode solid) necessary to make the sulfur composite cathode meet the slurry viscosity [58]. On the other hand, the NMC-type cathode requires approximately 0.82 kg per kg of NMC-electrode solids[58]. Furthermore, the energy consumption in NMP evaporation has also been identified as another contributor in the study of Deng et al. (2017) [289].

Our study has shown that the climate impact of Li-air batteries (4.86 kg CO₂eq. MJ⁻¹) is consistent with the result of Ribeiro (2019) [1040], who obtained 4.81 kg CO₂eq. MJ⁻¹. The main contribution is the production of the battery module (82%), followed by the cell assembling stage (10%). Unlike Li-ion and Li-S batteries considered in this analysis, where the impact is due to the presence of the active materials (anode and cathode) in the cell, Li-air batteries require O₂ as the active material transferred through the cell via the porous materials on the cathode side (e.g., graphite) [960]. Therefore, the lowest impact is due to no requirements of (climate impact-intensive) cathode processes which, in contrast, occur in the cases of Li-ion and Li-S batteries.

On top of that, the climate impacts of battery manufacturing cannot be directly compared owing to numerous factors such as the modeled battery (e.g., distinguish active materials, its energy density) and types of containers (e.g., pouch cell, cylindrical cell). However, two main contributors have often been reported:

(i) the source of energy, whether in the form of heat or electricity, whichever the battery manufacturing stages are considered (e.g., the preparations of cell compartments including an anode, cathode active materials, the battery cell assembling stage, the packaging productions), which agrees with the findings to other studies [289,1036,1040].

(ii) the emissions during the mine operation regarding the types of batteries. In case of Adv. Li-ion batteries, 26% out of the total impact belonged to the production of Nickel-Manganese-Cobalt (8:1:1) as a cathode active material, the dominant emissions coming from the mine operation stage of cobalt and nickel. Similar trends are observed in the production process of manganese oxide (used for LiMn₂O₄ (LMO) synthesis, as a cathode for the analyzed Li-ion battery), in which 50% of the impact is due to emissions to air. Their impacts are irrespective of the source of energy.

Hydrogen

For the H₂ electrolytic technologies, the climate impacts of alkaline and PEM-based approaches have been estimated at 0.010 and 0.007 kg CO₂eq. MJ⁻¹ H₂ produced, respectively, being lower than the range of other studies [68,69,207,987]. This is mainly determined by the recovered heat, which can potentially avoid the heat production from natural gas reaching 33% of the total impact. However, when the avoided heat impact is not addressed, the obtained results of around 0.02 kg CO₂eq. MJ⁻¹ H₂ is in the range of 0.02-0.032 kg CO₂eq. MJ⁻¹ for alkaline [207,987] and 0.018-0.096 kg CO₂eq. MJ⁻¹ H₂ for PEM electrolysis [68,69]. As reviewed, their climate impacts depend mainly on the electricity source, as also observed in our study. For instance, for the PEM electrolysis, high shares of renewable electricity such as wind generates 0.018 kg CO₂eq. MJ⁻¹ H₂ [68], while the impact increases to 0.096 kg CO₂eq. MJ⁻¹ H₂, where 40% of electricity comes from natural gas [69]. Although our results are generally in line with the existing studies, it highlights that there is no single answer, as the overall results depend on the assumptions and approaches for addressing the co-product generation.

4. Further contribution analysis

The additional results for the contribution analysis are further explained in this section regarding the assessed impacts and time scopes, corresponding to Figs. 4.3 and S4.5.

4.1 Near-term scenarios analysis

Climate change (CC)

Net negative climate impacts are observed from the biofuels FT and ethanol-to-jet approaches, irrespective of service segments. The PFR counterfactual use considered to decay on land is a meaningful contributor in both cases. This is due to the avoided biogenic methane ($27 \text{ kg}_{\text{CH}_4\text{bio}} \text{ kg}^{-1} \text{ CO}_2$ [853]) emitted during the decomposition process. The higher saving impacts are demonstrated in the international segment regarding the more considerable air demands (9 trillion RPK [458]) (saving up to 133-170% (for the FT and ethanol-to-jet) in comparison to fossil kerosene).

The lower impact is found in the case of the FT (reduction of 160-170% compared to the fossil kerosene) relative to the ethanol-to-jet (reduction of 133-144%). This corresponds to the avoided heat (from natural gas), in which recoverable heat is considered from the gasification and the FT processes (accounting for about 9% of the overall climate impact).

In terms of net impacts, the FT and ethanol-to-jet are followed by full electric systems (reduction of approx. 96% only considered for the domestic segment) and H_2 systems (reductions of 80-85%). The main contributor in the former case is the recharged electricity in the red bar. Battery manufacturing and its end-of-life management are insignificant climate contributors.

Electricity consumption in (low-temperature) water electrolysis is the key contributor (green bar). About 64% of its impact is due to the construction materials (e.g., concrete, steel, copper, glass fiber) required for wind turbines, while 16% is due to the refinery process of diesel used in harvesting the wood required for the wood-based electricity portion of the marginal electricity mix. This corresponds to its electricity-intensive processes ($55.90 \text{ kWh kg}^{-1} \text{ H}_2$ for alkaline and $57.12 \text{ kWh kg}^{-1} \text{ H}_2$ for PEM systems). Although the negative results are not addressed in the latter case, the H_2 systems provide better performance in terms of lower tailpipe emissions (NO_x and/or H_2O) from the fuel use (aircraft operations; red) when they are compared to (fossil) kerosene combustions. Additionally, the avoided marginal (natural gas) heat can be compensated with the generation of recoverable heat during water electrolysis (accounting for approx. 24% and 31% of the net performances for the alkaline and PEM electrolysis, respectively).

The equivalent performances to fossil kerosene are displayed in battery hybridization systems, followed by electrofuels. The mass penalty caused by the battery accommodation is of concern in the former case, in which fossil kerosene is required to compensate. In the electrofuels, electricity is the key contributor, derived mainly from H_2 -sourced-alkaline electrolysis (~11% climate impacts). The heat supplied for the DAC process is the second driver accounting for 13-14% of climate impacts (79-80% of the DAC climate standalone impacts). Although heat is avoided, as the recoverable heat becomes marginal heat whether from the FT (50-85% recoverable HT heat; $>100^\circ\text{C}$ [979,980]) or alkaline electrolysis (35-50% recoverable LT heat; $<100^\circ\text{C}$ [970,971]), it is insufficient to provide overall negative impacts. It only reduces the impact with 8-13% in comparison with the fossil kerosene system.

In contrast, the HEFA has the worst climate performance. This is due to the induced heat generated from natural gas ($0.0701 \text{ kgCO}_2 \text{ MJ}^{-1}$ heat produced) instead from WCO, in which the lower climate impact is obtained, i.e. $0.00068 \text{ kgCO}_2 \text{ MJ}^{-1}$ heat produced. This drives the overall impacts of HEFA to be +77-87% relative to the fossil kerosene.

Photochemical O_3 formation (POF)

Results indicate that the full-electric and H_2 systems perform the best (no negative) in the domestic and international segments, respectively. Full-electric and H_2 systems show a benefit of 93% and 54-70% over fossil kerosene. Electricity is observed as the main contributor in both best scenarios, as the recharged electricity for the full-electric (aircraft operation in red) and for water electrolysis (fuel production in green). Therefore, the overall impacts of the larger RPK in the international segment are increasing.

In the H₂ systems, electricity contributes to approx. 73% and 95% in fuel cell and combustion modes, respectively. This is mainly caused by the diesel refinery process utilized in the wood harvesting process (for wood-based electricity production) (63% electricity production impact) and the construction materials of wind turbines (e.g., concrete, steel) (28%). The NO_x emissions from H₂ combustion modes (red) drive the net impact 30-36% higher than fuel cells where only H₂O is considered to be emitted.

Tailpipe emissions generated from the combustions of (fossil) kerosene are the common contributor for all remaining scenarios. Based on the scenarios, this contributes with 21-80% of the net impact. Another common contributor is fossil kerosene production (yellow) owing to sour natural gas (burning) treatment in the extraction step, and heat required during the refinery process.

The best performance is provided by biofuel FT with a reduction of 47% relative to fossil kerosene, followed by the ethanol-to-jet (reduction of 39%). In both cases, the PFR decomposition (avoided 0.065 kg CH₄ biogenic kg⁻¹ PFR DM) results in a negative contribution (about 14% of net results). In the FT, the avoided co-products (e.g., gasoline, wax; ~6%) result in the lowest negative impact detected. On the other hand, the HEFA-induced natural gas for heat production generates 21% of the net POF. This reflects the higher impact from the combustion of WCO (2.20×10⁻⁶ kg NMVOCeq. MJ⁻¹ heat) compared to natural gas (6.08×10⁻⁵ kg NMVOCeq. MJ⁻¹ heat). One negative driver in the HEFA case is the avoided co-products (e.g., diesel, propane) contributing to around 8%. Overall, it is observed that avoiding the impacts of co-products is more significant than avoiding natural gas for heat.

The fossil kerosene system has the worst performance owing to tailpipe emissions (82% net impact). NO_x and NMVOC are associated pollutants accounting for 56% and 24% of net POF impact, respectively. The battery hybridization systems have similar behavior regarding the high volume of fossil kerosene requirements. In contrast, the electricity consumption for alkaline electrolysis is the main contributor for electrofuels (0.74 kWh_{elec} MJ⁻¹ electrofuel produced), representing approx. 27% of the net POF impact. Another contributor is the heat used for the DAC process accounting for 47-56% of the DAC impact (about 2% of the net POF performance). The impacts from avoided co-products and heat are minor (~7% net impact) compared to the positive contributors.

Particulate matter (PM)

The lowest net negative impact was obtained for biofuel FT, driven mainly by the impact of PFR counterfactual use (avoiding the decomposition; 82% net). Ammonia (NH₃) is the associated substance (0.0035 kg NH₃ kg⁻¹ PFR DM). The ethanol-to-jet system follows with the same contributor; however, its conversion yield is lower (0.17 kg PFR DM MJ⁻¹ fuel produced) relative to the FT (0.18 kg PFR DM MJ⁻¹ fuel produced). This results in higher PFR amount and thus in a higher impact of the avoided decomposition. As a result, the net impact of FT and ethanol-to-jet systems decreases with 689-695% and 608-614%, respectively, relative to fossil kerosene. On the other hand, the HEFA demonstrates up to 23% reduction corresponding to the impact of avoided co-product, including diesel and propane (21% of the net PM).

The battery hybridization systems have equivalent impacts compared to fossil kerosene. This is mainly due to the heat supplied (e.g., heavy fuel oil, hard coal) during the fossil kerosene refinery stage, accounting for about 65%. In comparison, the PM impact from the (fossil) kerosene combustion is much lower. Additionally, for the domestic segment, recharged electricity is the significant contributor in full-electric systems showing 40% reduction relative to fossil kerosene.

Electrofuels and H₂ systems here demonstrate worse performance, with a net impact increase of 192-211% and 169-189% relative to fossil kerosene. This is essentially due to electricity consumption of 0.54-0.55 kWh_{elec} MJ⁻¹ H₂ produced, while this amount is up to 0.78-0.79 kWh_{elec} MJ⁻¹ electrofuel produced. The marginal electricity mix owes 89% impacts to the diesel used in the wood harvesting process, and wind turbine construction materials. The NO_x, particulates (<2.5 μm), and SO₂ are the responsible pollutants.

Freshwater eutrophication (EUF)

Full electric (54% reduction) and biofuel FT (54% reduction) systems provide the best benefits (however no net negatives impacts are obtained) for domestic and international segments, respectively. The main contributor to the full electric system is the electricity required in the aircraft use phase. The electricity's impact is dominated by copper mining activities used in wind turbine constructions. In the FT, the impacts of co-products (e.g., avoided gasoline, wax) and a 44% lower impact of the conversion process (green bar), relative to the HEFA, is beneficial to FT's overall performance. Fossil kerosene production is another significant contributor to all hybridized

systems. This is mainly due to the supplied heat from lignite and hard coal used in the refinery process, where the mining operations are the significant sources of pollutants (phosphorus and phosphate).

Electrofuels show the worst impacts owing to electricity consumption, similar to the case of H₂ systems. In the former case, (alkaline) water electrolysis is the main impact generator (up to 69% conversion; 57-58% net impact) relative to the DAC process (contributed to 11-12% net impact). Albeit relatively small, the negative co-product credits reached approx. 13% net impact. As a result, the net impact of electrofuels increases, compared to fossil kerosene, up to 117-120%. EUF also increases up to 99-121% for hydrogen systems.

Marine eutrophication (EUM)

The FT shows the best result among the biofuels (reduction of 66%), followed by the ethanol-to-jet (reduction of 57%) in the international segment. This is due to the avoided PFR decomposition, in which the NH₃ is the associated substance in the EUM impact. In biofuels, the avoided co-products (e.g., diesel, gasoline, wax) resulting in avoided heat demand from hard coal and diesel used in the refinery process have detectable negative impacts. They account for 16% of the HEFA, 8% of the FT, and 3% of the ethanol-to-jet. In contrast, full electric systems demonstrate the best performance in the domestic segment; recharged electricity is the dominant contributor. 63% of its impact is mainly derived from heat sources used in the diesel refinery process, which is further used for wood harvesting. Mining operations to obtain lignite and hard coal as heat sources have been identified as impact sources where nitrogen compounds (e.g., NH₃, nitrite, nitrate) are discharged into the marine environment.

Aircraft operation commonly contributes to all combustible fuels owing to the NO_x emitted. Their contributions are varied from fossil kerosene (78%), to biofuels/electrofuel (37-51% regarding scenarios) and H₂ combustion (23-25%). Another (common) detectable contributor is the production of fossil kerosene (yellow), accounting for 8-21% net impact, depending on the scenarios. This is due to lignite mining operations for heat production to be utilized in the kerosene refinery process.

Electricity is identified as important (green bar) in electrofuels (reduction of 2-9%) and H₂ systems (reduction of 37-60%). The significant electricity impacts in the former case are obtained from alkaline electrolysis (85% conversion; up to 41% net impact) coupling with heat consumption (natural gas) and/or sorbent regeneration in the DAC process (representing 15-18% conversion; up to 8% net impact). This introduces an increase of 2-10% relative to fossil kerosene. However, the avoided credits from recovered heat and co-products (~6% net) are not enough to compensate for the positive impacts. The avoided marginal heat in H₂ systems has a small contribution (2-4% net).

Water scarcity (WS)

The HEFA provides the only net negative impact irrespective of service segments. The net impact decreases by 103%, relative to fossil kerosene, followed by the full electric scenario (only in domestic; reduction of 74%). This is owing to the avoided credits from co-product generation, namely palm oil refinery and petroleum refinery processes (e.g., diesel, propane, and naphtha). They reached about 51% of the overall impact. On the other hand, electricity is a key contributor in full-electric, electrofuels and H₂ scenarios due to cooling water required for heat production, which is further used for the construction materials for wind turbines (e.g., steel, copper, and glass fiber).

H₂ systems do worse than others (+197-224% compared to fossil kerosene) except for electrofuels. The water consumption for electrolysis and liquefaction (approx. 15 kg H₂O kg⁻¹ liquefied H₂[1041]) is another essential driver contributing to 22-23% net. For electrofuels, liquid sorbent has a significantly higher result (+174%) relative to solid sorbent scenario, the water requirement for the sorbent additionally causes this (such as Ca(OH)₂ regeneration) (approx. 12 kg H₂O kg⁻¹ CO₂ captured) accounting for 71% of the conversion (67% net impact result).

4.2 Long-term scenarios analysis

Climate change (CC)

The PFR-based biofuels (whether FT or isobutanol-to-jet) benefit from the PFR counterfactual use (decay on land), for both segments, corresponding to the biogenic CH₄ emission. The net reductions are 309-328% and 260-276% for FT and isobutanol-to-jet. Avoided co-product credits such as diesel, propane, gasoline, etc., are more important relative to the avoided electrified heat in the case of FT, isobutanol-to-jet, and electrofuels.

Full electric and H₂ are the second-best systems in domestic and international services, respectively. Recharged electricity is the main contributor in the former case (reduction of 96%), while the latter is caused by electricity consumption for H₂O electrolysis (accounting for 60–61% net impact). In addition, NO_x emissions contribute to the impact of H₂ combustion modes (up to ~6% higher than fuel cell modes).

Electricity is detected as important contributor to electrofuels impact. It reaches 40–41% of the net impact owing to electricity consumption for alkaline electrolysis (~73–74% conversion) and for the electrified heat (~26–27% conversion for the DAC process). Tailpipe emissions, namely CO_{2fossil}, AIC, NO_x, and H₂O, are crucial contributors in case of fossil kerosene and the hybridized systems, contributing with 85–96% to the overall impact. However, due to technical improvements, the tailpipe emissions contributions is lower (8–30%) for biofuels/electrofuels, while no longer blending mandate with fossil kerosene is required.

Photochemical O₃ formation (POF)

Biofuel FT shows the best performance, irrespective of the segments, owing mainly to the avoided PFR decomposition (CH₄ as the main pollutant). The net impact decreases 97–99% relative to fossil kerosene. Avoided electrified heat has more significant contribution than avoided co-products in most assessed systems, with similar impact contributions (11% net impact of each avoided activity). Among biofuels, HEFA has the worst impact regarding the induced electrified heat (8.29×10⁻⁵ kg NMVOC MJ⁻¹ heat), relative to WCO-based heat (2.2×10⁻⁶ kg NMVOC MJ⁻¹ heat). Full electric systems are the best in POF impact (reduction of up to 93%), the recharged electricity (red bar) being the main contributor.

Electricity-consumption also explain the significant impact of conversion processes (green) in cases of H₂ (reductions ranging from 28–65%) and electrofuels (reduction up to 20%, international). Electricity contributes with 73–97% in H₂ and 58% in electrofuels (whether directly used electricity or electrified heat). H₂ combustion scenarios reach 28–30% larger impact than fuel cell scenarios due to NO_x emissions. Although they are relatively small compared to fossil kerosene impact (almost 80% net impact), the inclusion of tailpipe emissions has influence for electrofuels (~23% net impact) and biofuels (23–30% net impact), because of the emitted NO_x, CH₄, SO_x and NMVOC.

Particulate matter (PM)

Net negative impacts are observed in case of biofuels based on PFR, with reductions of 1,400% (the FT) and 150% (the isobutanol-to-jet system). This is mainly due to the avoided PFR decomposition (~77% net FT impact). On the other hand, the higher conversion of the isobutanol-to-jet (0.15 kg PFR DM MJ⁻¹ fuel produced) with respect to FT (0.18 kg PFR DM MJ⁻¹ fuel produced) process, results in lower impact from PFR decomposition. In addition, the avoided heat (about 6% net) and co-products (2% net) are beneficial to the overall FT system.

Another promising (domestic) scenario is full-electric (-93%), which impact is essentially due to the recharged electricity.

Electricity consumption makes the H₂ and electrofuels to behave worse relative to fossil kerosene. An impact increase of +163–364% and +392–422% is observed for H₂ and electrofuels, respectively. Approx. 95–96% of net impact of the H₂ systems is due to electricity, while the remaining is mostly generated from avoided electrified heat. Similarly, (alkaline) water electrolysis dominates the impact, accounting for 82% of the total impact. This is in addition to the impacts generated from electrified heat requirement and the sorbent production (e.g., NaOH; 44% for the DAC liquid sorbent and polyethyleneimine (PEI); 56% for the DAC solid sorbent). The negative impact (around 15% net from avoided heat and co-product generations) is insufficient to compensate for the overall positive impacts. The HEFA is the worst scenario (+450–461%) due to the induced electrified heat (~71% of the net impact), generating higher PM emissions than WCO-based heat (with a magnitude of +25X; due to PM<2.5μm).

Freshwater eutrophication (EUF)

Isobutanol-to-jet biofuel has the best performance with the lowest net negative result (about 185% reduction). This is because of the avoided petroleum-based co-product (naphthalene sulfonate (NS) production; approx. 48% net impact). This results in the heat generation as a by-product during the pretreatment of coal tar, which avoids using heat from e.g., lignite or hard coal, having more significant emissions owing to the mining operations. Another negative result is provided by FT (138% reduction), where the avoided credits from co-products (30%) and heat (25%) are the main contributors. The HEFA performs the worst system with additional burdens of 277–278%

relative to fossil kerosene. The induced electrified heat is the main contributor owing to a higher positive impact (about 13X increase) relative to WCO combustion. In comparison, the impacts of battery hybridization systems are mainly driven by fossil kerosene production (up to 96% of the net impact), followed by recharged electricity.

H₂ systems show worse performances (+92-233%) due to electricity consumption in electrolysis and liquefaction processes. Electrofuels do even worse because of high electricity demands (particularly for alkaline electrolysis, representing 56-57% net impact). This includes the DAC activities in which electrified heat (representing 8-19% of the net impact) and/or PEI production (48% net for the solid sorbent) are taken into account, depending on the scenario. As a result, negative credits can be observed (approximately 22-23% of the net impact); however, they are insufficient to provide the overall net negative results.

Marine eutrophication (EUM)

The FT route generates the highest impact saving in both segments (reduction of 137-141%; slightly negative impact). These avoided impacts derived from i) 39% PFR decomposition (NH₃ as a responsible pollutant), ii) 13% petroleum co-products, and iii) 14% electrified heat. The FT is followed by the isobutanol-to-jet (-92%) and full-electric systems (-91%, only for domestic). In the isobutanol-to-jet system, the avoided co-products (from the NS production) are more important (about 12% of net impact) than avoided heat (~6% of net impact). This is mainly due to the avoided heat production from lignite, hard coal, where the nitrogen compounds are discharged during the mining activities. Albeit the negative impact of 20% obtained from the avoided co-products (e.g., diesel, propane, palm oil production), the HEFA is the worst biofuel providing only a 12-13% reduction. This is due to the induced electrified heat (44 times increase, owing to NO_x) in comparison to WCO-based heat.

In comparison, electricity significantly contributes to aircraft operation (the full-electric scenarios) and fuel production in H₂ and electrofuel systems. The NO_x generation introduces +32-34% for H₂ combustion relative to the fuel cell scenario. 72-97% of the net impact is dominantly generated from electricity consumption used in water electrolysis. A similar trend has been observed for the electrofuels, where (direct use) electricity for electrolysis and electrified heat for the DAC systems contributed to 59-71% and 3-14% of the net impact, respectively. The PEI sorbent production is another detectable contributor with 6% of the net impact due to the NH₃ and NH₄⁺ emissions during the monoethanolamine production (about 58% in the standalone solid sorbent). This explains better performance of the electrofuel systems, with 10-18% reduction potential than fossil kerosene system.

Tailpipe emission is the dominant contributor, particularly in the scenarios using fossil kerosene (78-98% of the net impact as the worst performance), followed by the fossil kerosene production with 21%. On the other hand, NO_x emissions contributions are found to be lower in biofuels (8-10% depending on scenarios) and electrofuels (approx. 9% of the net impact) in comparison with fossil kerosene. This is because a lower NO_x emission factor (2.10 g kg⁻¹ biofuels/electrofuel combusted[47,49,500,846,995]) is considered compared to fossil kerosene combustion (6.03 g kg⁻¹ fossil kerosene combusted[501,996]).

Water scarcity (WS)

Full electric and the FT systems provide the best result for the domestic and international segments, respectively. They have a 97% and 74% reduction relative to fossil kerosene. The impact of avoided co-products (31% of the net impact) is of higher contribution to FT than the avoided electrified heat production (15%). The isobutanol-to-jet system is the following best scenario because of the avoided co-product credits (from the NS production; 37% of the net impact). The HEFA here has the worst saving impact among the biofuels, and is worse than fossil kerosene (+33-35%). The induction of electrified heat is the cause of higher WS (for electricity production) relative to WCO-based heat showing an increasing of 17 times.

H₂ systems have the worst impact except when compared with the electrofuels. This is due to the water required for electricity generation, which is subsequently applied in the water electrolysis (68% of total impact) and liquefaction process (21-22%). It drives +190-396% overall impact compared to fossil kerosene. The additional water consumption required in the liquid sorbent regeneration put this system at the worst performance (+1,115-1,212%). It has +130% relative to the solid sorbent system, where alkaline electrolysis is a key contributor (~70% of the net impact). It should be highlighted that the production of solid sorbent also contributes to the net impact (11%), almost 79% for the solid-based CO₂ capturing systems.

5. Supplementary figures

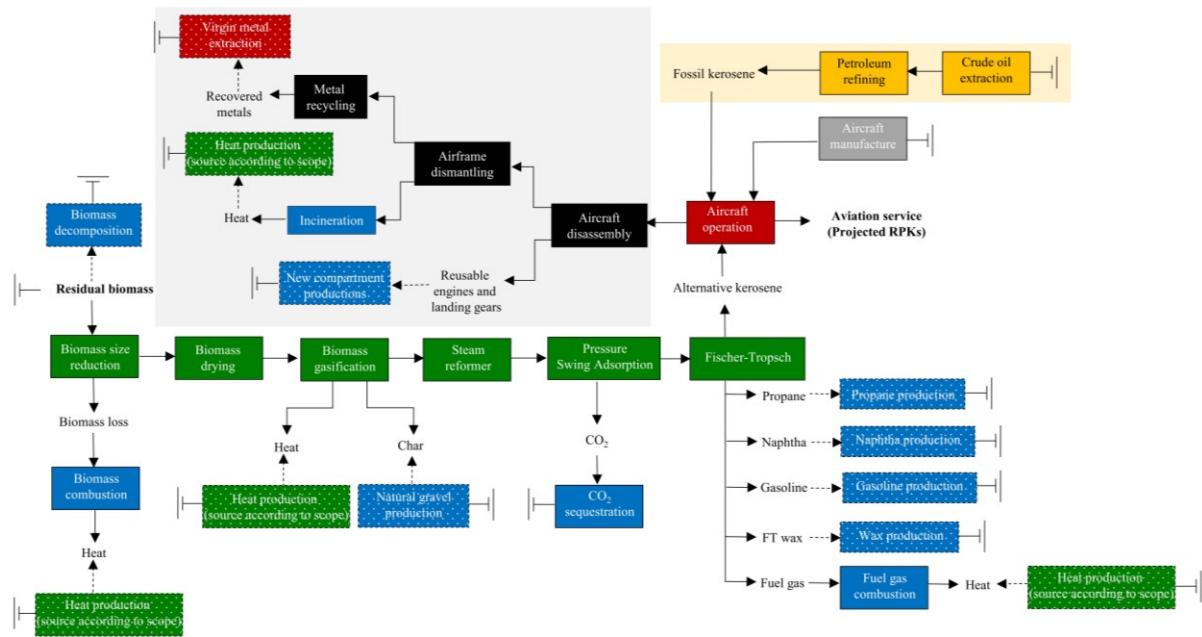


Fig. S4.2 System boundary for the biomass gasification & the Fischer-Tropsch process (FT)

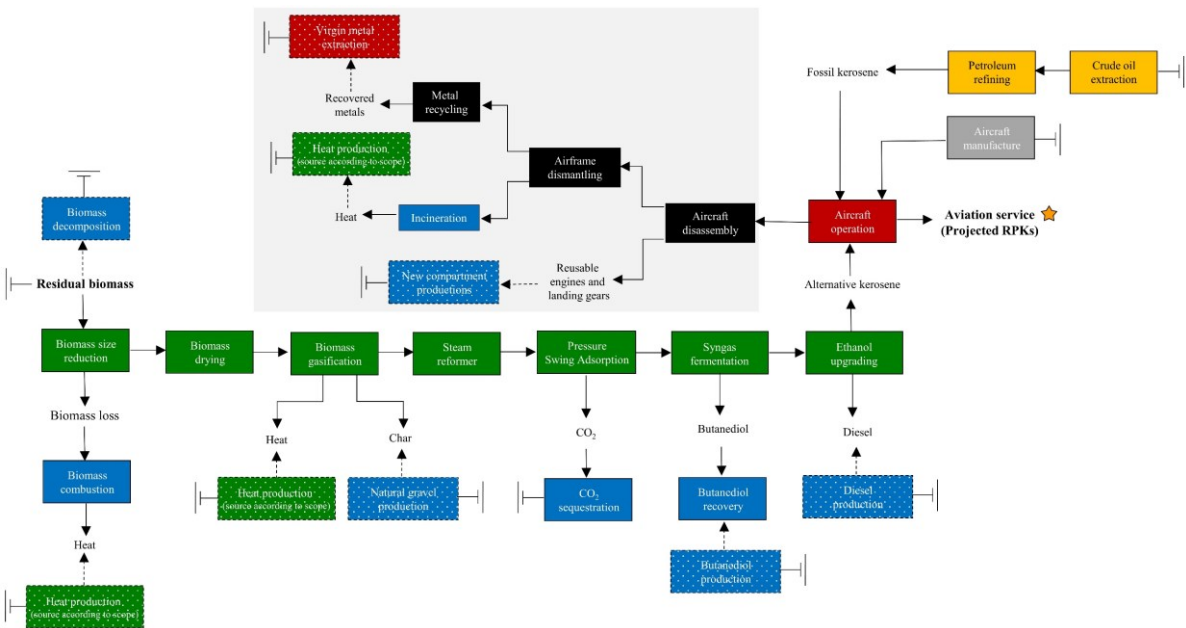


Fig. S4.3 System boundary for the biomass gasification, syngas fermentation & alcohol upgrading (Ethanol-to-Jet) process, applied only for the near-term scope

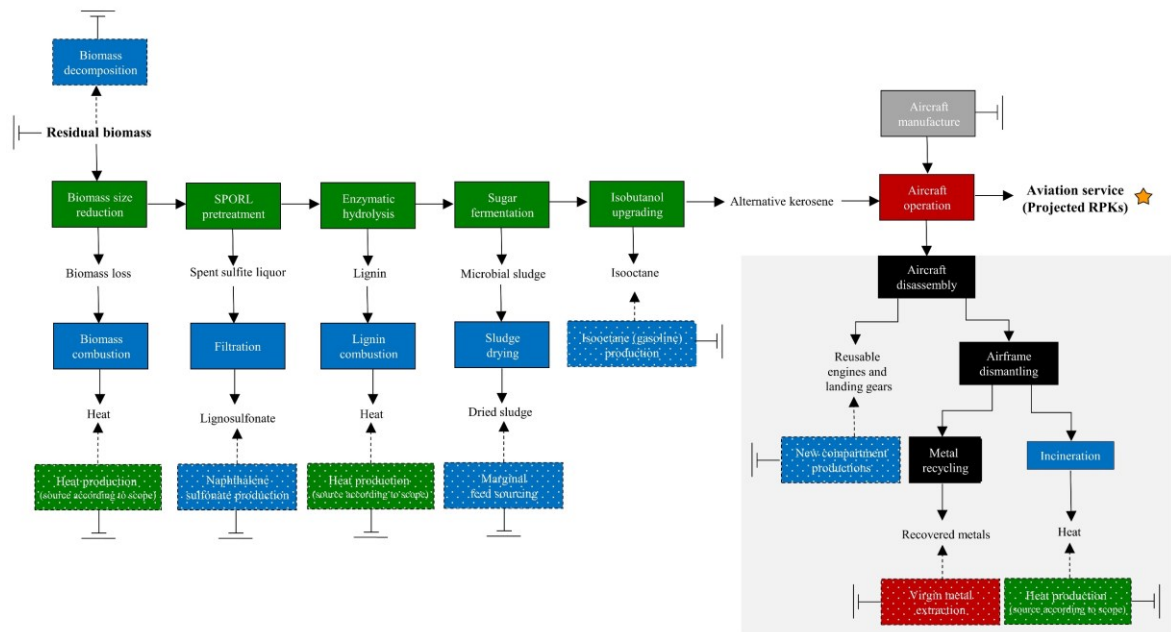


Fig. S4.4 System boundary for the sugar fermentation & alcohol upgrading (Isobutanol-to-Jet) process, applied only for the long-term scope

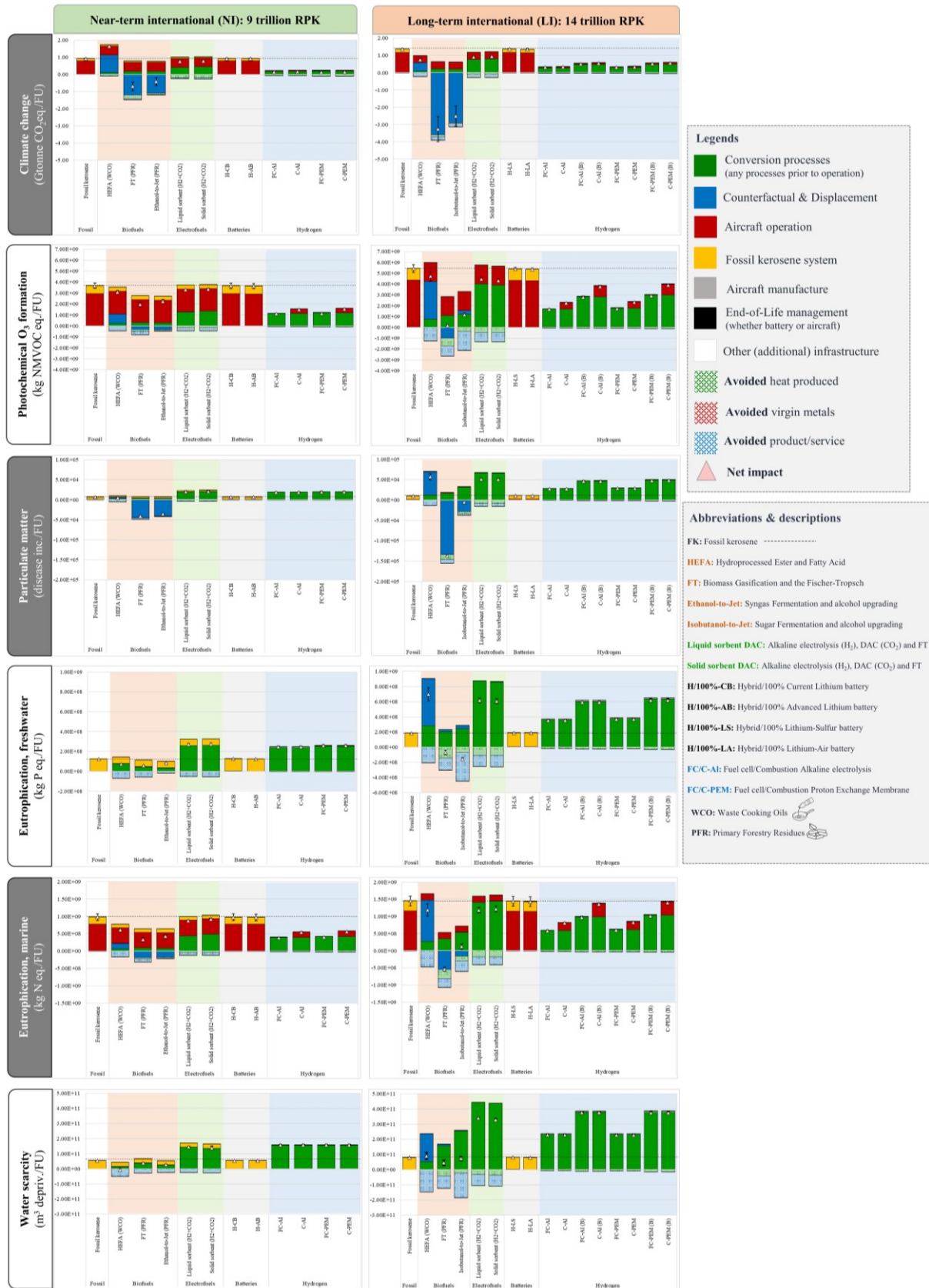


Fig. S4.5 Contribution analysis for near- and long-term time scopes for the international segment of the six assessed environmental impact categories for fossil kerosene (reference system), biofuels, electrofuels, electric (batteries), and H₂ systems. (B): Blended wing body plan's configuration. The contribution analysis for the domestic segment can be retrieved in Fig. 4.3.

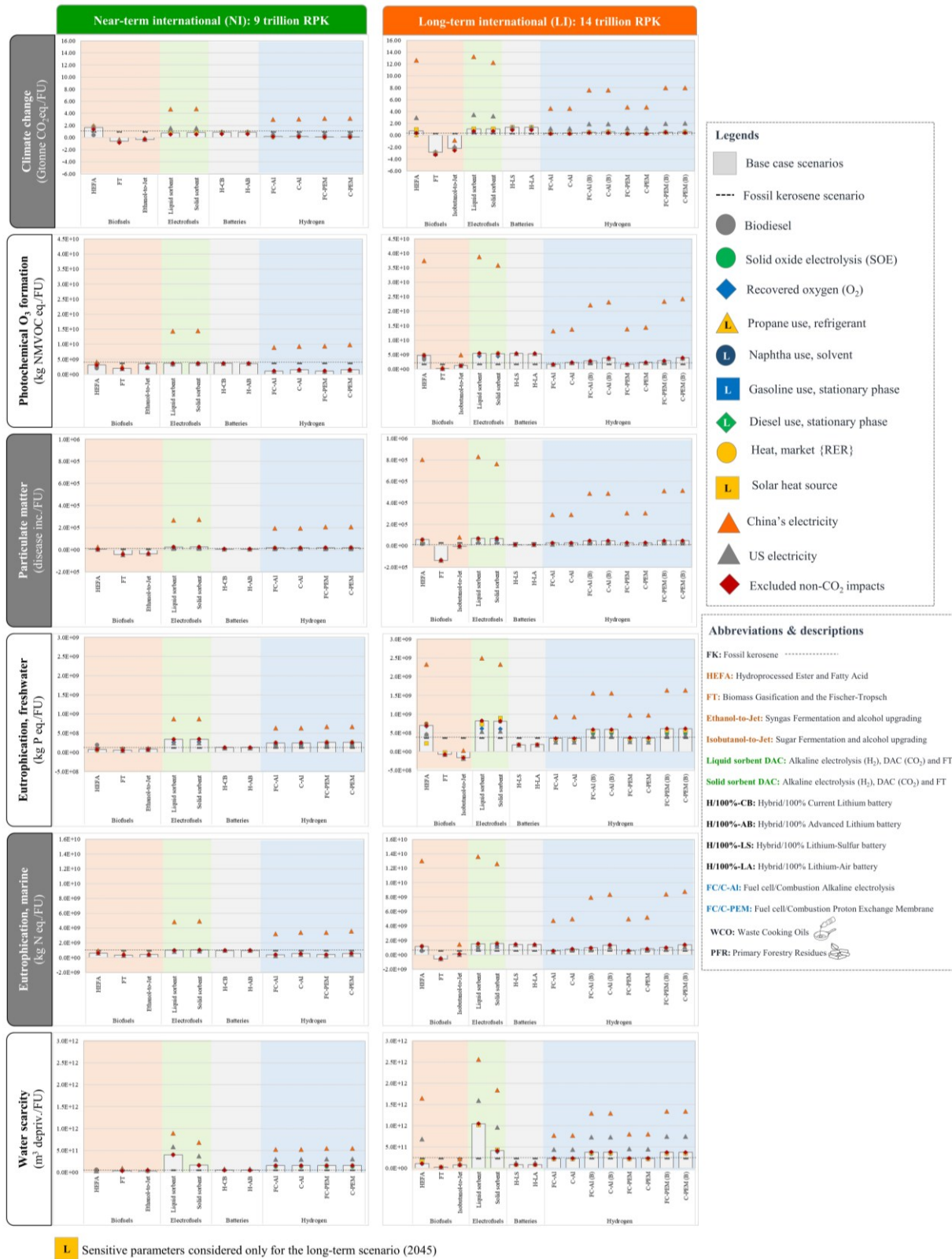


Fig. S4.6 Sensitivity analysis for near- and long-term time scopes for the international segment, of the six assessed environmental impact categories, for fossil kerosene (reference system), biofuels, electrofuels, electric (batteries) and H₂ systems. (B): Blended wing body plane configuration. The sensitivity analysis for the domestic segment can be retrieved in Fig. 4.4.

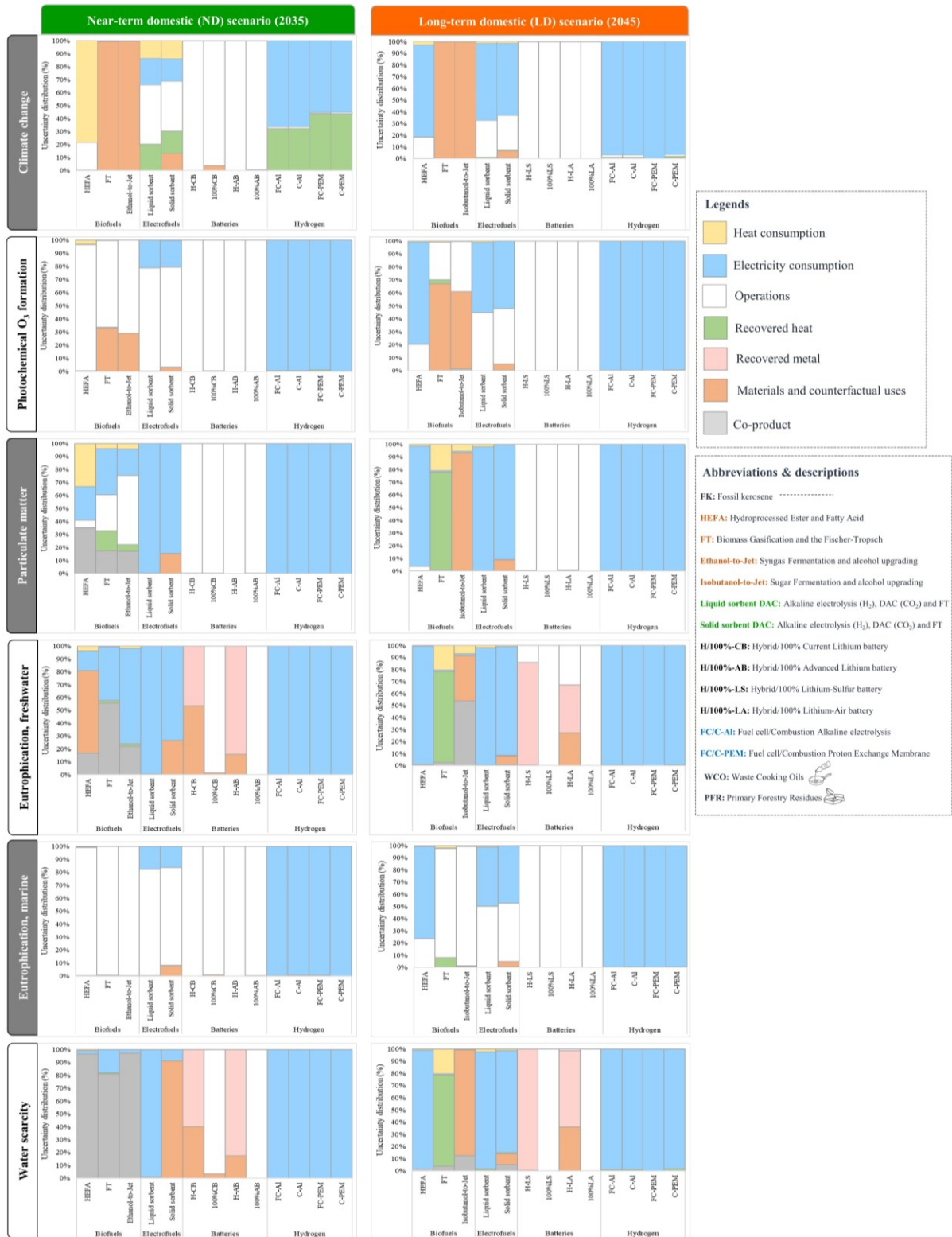


Fig. S4.7 Uncertainty contributions of considered parameters for for the domestic segment (in both time scopes), of the six assessed environmental impact categories, for fossil kerosene (reference system), biofuels, electrofuels, electric (batteries) and H₂ systems. Further details can be retrieved in SM 4.2 GSA folder.

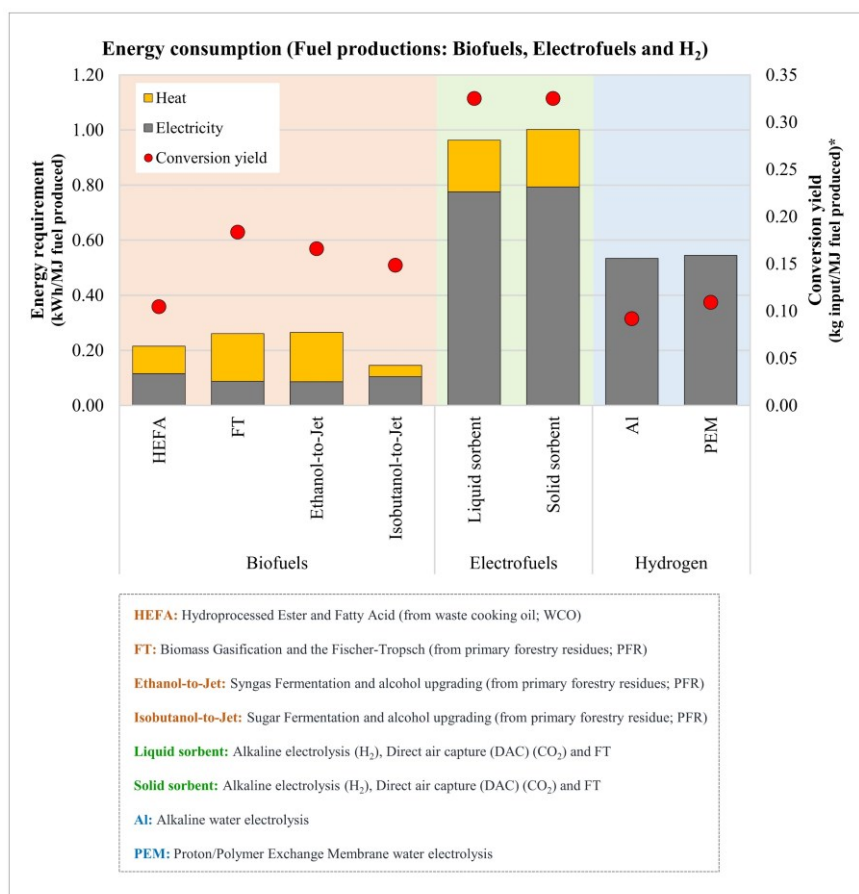


Fig. S4.8 Energy consumption and conversion yields for fuel productions (including biofuels, electrofuels, and H₂). *Biofuel feedstocks are expressed in terms of dry matter (DM), whether waste cooking oil (WCO) or primary forestry residues (PFR). For electrofuel productions, the captured CO₂ and water (for electrolysis) are the primary feedstocks.

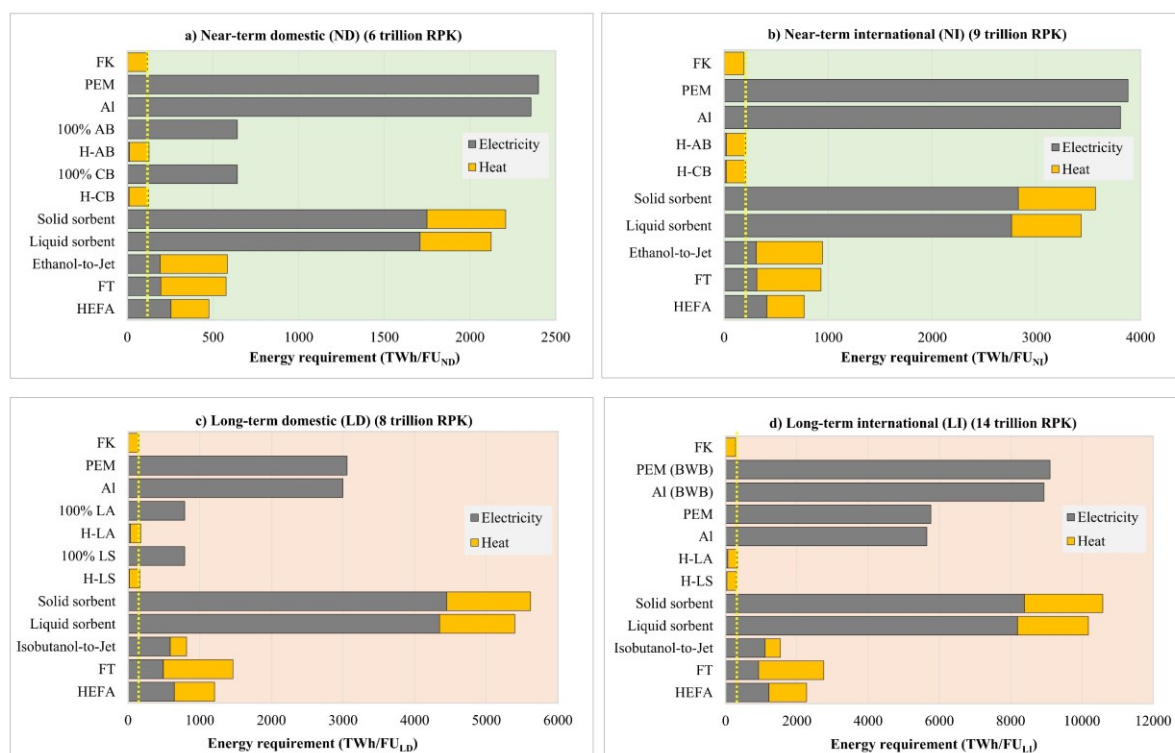


Fig. S4.9 Energy consumption per accessed functional units. A 50% blending mandate is considered for near-term uses of biofuels/electrofuels. Displayed energy consumptions include electricity and heat

demands. For the full-electric systems (100% CB, AB, LS, and LA), this includes recharged electricity (aircraft operation phase; red bar) and battery manufacturing (conversion phase; green bar). The additional energy consumed for fossil kerosene production is further considered in case of battery hybridization systems (H-CB, H-AB, H-LS, and H-LA).

Table S4.2 Key parameters for the GSA (Near-term domestic segment) (Further details in SM 4.2 GSA folder)

Categories	No.	Description (or process considered)	Unit	Baseline values	-10% values
Heat consumption	P1	Hydrodeoxygenation	MJ per kg oils input	3.09	2.78
	P2	Hydrocracking	MJ per kg paraffins	4.17	3.75
	P3	Induced heat, natural gas	MJ per MJ heat produced	1.01	0.91
	P4	Ethanol upgrading	MJ per MJ kerosene produced	0.16	0.15
	P5	Steam reformer	MJ per kg reformed gas	1.02	0.91
	P6	Liquid sorbent direct air capture (DAC)	MJ per kg CO ₂ captured	4.98	4.48
	P7	Solid sorbent direct air capture (DAC)	MJ per kg CO ₂ captured	5.52	4.97
Electricity consumption	P8	Biomass drying	kWh per tonne biomass dry matter (DM)	97.04	87.34
	P9	CO ₂ compression for sequestration	kWh per tonne CO ₂	0.089	0.080
	P10	Alkaline water electrolysis	kWh per kg H ₂	55.90	50.31
	P11	PEM water electrolysis	kWh per kg H ₂	57.12	51.41
	P12	Hydrogen liquefaction	kWh per kg LH ₂	7.53	6.78
Aircraft operations	P13	CO ₂ emissions from fossil kerosene combustions	g CO ₂ per kg fuel combusted	3152	2837
	P14	CO ₂ emission from biofuels/electrofuels combustions	g CO ₂ per kg fuel combusted	3000	2700
	P15	Contrail formation from fossil kerosene combustion	g CO ₂ per kg fuel combusted	3152	2837
	P16	Contrail formation from biofuels/electrofuels combustions	g CO ₂ per kg fuel combusted	30000	2700
	P17	NO _x emissions from fossil kerosene combustions	g NO _x per kg fuel combusted	14.10	12.69
	P18	NO _x emissions from biofuels/electrofuels combustions	g NO _x per kg fuel combusted	2.10	1.89
	P19	NO _x emissions from hydrogen (H ₂) combustions	g NO _x per kg H ₂ combusted	7.87	7.08
	P20	H ₂ O emissions from hydrogen use phase	g H ₂ O per kg H ₂ used	8575	7718
	P21	Recharged amounts of electricity (for full electric aviation)	% overall propulsion efficiency	78%	0.70
Recovered heat	P22	Low-temperature heat recovered (<100°C)	% heat recovered	42%	38%
	P23	High-temperature heat recovered (>100°C)	% heat recovered	71%	64%
Recovered metals	P24	Recovered aluminium	% recovered mass	94%	84%
	P25	Recovered nickel	% recovered mass	100%	90%
Material	P26	Platinum catalyst for hydrodeoxygenation and hydrocracking	Platinum loading (%)	1.20%	1.08%
	P27	PEI used for solid sorbent DAC	g per kg CO ₂ captured	5.25	4.73
	P28	Nickel-Manganese-Cobalt (NMC-811) synthesis	kg NMC111 oxide per kg NMC811	0.92	0.83
	P29	Copper current collector	kg Cu per kg current collector	0.99	0.89
	P30	Al consumption for battery module production	Battery module production	0.61	0.55
	P31	Al consumption for aircraft manufacture	% aluminium contained	59%	53%
	P32	CH ₄ emissions to air from the PFR decomposition	% carbon lost from biomass content	10%	9%
	P33	N ₂ O direct emissions to air from the PFR decomposition	kg N ₂ O-N per kg N (content in biomass)	0.006	0.005

	P34	N ₂ O indirect emissions to air from the PFR decomposition	kg N ₂ O-N per kg NH ₃ -N (content in biomass)	0.014	0.013
Co-products	P35	Replacement of the production of fossil propane	% mass	1.00	0.90
	P36	Replacement of the production of fossil naphtha	% mass	1.00	0.90
	P37	Replacement of the production of fossil gasoline	% mass	0.99	0.89
	P38	Replacement of the production of fossil diesel	% mass	1.08	0.97
	P39	Replacement of the production of petroleum wax	% mass	1.12	1.01

4.6 Appendix: Insights from the first Life Cycle Assessment comparing biofuels, electrofuels, electric and hydrogen systems for aviation

ABSTRACT

This work proposes and applies a methodology to compare, quantify and anticipate, by life cycle assessment (LCA), the environmental consequences of investments into four key emerging alternatives to fossil kerosene for commercial domestic aviation. This includes biofuels, electrofuels, electric battery and H₂ systems. A total of 12 pathways are assessed, for the six following environmental impacts: climate change, photochemical ozone formation, particulate matter, freshwater & marine eutrophication, and water scarcity. The proposed methodological framework includes suggestions for the inclusion of the climate effect generated by non-CO₂ tailpipe emissions, as well as for handling issues of blending, weight penalty or constrained resources while ensuring fair comparisons. It considers two time scopes, namely 2030 and 2050, where different levels of technological advancements are assumed.

Results shows that full electric (batteries) aviation tend to present the greatest environmental performance, over all impacts categories and time scope assessed. This, however, is not true for particulate matter and water scarcity impacts (near-term), where the biofuel “hydroprocessed esters and fatty acids” (HEFA) is not only the system with the lowest impact, but also the only one with a net negative impact. Another exception is for the freshwater eutrophication impact (long-term), where the biofuel isobutanol-to-jet is the only option to display a net negative impact. For all impact categories (but climate change), electrofuels showed the worst performance, reflecting their high electricity demand per functional unit (corresponding to the generation capacity of ca. 5-14 power plants). Hydrogen (H₂) systems generally showed better performance relative to biofuels and fossil kerosene in the climate change and photochemical ozone formation impacts.

This study provides first preliminary results, but additional work will be carried to complete the results. This includes global sensitivity analysis and scenario analysis, among others. International flight segments will also be covered.

Keywords: Electric aviation; Biofuels; Electrofuels; Hydrogen; Life cycle assessment (LCA); Sustainable aviation fuels (SAF); Aviation kerosene

1. Introduction

Commercial aviation (passenger and cargo) represents 88% of global aviation CO₂ emissions, with [13]. ca. 810 Mt CO₂ emissions per year (2019 baseline [1]). Therefore, sustainable aviation fuels (SAF) are encouraged in the endeavor of reducing environmental impacts from the aviation industry. This is for example reflected by the ReFuelEU Aviation initiative (part of the fit for 55 package) [18], where the enhanced use of alternative fuels in aviation, along with the enhanced deployment of the infrastructure they require are explicitly proposed as a measure to achieve the targets of the European Climate Law.

SAF typically refers to drop-in aviation fuels, including liquid biofuels and electrofuels (also known as synthetic kerosene and power-to-liquid) that do not require any engine modification. Here, we instead use the term Sustainable Aviation (SA) systems to extend this definition to emerging alternatives, among others batteries and fuels that could not be directly blended with conventional (fossil-based) kerosene, such as cryogenic hydrogen. In this study, we are interested into four specific categories of SA, which we define as follows:

- Biofuels: Kerosene entirely bio-based, produced either from land-dependent biomass, or from residual biomasses (e.g. waste cooking oil). The sustainability of the biomass feedstock is addressed within the

RED II [19], and six production pathways are already certified by the American Society for Testing and Materials (ASTM) International.

- **Electrofuels:** Kerosene produced from independent H₂ and carbon sources. The vision typically promoted is that these stem from non-biological origin (e.g. CO₂ from the atmosphere and H₂ from water electrolysis, itself power by renewable electricity), but it is not necessarily always the case. Fischer-Tropsch (FT) is the only certified pathway for these kerosene production [733].
- **Battery-electric:** This refers to systems involving the use of batteries as energy sourcing to power aircraft (whether for propulsion, on-board operating systems, or both in a hybridized mode). In contrast with other widely used terms (e.g. all electric systems), it does not encompass all systems involving an electric engine, but those using batteries. Here, two cases are considered: (i) Batteries as the sole energy source to power the aircraft and (ii) Batteries used in hybridization with fossil kerosene. The former system is limited to short-range flights (e.g., approx. 400 km flew by the Heart Aerospace ES-19 [1009]), for planes carrying up to 19 passengers [1009].
- **Hydrogen:** Hydrogen can propel planes via direct combustion, electricity supplied via a fuel cell, or a combination of the two. Renewable hydrogen from water splitting technologies is a prioritized source of H₂. Storing liquid H₂ onboard implies cryogenic temperatures (ca. -253°C; 20K), and the overall system requires many components change in comparison to fossil kerosene systems (e.g. changes in the combustion chamber, H₂ pump, eventual cryogenic heat exchangers, etc.)

Nevertheless, it remains unclear which approach should prevail from an environmental standpoint. While life cycle assessment (LCA) is an acknowledged methodology to quantify and compare the environmental impacts of such emerging alternatives [79], the particular case of Sustainable Aviation poses several methodological challenges that need to be addressed to allow meaningful comparisons via LCA. In an endeavor to bridge this gap, this study proposes and applies a methodology to compare the environmental impacts of the emerging SA systems cited above.

2. Materials and Methods

Emerging technologies selection

For each SA category, the technologies considered as the most relevant for a full LCA were identified through a semi-quantitative ranking framework described in Su-ungkavatin et al. (2021) [1042]. Three key performance indicators (KPI), including costs (CAPEX and OPEX), technology advancement, and foreseen environmental performances, are considered for two future time scopes: near-term (2030) and long-term (2050). Nine production approaches for biofuels, eight possible approaches for electrofuels (with a variety of carbon capture technologies and water electrolysis), five lithium-based batteries, and four water-splitting H₂ production technologies have been selected. The selected technologies, as well as the general technological advancements considered for the two representative time scope, are presented in Fig.4.6.1.

As shown in Fig.4.6.2, two modes of propulsion systems are identified. Combustion mode refers to the system where fuel is combusted to generate a mechanical force that is further used to drive the propeller. In contrast, the electric mode refers to the system where the mechanical force is generated by electricity (from the battery as electricity storage or fuel cell as electricity converter). Currently, at least 50% by vol. fossil kerosene is required to be blended with biofuels/electrofuels on the basis of applying safety standards (e.g., ASTM D7566 [733]). Furthermore, mass penalty indicates that fewer passengers can be carried in a plane compared to the (conventional) kerosene system due to the additional masses (e.g., battery packs; H₂ storage tanks) introduced. End-of-life encompasses the fate of battery packs and aircraft frames, including all disassembling, dismantling and recycling activities, as detailed in [1043].

Life cycle assessment (LCA)

Life Cycle Assessment (LCA) was performed in accordance with ISO 14040/44:2006 [927,928]; accordingly, multifunctionality was handled with the so-called system expansion approach, and the consequences of using constrained resources whose production cannot increase on demand (e.g. waste cooking oil, arable land) are taken into account. This is done by considering the counterfactual use of the resource (i.e. what would have otherwise happened, e.g. combustion for heat production for the waste cooking oil; on-land decay for the primary forestry residues), including the resulting avoided/induced associated effects (e.g. heat no longer produced and compensated for by another heat source for the waste cooking oil case). A generic representation of the actual

system boundary considered is given in Fig. 4.6.2, where all involved processes and activities are classified into seven categories.

The analysis considers that the fuels (biofuels, electrofuels, hydrogen) are produced in France (geographical scope of the analysis), while batteries and other goods typically traded on global markets stem from the international market. To the extent possible, only marginal suppliers, i.e. those reacting to a demand change, are considered. Foreground Life Cycle Inventories (LCI), i.e. those specific to this study, were established based on literature reviews, estimations based on stoichiometry, and advices from experts, as further detailed in Su-ungkavatin (2022; unpublished data) [1044]. Heat recovery with an efficiency of 35-50% [970,971] (for low-temperature heat; $<100^{\circ}\text{C}$), and 50-85% [979,980] (for high-temperature heat; $>100^{\circ}\text{C}$) was considered for all foreground processes generating heat. Besides the H_2 systems, most of the pathways illustrated in Fig. 4.6.1 involve the supply of H_2 . For these, the production of H_2 through alkaline electrolysis was considered; different types of H_2 production are considered only in the H_2 systems (Fig. 4.6.1). All H_2 production systems consider no recovery of the co-produced O_2 . Background (or generic) LCI data were retrieved from the Ecoinvent v. 3.8 consequential database [14]. This among others covers the marginal electricity mix of France (the same mix is considered for the near- and long-term), consisting of 62.20% onshore wind power, 21.85% offshore wind power, and 13.22% biomass (wood) combustion.

LCI dataset detail all input and output flows for each unit operation involved in the system. These flows are translated to actual environmental impacts with the Environmental Footprint (EF) Life Cycle Impact Assessment (LCIA) methodology [1045], as recommended by the European Commission [1046]. Six (out of 16) environmental impacts are addressed. Climate change with an horizon time of 100 years (CC; key contributing substances being well-mixed GHGs, namely CO_2 , CH_4 , N_2O) is considered, being a driver of public decision making due to the climate urgency [978], Photochemical ozone (O_3) formation (POF; CH_4 , CO , NMVOC) and particulate matter (PM; soot, NO_x , SO_2) are chosen because their contributing substances are emitted as tailpipe emissions. In addition, the eutrophication derived from exceeding phosphorus and nitrogen emissions in water compartments is considered, both being identified as vulnerable planetary boundaries [364]. Water scarcity (WS), because of the heavy water demand from both hydrogen production and cooling systems, is also considered as a particularly important impact for the LCA interpretation.

In accordance with the EF LCIA method, the absorption and emission of biogenic C is accounted for with a global warming potential (GWP_{100}) of zero. Negative emissions are accounted for only in the case where a portion of absorbed biogenic carbon, or captured atmospheric C, is not re-emitted within one year, or when a process is avoided. In this study, only the latter case is involved.

The EF methodology is slightly adapted for CC in order to (i) update it with the latest AR6 characterization factors and (ii) include the impact non- CO_2 climate forcers. To this end, the climate characterization factors (CFs; GWP_{100}) of well-mixed GHGs (CO_2 , CH_4 , and N_2O) [853], CO [851], and non-methane volatile organic compounds (NMVOC)[1047] are adjusted according to the latest IPCC Assessment Report (AR6; IPCC 2021). CF for the other aviation forcers (GWP_{100}), including NO_x , soot (black carbon), water vapour, aviation-induced cloudiness (referred to as contrail and cirrus cloud formations), and SO_2 , were retrieved from Lee et al. (2021) [354].

ICAO's projected revenue passenger kilometer (RPK) for 2035 and 2045 has been selected as the functional unit, with a distinction for domestic and international segments. The present study only addresses the domestic segment. Accordingly, the functional unit of this study is to supply 6 trillion RPK and 8 trillion RPK for near- and long-term scopes, respectively.

To relate this functional unit to the four systems assessed herein, hypotheses had to be made on the type of planes used for each system, and on the amount of passengers and cargo carried on these planes, as further detailed in Fig. 4.6.1, and in [1043], along with the full LCA methodological approach.



Fig. 4.6.1 Selected technologies and general technological advancements considered for the two representative time scopes of the analysis. Elements in red highlight differences for the long-term perspective in comparison to the short-term perspective.

Notes.

- ^a A320 is considered a representative model for all scenarios except all-electric batteries planes. The overall propulsion efficiency (OPE; %) for near-term and long-term scopes are 58% and 65%, respectively [332,394], and are shown in the parenthesis.
- ^b The ES-19 is considered a representative model for an all-electric scheme, capable of carrying up to 19 passengers. The overall propulsion efficiency (OPE; %) has been estimated to be improved from around 78% (in the near term) to 87% (in the long term), shown in the parenthesis. They are calculated upon the projected power density of electric motors, converters, and generators[1010,1048,1049].
- ^c The heat sources are selected as illustrative examples for the different time scopes. These options might be locally different regarding resource availability. Low- (LT) and high-temperature (HT) heat are referred to as delivery temperatures of 100°C and >100°C, respectively.
- ^d Mass penalty indicates that less passengers can be carried in a plane compared to the (conventional) kerosene system due to the additional masses (e.g., battery packs) introduced. The all-electric aircraft is not considered as mass penalty because it implies a different aircraft' model (19 passenger plane; the ES-19).

Acronyms (not shown in the figure): PFR (Primary Forestry Residues); WCO (Waste Cooking Oils)

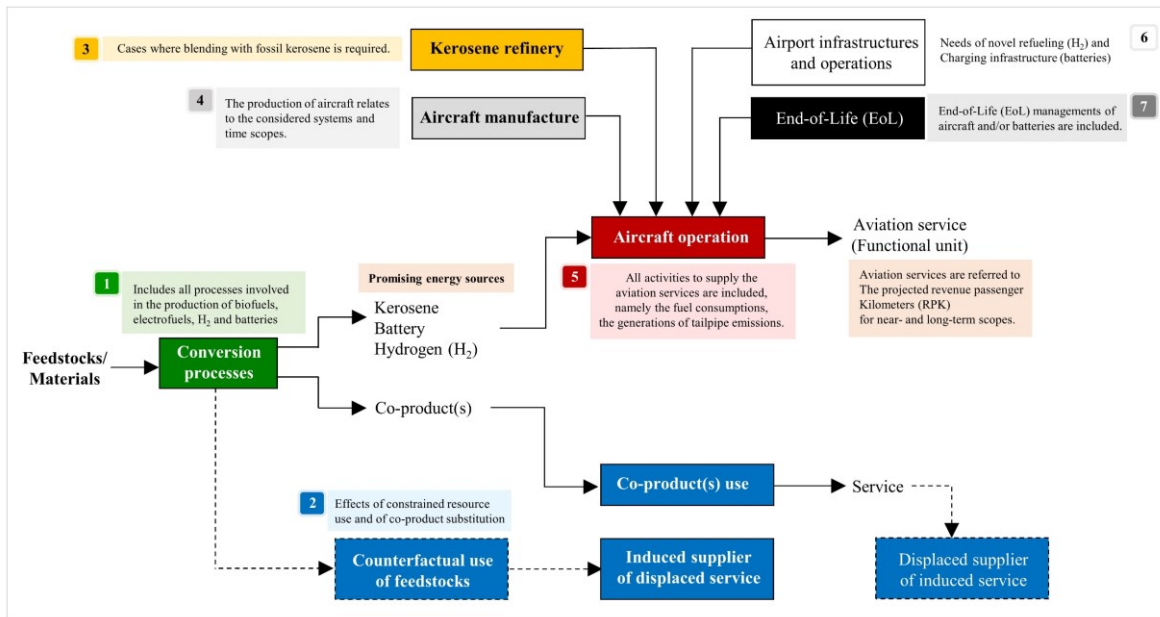


Fig. 4.6.2 System boundaries applied in this LCA framework

Seven categories are defined: conversion process (■), counterfactual use of constrained resources and displacement effect of cro-products (■), fossil kerosene production (■), aircraft manufacture (■), aircraft operation (■), airport-related infrastructures and operations (□), and end-of-life management (■). For the blue category, dotted lines represent avoided processes, and full lines represent induced ones.

4.6.3. Results and discussion

In Fig. 4.6.3, twelve scenarios for each time scope are presented with impacts split in ten contributors (distinguished by color and shade). Results with positive and negative bars indicate the environmental impacts induced and avoided, respectively, while triangles indicate the net scenario performance. Results for other impact categories with their contribution analysis can be retrieved in SM 4.2. It should be highlighted that the functional unit of the two time scopes is different, as described in section 4.6.2.



Fig. 4.6.3 Contribution analysis for near- and long-term time scopes of the six selected environmental impact categories for fossil kerosene (reference), biofuels, electrofuels, batteries (electric) and hydrogen systems.

4.6.3.1 Analysis per environmental impact

In this section, the term reduction refers to reductions in comparison to the fossil kerosene system.

Climate change

Results indicate, for the near-term scope, the full electric system as the one with the lowest net climate impact (reductions of about 96% in comparison to the fossil kerosene), with recharged electricity as the only meaningful

contributor. Battery production and end-of-life, in fact, are shown with negligible climate contributions. In terms of net performance, the full electric system is followed by H₂ systems (reductions of 80-84%) and two biofuels (FT and ethanol-to-jet; reductions of 42% and 26%, respectively). In contrast, electrofuels as well as battery hybridization systems, are shown as equivalent to fossil kerosene. In the latter case, this reflects that the benefits from kerosene are compensated by the mass penalty induced by accommodating the batteries. The HEFA from WCO demonstrates the worst performance, with an increased net impact in comparison to fossil kerosene (+ 63%). This is due to the fact that the WCO is no longer used to deliver heat, thereby inducing the need for equivalent heat from natural gas. Natural gas heat has a higher climate impact (0.065 kgCO₂eq. MJ⁻¹ heat) relative to heat from WCO (0.00085 kgCO₂eq. MJ⁻¹ heat).

Hydrogen systems have the advantage of coupling low (despite not negligible when non-CO₂ forcers are accounted) tailpipe emissions from the fuel use (aircraft operation), with the generation of recoverable heat during water electrolysis. Recovering this heat avoids the use of marginal heat. This also applies for biofuels, and more precisely FT and ethanol-to-jet due to the recoverable heat generated during biomass gasification and the FT process. Similarly, heat is generated and recovered from the FT process involved in electrofuels production. However, it is not enough to compensate the important heat consumption of the direct air capture (DAC) process (representing 13-15% of the contribution to the conversion process in Fig. 4.6.3).

This heat advantage is no longer applying in the long-term results, due to the underlying premise of electrified heat (instead of natural gas; Fig. 4.6.1). Consequently, the gap with fossil kerosene is reduced for the hydrogen systems (reductions of 73-75%), while the counterfactual effect of HEFA is not as important as in the short-term, leading to an overall improvement of the climate effect in comparison to fossil kerosene for HEFA (reduction of 51%). Similarly, a greater gap (reduction of 12-13%) is observed for electrofuels. The overall net improvement for biofuels and electrofuels is also due to the premise that blending with fossil fuels is no longer required, due to the assumed technical improvements (Fig. 4.6.1). For these, the enhanced benefits from avoided co-products is due to two facts (i) there is no blending and (ii) the functional unit (i.e. RPK to supply) is more important. As a result, more co-products are generated, and hence more fossil-based products are avoided (these co-products being essentially diesel, naphtha, propane, etc.).

Photochemical ozone (O₃) formation

The dominant contributor to all systems (except hydrogen), is aircraft operation (red). This reflects the tailpipe emissions of CO, non-methane volatile organic compounds (NMVOC), CH₄, NO_x during combustion of kerosene, electrofuels and biofuels. Based on the inventory data, these emissions are less important than fossil kerosene for all biofuels/electrofuels, as reflected in Fig. 4.6.3. Electricity, on the other hand, is the main contributor to the all-battery operation phase; 63% of its impact is due to the diesel used to harvest the wood required for the wood-based electricity portion of the electricity mix, while 28% is due to the construction materials (e.g., concrete, steel) required for wind turbines.

These electricity-related processes also explain the important impact of conversion processes for hydrogen and electrofuels. Similarly, because the electricity required to produce biofuels (0.09 to 0.34 kWh MJ⁻¹ fuel produced) is lower than the requirements for electrofuels (varying from 0.59-1.00 kWh MJ⁻¹ fuel produced [28,206,955]), the contribution of conversion process to the overall impact is relatively smaller for biofuels. For the avoided contributions, it can be observed that the impact of co-products (avoiding fossil diesel, propane, naphtha, wax) is more important than the one of avoiding natural gas for heat.

In long-term scenarios, when unblended biofuels/electrofuels are considered, the impacts from aircraft operation are significantly decreased. All biofuels involve reductions from fossil kerosene (50 to 65%), among others due to their avoided co-products. On one hand, additional avoided electrified heat makes the FT is the best among biofuels. On the other hand, regarding the induced electrified heat, the HEFA demonstrates higher impact compared to the FT and isobutanol-to-jet route. It should also be highlighted that the counterfactual for biofuels based on PFR appears visible in the long-term where a higher production is involved. All H₂ scenarios provide larger impacts (31-36%) relative to the FT biofuel, except for FC-Al (-0.1%), while electrofuels provided the highest impact, reflecting their high electricity (and electrified heat) demand.

Particulate matter (PM)

Conversion process are shown as important here (green bar), and this is essentially due to electricity. The net impact of H₂ systems increases, relative to fossil kerosene, up to 198%, while this is up to 662% for electrofuels.

For all-battery systems, electricity also contributes to the use phase because of the battery recharge. In turns, the electricity consequential mix owes its impacts to the diesel used for wind turbine construction and the wind turbines construction. The pollutants responsible for the impact mainly comprise NO_x , particulates ($<2.5\mu\text{m}$), and SO_2 . Another detectable contribution is derived from the fossil kerosene refinery, namely the burning of heavy oil in the refinery furnace. Albeit there is a relatively small fraction, the impacts from the combustion of fossil kerosene and biofuels/electrofuels (red bars) can be observed.

HEFA here demonstrates the best performance, with a net negative impact. This is due to the avoided co-products (diesel and propane refinery) and associated substances (particulates $<2.5\mu\text{m}$). In addition, the induced heat from natural gas provides better performance (reduction of 75%) compared to the use of WCO with higher emissions of NO_x and SO_2 . Furthermore, it is found that the biomass (and biomass loss) resulting from size reduction process, whether for the FT or ethanol-to-jet routes, should not be combusted otherwise the PM impact would significantly increase (about +100X magnitudes; due to particulates $<2.5\mu\text{m}$) compared to natural gas-based heat.

Similar trends are found for the long-term scenarios, but here the impact of the counterfactual is notable for HEFA and isobutanol-to-jet, making these two pathways worse than fossil kerosene. Isobutanol-to-jet scenario (+994% relative to fossil kerosene) exhibits the worst performance. This is due to the combustion of lignin (for heat generation) providing higher emissions than avoided electrified heat (with a magnitude of +10X). Albeit the high energy content of lignin (lower heating values (LHV) ranging from 11.2 to 25.6 MJ kg^{-1} [1050]), the other counterfactual use should be considered if the PM is the primary concern.

Eutrophication freshwater (EUF)

All-electric batteries provide the best benefits in the near term. Electricity is the main impact contributor in their aircraft use phase owing to the wind turbine construction (wind power represents 80% of the French marginal electricity mix), which, in turn, is dominated by copper mine operation where the water emissions are mainly derived from the generated tailing streams. Similarly, the impact in case of electrofuels and hydrogen (+204% and +121%, respectively, relative to fossil kerosene), is due to the electricity consumption. Fossil kerosene production has also an important EUF impact and contributes to the impact of all hybridized systems. This is due to the heat source, based on lignite and hard coal, for the refinery process, where the coal mining activities have significant emissions. Biofuels show lesser impacts compared to others, excepting all-electric scenarios. The best biofuel performance is the HEFA, followed by the FT, owing mainly to avoided (fossil-based) co-products (e.g., diesel, gasoline). In addition, avoiding the petroleum products reduces the heat demand and phases out the mine activities where the major impacts are generated.

Electrofuels exhibit the worst results for both near and long term, due to the electricity consumption (with the addition of electrified heat in the long term). The HEFA provides the second worst performance and differs in near and long term. This is because the induction of electrified heat (~50% of the net impact) causes a higher positive impact relative to the heat from combustion of WCO (10X increase). On the contrary, the isobutanol-to-jet scenario shows the best performance with the only net negative result. Avoided petroleum-based co-product (naphthalene sulfonate production) is a significant contributor. This is due to the coal tar pretreatment in which heat is a by-product. The heat generated is avoided by coal-based heat (e.g., lignite, hard coal), with higher impacts due to the mining activities.

Eutrophication marine (EUM)

Aircraft operation (red) is a significant contributor to this impact for all combustible fuels. This is mainly due to the generation of NO_x from fossil kerosene (78%), biofuels/electrofuels (from 32-63% depending on scenarios), and H_2 combustion (23-25%). In case of all-electric scenario and in H_2 systems, electricity is the key contributor. Fossil kerosene production is another contributor for all scenarios using this fuel for hybridization. Heat from lignite and hard coal, applied during the refinery process, is an impact source with nitrogen compounds discharged into the marine environment during the coal mining.

The additional shared impact (27%) is due to the wind turbine construction (e.g., copper mining). Albeit insufficient to drive net negative impacts, the avoided co-products are contributors in the case of HEFA and FT, and electrofuels. The avoided fossil diesel and palm oil (as a substituted lipid source) refineries are significant contributors in the HEFA system. In contrast, the avoided impact from fossil gasoline refinery coupled with the avoided heat (based on natural gas), provide the benefit to the FT and electrofuels, compared with the identical kerosene production (FT) technology.

Although NO_x derived from the combustion of 100% biofuels/electrofuels are significantly decreased in the long-term future (reduction of 85% compared to fossil kerosene), the electrofuels still present the worst performance due to the intensive electricity demands, whether for the electricity itself or electrified heat. To some extent, H_2 combustion systems demonstrate worse performances compared to biofuels. This is owing to the lower NO_x emission factor of about 2.10 g kg^{-1} biofuels/electrofuels combusted [47,49,500,846,995], relative to H_2 combustion ($\sim 7.87 \text{ g kg}^{-1} \text{ H}_2$ [758]). This is additionally due to the avoided impacts from their refinery co-products (gasoline, wax, diesel, propane, palm oil) and recovered heat, particularly detected in the FT case.

Water scarcity (WS)

The HEFA shows the best benefit for the near future (reduction of 105% relative to fossil kerosene), followed by the all-electric scenarios. This result of HEFA is due to the avoided credits from co-products generations, including palm oil refining process and petroleum products refinery (diesel, propane, and naphtha), accounting for 51% net impact. In comparison, electricity is a crucial contributor to all-electric cases, electrofuels and H_2 systems, because of the construction of wind turbines in which metals (like copper, steel) and glass fiber are necessary. In case of electrofuels production, the major contributor is the DAC process (with liquid sorbent) with an increase of +673% compared to fossil kerosene.

Another contributor is the production of fossil kerosene observed in all fossil-hybridized scenarios. This relates to the water required for heat generation necessary in the refinery process. H_2 scenarios are even worse than the others, excepting electrofuels. This is due to water consumption for H_2 production and liquefaction (approx. $15 \text{ kg H}_2\text{O kg}^{-1}$ liquefied H_2) [1041], and to the electricity consumption (through wind infrastructure construction).

All-electric scenarios demonstrate the best results in the long-term scope (reduction of 74-76% relative to fossil kerosene), followed by the biofuel scenarios. Again in case of biofuels, the avoided credits of co-product productions are key contributors (varying according to the scenario), higher than the avoided credits from the electrified heat. The positive impact of the HEFA, out of biofuels, is due to the induced electrified heat which has a higher impact than WCO-based heat. Electrofuels and H_2 have similar trends in the near- and long-term futures. There are no more impacts from fossil kerosene production because the blending is no more necessary for the biofuels/electrofuels utilization.

4.6.3.2 Summary of environmental hotspots

In a nutshell, five key processes can be highlighted as significantly contributing to the six selected environmental impact categories, in either near- or long-term scopes: i) energy consumption (electricity and heat sources), ii) tailpipe emissions, iii) fossil kerosene production, iv) avoided (petroleum)-based products generation, and v) avoided heat production (varying on time scope). This is summarized in Fig. 4.6.4, along with the key activities or substances behind these processes. Electricity (and heat when supplied with electricity) is a particularly important contributor, notably for H_2 and electrofuel systems, for all studied impact categories. It should be highlighted that the electricity considered herein has a high share of renewable electricity ($\sim 80\%$ wind power in the case of the French electricity mix); climate change results would be significantly impacted by the use of a mix considering more fossil resources.

As a general remark, the net impact results are positive values for almost all SA systems, with few exceptions for the biofuels, namely HEFA (near-term) for the WS impact and isobutanol-to-jet (long-term) for the PM impact. This implies that SA systems, even if sometimes mitigating impacts in comparison to fossil kerosene (Fig. 4.6.3), do imply the generation of net environmental impacts. In both scopes, electric aviation scenarios allow significant reductions relative to fossil kerosene (climate change, photochemical O_3 formation, marine eutrophication), but only when batteries are used as the sole energy source. Moreover, it can be noted that for batteries, the type of lithium battery used (current or advanced) does not seem to affect the LCA results; this also applies to the type of conversion considered for H_2 into thrust (combustion or fuel cell mode).

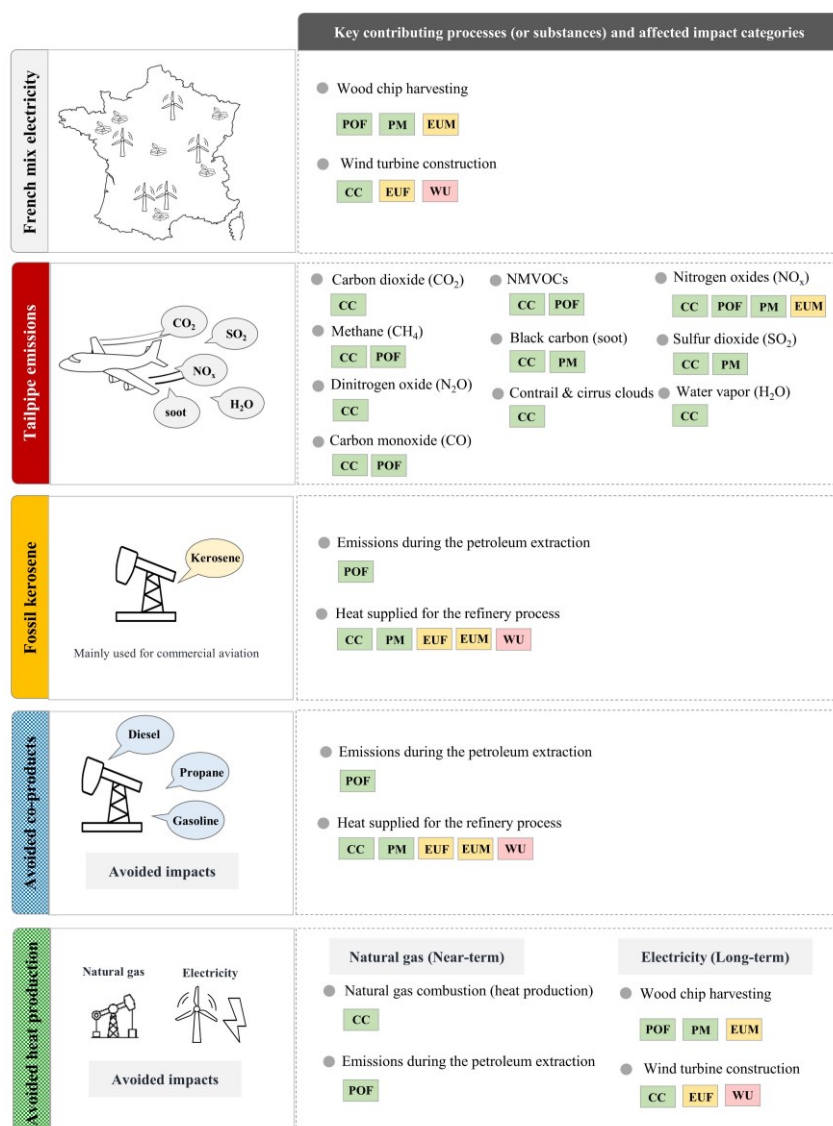


Fig. 4.6.4 Summary of key contributing processes to the environmental performance of the sustainable aviation systems.

Acronyms:

CC (Climate change); EUF (Freshwater eutrophication); EUM (Marine eutrophication); NMVOC (Non-methane volatile organic compounds); PM (Particulate matter); POF (Photochemical O₃ formation); WS (Water scarcity)

4.6.4. Limitations and perspectives

A few limitations of this work in progress should be highlighted:

- A few LCI dataset were approximated by the authors, due to the lack of available public data. This includes, but is not limited to, the production of new types of batteries, as well as most end-of-life processes (recycling of batteries and of novel aircraft compartments composed of new composite materials).
- Non-CO₂ impact calculations: pollutants can have different behaviors depending on where they are emitted. Here, no distinctions were applied in accordance to the specific amount of fuel released in each flight phase, but this may need to be considered in the future. Moreover, the commonly used GWP metric applied in LCA studies cannot fully address non-CO₂ impacts (such as NO_x, contrails, SO₂); here, the characterization factors proposed Lee et al. (2021) [354] were used, but their validity remain challenged.
- The sensitivity of model choices (e.g. the actual counterfactual for the WCO, the actual displacement of biofuels and electrofuels co-products, the heat and electricity marginal mix) has not been tested and should be quantified in future work.

Accordingly, future work includes global sensitivity analysis[986], to uncover to which parameters the LCA results are the most sensitive to, and how uncertain the net LCA results are. Moreover, scenario analysis will be perform

with one-at-the-time scenario change to test: i) the counterfactual use of WCO, ii) the application of high-temperature solid oxide electrolysis (SOE) for H₂ production, iii) the potential of recovering O₂ from water electrolysis, iv) the use of solar heat in long-term, v) the variable sources of marginal electricity (US and China), and vi) the impact of exclusion non-CO₂ tailpipe emissions.

4.6.5. Conclusions

This study compares the environmental performances of four emerging aviation systems: biofuels, electrofuels, electric (batteries), and H₂. Electric aviation systems powered by batteries only were shown as the approach allowing the greatest reductions, relative to fossil kerosene, in both scopes, for most impact categories. This, however, is not true for particulate matter and water scarcity impacts (near-term), where HEFA biofuel is not only the SA system with the lowest impact, but also the only one with a net negative impact. Another exception is for the freshwater eutrophication impact (long-term), where isobutanol-to-jet is the only option to display a net negative impact.

Accounting for the counterfactual use of input residual feedstock, in particular waste cooking oil, had a significant impact on the climate change result (short-term where natural gas heat is induced) and freshwater eutrophication/particulate matter (long-term where electrified heat is induced) for the HEFA pathway.

For all impact categories (but climate change), electrofuels showed the worst performance, reflecting their high electricity demand per functional unit (corresponding to the generation capacity of ca. 5-14 nuclear power plants).

Hydrogen (H₂) systems generally showed better performance relative to biofuels and fossil kerosene in the CC and POF impacts. Battery hybridization is similar to fossil kerosene due to the low degree of hybridization hypothesized.

This study provides first preliminary results, but additional work will be carried to complete the results. This includes global sensitivity analysis and scenario analysis, among others. International flight segments will also be covered.

5

GENERAL CONCLUSIONS & LIMITATIONS AND PERSPECTIVES



CONCLUSIONS

The conclusions regarding the research questions elaborated in **Chapter 1** have been addressed.

1) Biofuels, Electrofuels, Batteries (Electric), and H₂ were reviewed as four promising Sustainable Aviation (SA) systems. This regards their comprehensive attention (with several ongoing projects) in the aviation sector from aircraft manufacturers (including engines and airframes), fuel producers, and policymakers, encouraging their implications in the future. Albeit relevant, other alternatives comprising of liquefied natural gas (LNG), ammonia (NH₃), direct use of alcohol-based fuels (e.g., methanol, ethanol), and solar power, were not considered concerning, for example, the integration systems in the commercial aircraft (although potentially applied), the constraint of renewable production technologies (such as the NH₃), the improved technologies requirements (e.g., photovoltaic cells).

2) The semi-quantitative tool was established in the light to uncover the SA potential. Three key performance indicators (KPI) are identified, including i) four economic perspectives criteria, ii) four technology advancements criteria, and five criteria for foreseen environmental performances, and considered for two future time horizons: near-term (2035) and long-term (2045). In total, 32 approaches, consisting of fourteen production approaches for biofuels (with the possible feedstocks), nine approaches for electrofuels (with a variation of CO₂ capturing technologies and H₂O electrolysis, five lithium-based batteries, and four H₂O splitting H₂ production approaches, were analyzed. In addition, numerous supporting data sources, namely literature, scientific papers, patents, industrial/research organization reports, and announcements, were extracted to score for all addressed criteria and all approaches. In this sense, it thoroughly represents a pre-screening platform that can be further applied and developed to reveal each system's most promising approaches.

Overall, the hydroprocessed esters and fatty acids-based-waste cooking oil (HEFA-WCO), biomass gasification and Fischer-Tropsch process-based primary forestry residue (FT-PFR) were the most promising approaches for biofuels, irrespective of time scopes. In the HEFA, this is due to its high production capacity (only for the near term) or no additional arable land demands to access the feedstock (WCO). For the comparison, the FT benefits from the addition of land demand coupling with its low well-to-wake greenhouse gas (GHG) emissions (around 100% reduction relative to fossil kerosene system). In the near-term, syngas fermentation and alcohol upgrading (SF or ethanol-to-jet derived from lignocellulosic biomass) was the additional promising biofuel owing to its high production capacity. In contrast, the SuF (or isobutanol-to-jet; sugar fermentation and alcohol upgrading from lignocellulosic biomass) was observed in the long term. This is essentially due to its high GHG reduction potential (a reduction of 69%).

For the electrofuels disregarding the assessed time scopes, the alkaline H₂O electrolysis, direct air capture (DAC), and the FT process were the only standing out approaches. This corresponded to its expected 90% well-to-wake GHG emissions reduction when the fossil kerosene is compared. Lithium-ion batteries were the emerging approaches regarding their great maturity. In comparison, lithium-sulfur and lithium-air batteries were the standing-out approaches benefiting from their greater capacity (900-1,300 Wh kg⁻¹ cell) than lithium-ion batteries (400-500 Wh kg⁻¹ cell).

3) A comprehensive and full life cycle assessment (LCA) framework was proposed to ensure transparent comparability of four SA systems. A framework allowing to handle the main challenges includes the blending mandate (for the current use of biofuels and electrofuels) and the mass penalty when introducing the aircraft's batteries and H₂ onboard storage tanks. Ten main activities were simplified to cover the cradle-to-grave approach. This consists of i) the conversion process (fuel production and battery manufacturing), ii) induced activities of services/products, iii) manufacturing of aircraft, iv) the fossil kerosene productions (extraction and refinery), v) fuel/battery use phase in the aircraft, vi) additional requirements of infrastructure, vii) end-of-life management of aircraft and batteries, viii) avoided heat production, ix) avoided services/products, and x) avoided virgin metal productions.

The impacts of non-CO₂ tailpipe emissions are high uncertainty, with the main challenges regarding the limited scientific understanding of the non-CO₂ impact phenomena and the appropriate climate metrics (for short-lived climate forcers such as contrails and water vapor). This is particularly concerning in the perspective approach

when the emission changing rates are not accessible with the new climate metrics (e.g., GWP*, combined global temperature change potential, CGTP). Here, two calculation approaches for non-CO₂ emissions, using the GWP 100 years (GWP₁₀₀), were analyzed: characterization factors (CF) and emission weighting factors (EWF). Approx. 40% climate impact reduction was obtained when the non-CO₂ impacts were excluded, irrespective of the calculation approach. In this sense, they are suggested to include rather than putting a negligible score.

4) Environmental performances of the promising approaches in each system (mentioned in 2)) were studied using the established LCA in 3). Here, it is considered that a technology showed the best performance if it presented the lowest environmental impact for at least four out of six of the environmental impacts studied. In a nutshell, all considered systems demonstrated better environmental impacts for all six accessed categories relative to the fossil kerosene system. This excepts for two cases: i) the HEFA -based WCO for the near-term time scope (for the climate change) and for the long-term time scope (for the particulate matter and freshwater eutrophication), ii) the electrofuels & H₂ systems disregarding time scope for the particulate matter, freshwater eutrophication and water scarcity impacts.

The biofuels were the most promising approach (FT and HEFA) for the near term, followed by the full-electric systems considered only for the domestic segment. On the one hand, the FT gained environmental benefits from the avoided biomass degradation on the land in the climate change, particulate matter, and marine eutrophication (international segment). On the other hand, it should be highlighted that the results heavily depended on the assumption of associated substances (emissions to the air, including NH₃ and CH₄). The HEFA performed the best water scarcity impact associated with the negative impacts of co-products (e.g., avoided palm oil refinery, fossil fuels refinery including diesel, propane). On the other hand, full-electric systems perform better than biofuels. This result is explained by benefiting from no tailpipe emissions in the photochemical O₃ formation and marine eutrophication and no fossil kerosene requirement in the freshwater eutrophication. However, for the international segment, the FT became the best approach in freshwater, and marine eutrophication due to avoided co-product impacts (e.g., gasoline, naphtha) and the avoided PFR degradation (mainly in marine eutrophication). In the photochemical O₃ formation impact, the H₂ fuel cell system provided the best environmental impact owing to lower tailpipe emissions (only H₂O) compared to the biofuel systems (NO_x, NMVOC, CO, and CH₄ as responsible substances).

The HEFA showed the worst climate performance owing to the induced natural gas-based heat (a magnitude 100X higher than WCO combustion). It implied that the WCO should be prioritized for heat production rather than biofuel generation. Electricity is a key contributor in producing electrofuels and H₂ for all accessed impacts and in the aircraft used phase for the full-electric system. On the one hand, the construction materials for the wind turbine are the main contributors to climate change, freshwater eutrophication, and water scarcity impact. On the other hand, the impacts of energy consumption during biomass harvesting were shown in the photochemical O₃ formation, particulate matter, and marine eutrophication.

For the long-term scope, PFR-based biofuel systems perform the best environmental standpoint (four out of six assessed impacts), with avoided PFR degradation as a similar driver in the near term. The FT was the lowest system for all impacts. This excepts for i) the isobutanol-to-jet in the freshwater eutrophication and ii) full-electric systems in the water scarcity (domestic). The avoided naphthalene sulfonate production and recharged electricity were investigated as the key driver, respectively. The HEFA showed a 43–45% reduction relative to fossil kerosene when the electrified heat was induced (<17X lower than WCO combustion), implying WCO is recommended as biofuel feedstock rather than heat production as the opposite to the near-term. The impacts of fossil kerosene production were phased when the no-blending mandate was considered. The induced electrified heat causes the HEFA as the worst performances in the PM (>25X higher than WCO combustion) and EUF (>13X) impacts.

Irrespective of time scopes, battery hybridization systems demonstrate a similar behaviour as fossil kerosene systems, essentially due to batteries' low gravimetric energy density. The type of lithium-based batteries did not insignificantly affect the overall LCA results. This was also applied to the H₂ aircraft's configuration (blended wing body; BWB), considered only for the long-term international segment. Albeit not providing the best systems (except for the near-term international POF), H₂ systems show better relative fossil kerosene performance in climate change, photochemical O₃ formation, and marine eutrophication. The main driver was the lack of non-CO₂ tailpipe emissions (NO_x and/or H₂O).

LIMITATIONS AND PERSPECTIVES

A few limitations and recommendations for further research have been addressed:

- As the full LCA framework, life cycle inventory (LCI) was limited by the lack of available public data, especially for immature approaches/technologies, including the new aircraft systems, the new lithium-based batteries, and their end-of-life management. The future LCA models can be improved when the updated data is accessible.
- Albeit important and impactful, the inclusions of non-CO₂ tailpipe emissions have remained challenging. Their characteristics are varied upon numerous factors, such as reasons, altitude, latitude, and atmospheric conditions (temperature, pressure, humidity), and the complete understanding of their impacts, particularly for contrail formation, is questionable. To which extent and which climate metrics should be applied in the LCA remains unclear. Although the GWP metric might not be able to address those impacts, it was applied regarding its commonly applied in the current LCA studies. Emission factors depending on the flight phase (Landing and take-off; LTO and Climb, cruise and descent; CCD) will be further used to translate the fuel consumption if their data are available. It is suggested that standard procedure for non-CO₂ emissions calculation should be provided at least for the particular context (e.g., national, regional, and global scale).
- It should be aware that environmental impacts depend heavily on the assumption. This is included the mass penalty calculation for the hybridization batteries and hydrogen systems. This also covered the substrates' counterfactual activities (e.g., decomposition of PFR and heat production from WCO).
- It is clear that only one system cannot make the aviation sector reach environmental goals (like carbon neutrality in 2050). Therefore, analyzing several potential approaches (biofuels, electrofuels, batteries, and H₂) is encouraged to demonstrate the possible market share. This should cover the point of the sustainable availability of feedstocks (is it sufficient in amount?), the potential productions from fuel producers (can the technology be improved?), and the readiness of infrastructure (e.g., blending facilities, charging stations). On top of that, the techno-economic analysis is recommended to include to reveal their implications in the future.



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