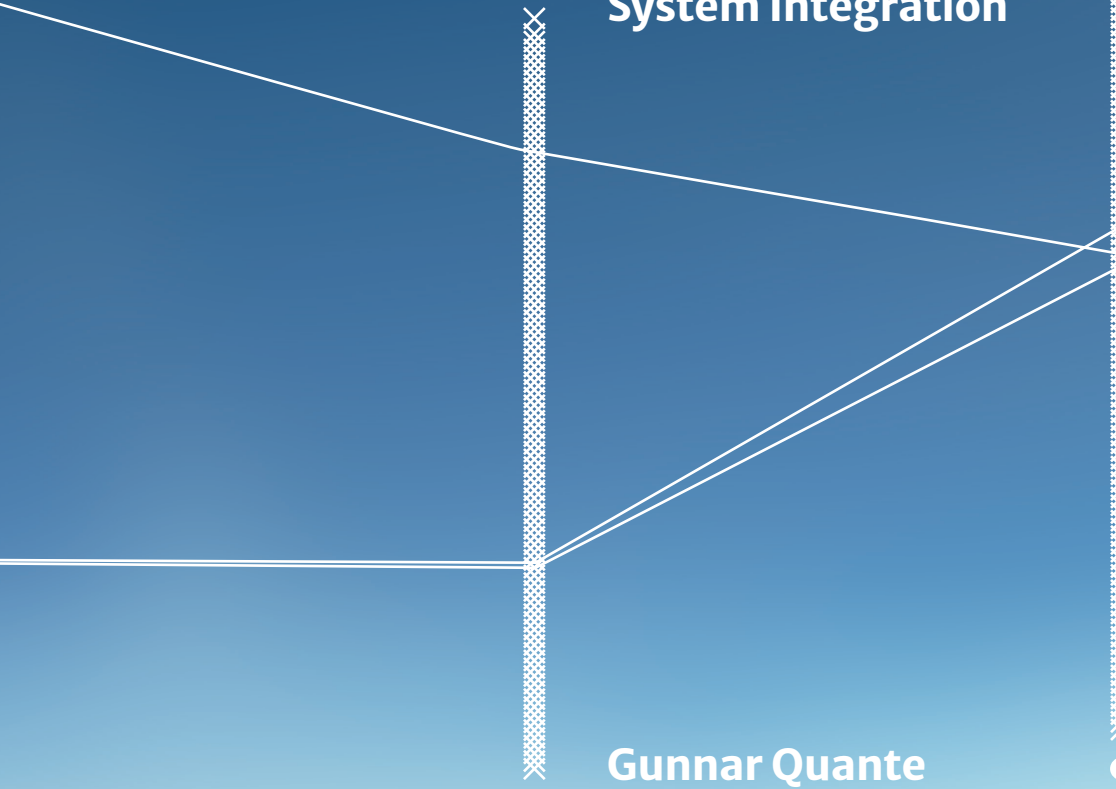
FUEL-RELATED MEASURES TO MITIGATE CLIMATE FORCING OF AVIATION

Fuel Provision and System Integration



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Fuel-related Measures to Mitigate Climate Forcing of Aviation

– Fuel Provision and System Integration –

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ABSTRACT

Climate change is an undeniable reality, with its increasingly severe consequences becoming more evident year by year. Due to its considerable contribution to climate change, also commercial air transport needs to mitigate its climate forcing. Main causes for aviation's climate forcing are contrails, fossil fuel-based carbon dioxide emissions, and nitrogen oxide emissions. These causes are all directly related to the combustion of conventional, i.e., crude oil-based, kerosene in aircraft engines. Thus, identification and integration of alternatives to conventional kerosene might be an option to lower the climate forcing of commercial aviation.

Within this context, the overarching goal of this thesis is to develop a better understanding about the role of fuel-related measures to mitigate climate forcing of aviation and about the factors mainly influencing their climate forcing mitigation potential. Two aspects are examined in detail: The identification of pathways to provide alternative aviation fuels and the integration of such alternative aviation fuels into the commercial air transport system. Concerning fuel provision pathways, altering the properties of conventional kerosene by hydroprocessing is studied as well as the provision of aviation fuels from renewable sources of energy. For the system integration, various strategies to maximize the reduction of climate forcing for a given amount of alternative kerosene are explored and associated operational efforts required to implement such strategies are discussed. Furthermore, central levers for a timely market introduction of alternatives to conventional kerosene are identified.

For a transitional period, additional hydroprocessing of conventional kerosene to lower its aromatics content would allow for substantial short-term contrail-related climate forcing reductions, even when considering additional carbon dioxide emissions released by hydroprocessing itself. Renewably sourced kerosene is essential to mitigate aviation's carbon dioxide-related climate forcing, since it allows to substitute the presently used fossil fuel-based kerosene used in aviation. Furthermore, targeting paraffinic kerosene (either from renewable sources of energy or hydroprocessed crude oil-based kerosene) to flights with a particularly high contrail-related climate forcing can substantially mitigate contrail-related climate forcing. But the associated implications for the system integration of such a strategy become increasingly complex, the more specifically individual flights or even segments of flights are targeted.

ACKNOW-LEDGEMENTS

Pure Vernunft darf niemals siegen
für das Verständnis von Unvernünftigem
Wir brauchen dringend neue Lügen
für die Suche nach Erkenntnis
Die uns den Schatz des Wahnsinns zeigen
für bedingungslosen Rückhalt
Und sich danach vor euch verbeugen:

In its present form, this work appears as if it were the work of an individual. This is clearly not the case. This thesis needs to be viewed rather as the collective effort of several teams, for which I had the lucky opportunity of connecting them.

Team Science: Martin Kaltschmitt and Christiane Voigt – for offering endless learning opportunities, for challenging my assumptions and for constantly raising the questions beyond the question at hand. I would like to express my gratitude towards Professor Hecker and Professor Skiborowski for literally asking the important questions during the defense of my thesis. Furthermore, I would like to acknowledge the importance of the team at aireg e.V. as a bridge towards implementation.

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TABLE OF CONTENTS

ACRONYMS

Acronym	Expansion
ABE	Acetone Butanol Ethanol
ADS–B	Automatic Dependent Surveillance Broadcast
AGWP	Absolute Global Warming Potential
ASTM	American Society for Testing Materials
AtJ	Alcohol-to-Jet
ATP	Absolute Temperature Potential
ATS	Air Transport System
BADA	Base of Aircraft Data
BM	Biomass
BtL	Biomass to Liquid
CH	Catalytic Hydrothermolysis
CoCiP	Contrail Cirrus Prediction Model
CONSAVE	Constrained Scenarios on Aviation and Emissions
COP	Conference of the Parties
CORSIA	Carbon Offsetting and Reduction Scheme for Intl Aviation
DAC	Direct-Air-Capture
DefStan	Defence Standard
dmnl	Dimensionless
ECMWF	European Centre for Medium-range Weather Forecast
EDB	Emission Databank
EF	Energy Forcing
ERA	ECMWF Re-Analysis
ERF	Effective Radiative Forcing
EtJ	Ethanol-to-Jet
ETS	European Emissions Trading Scheme
EU	European Union
EUROCONTROL	European Organisation for the Safety of Air Navigation
FAA	Federal Aviation Administration
FAME	Fatty Acid Methyl Ester
FT	Fischer-Tropsch

Acronym	Expansion
GDP	Gross Domestic Product
GHG	Greenhouse Gas
GtL	Gas-to-Liquid
GWP	Global Warming Potential
HBBA	High-Biofuel-Blends in Aviation
HC	Hydroprocessed Hydrocarbons
HEFA	Hydroprocessed Esters and Fatty Acids
HFS–SIP	Hydrofermented Sugars Synthesized Isoparaffins
IAGOS	In-flight service Aircraft for a Global Observation System
IATA	International Air Transport Association
ICAO	International Civil Aviation Organisation
ISSR	Ice Super Saturated Region
LC	Lignocellulosic
LPG	Liquified Petroleum Gas
MtJ	Methanol-to-Jet
MtO	Methanol-to-Olefins
N/A	Not Applicable
nvPM	non-volatile Particulate Matter
PQIS	Petroleum Quality Information Service
PtL	Power to Liquid
RF	Radiative Forcing
RQL	Rich-Quench-Lean
RWGS	Reverse Watergas Shift Reaction
S	Sugar/Starch
SAC	Schmidt-Appleman Criterion
SAF	Sustainable Aviation Fuel
SK	Synthesized Kerosene
SKA	Synthesized Kerosene with Aromatics
SMR	Steam Methane Reforming
SPK	Synthesized Paraffinic Kerosene
TAPS	Twin Annular Pre-mixing Swirler
TH	Time Horizon
TRL	Technology Readiness Level
TtW	Tank-to-Wake
UCO	Used Cooking Oil
UN	United Nations
USA	United States of America
WtT	Well-to-Tank
WtW	Well-to-Wake

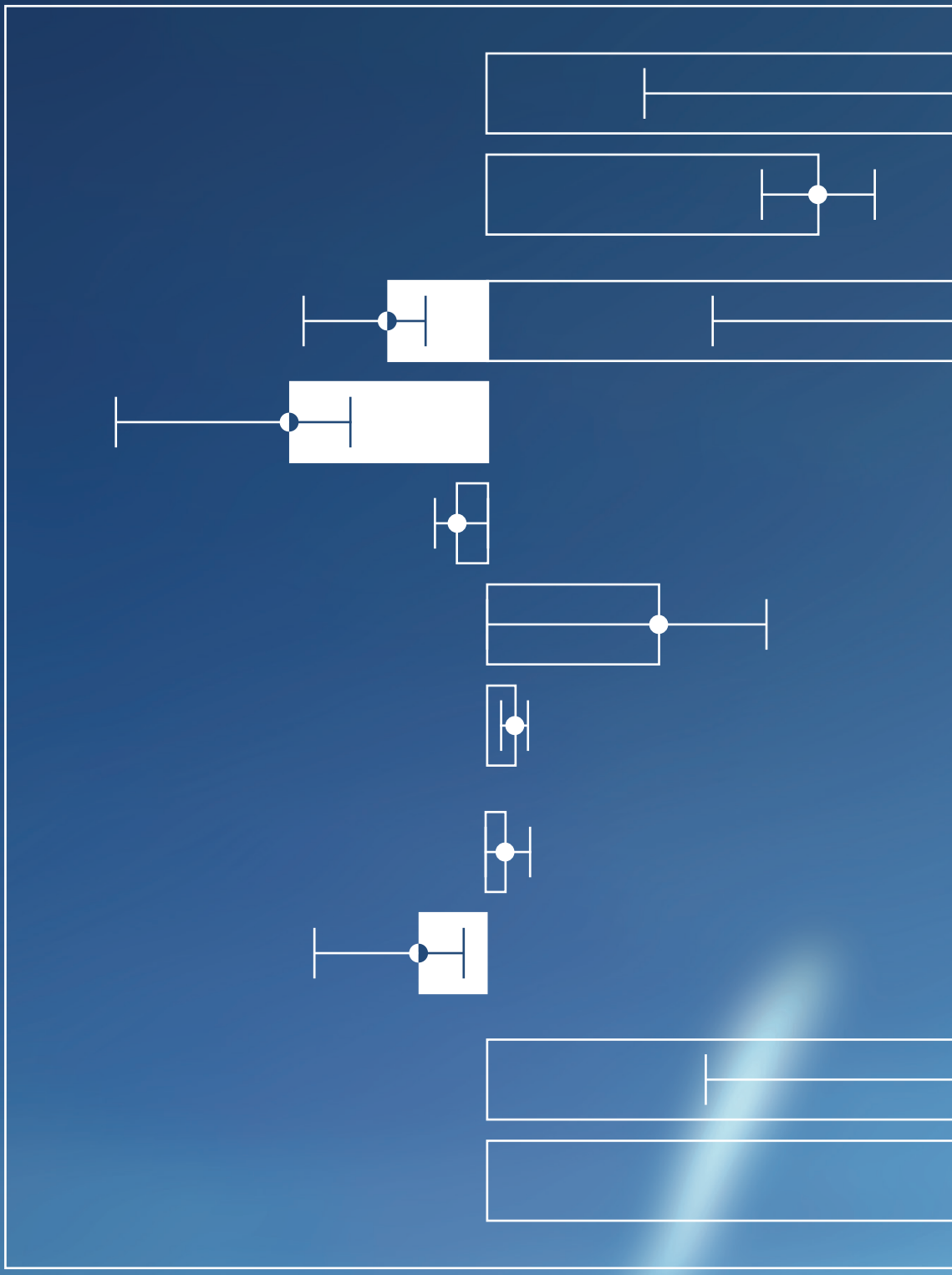
SYMBOLS

Symbol	Expansion
γ^{AF}	Sensitivity to Airline Fares
γ^{C}	Sensitivity to Competition
γ^{CG}	Sensitivity to Congestion
γ^{GDP}	Sensitivity to Gross Domestic Product
γ^{LF}	Sensitivity to Load Factors
γ^{OM}	Sensitivity to Operating Margin
γ^{UC}	Sensitivity to Unit Costs
τ^{AF}	Time to Adjust Airline Fares
τ^{AL}	Aircraft Lifetime
τ^{CA}	Time to Adjust Capacity
$\tau_{contrail}$	Contrail Optical Depth
τ^{CG}	Time to Adjust to Load Factor
τ^{CX}	Time to Cancel an Order
τ^{DT}	Target Aircraft Delivery Time
τ^{E}	Time to Launch/Close an Airline
τ^{ED}	Estimated Delivery Time
τ^{ISER}	Time to Return an Aircraft into Service
τ^{ISTO}	Time to Store an Aircraft
τ^{MC}	Time to Adjust Manufacturing Capacity
τ^{PC}	Time to Adjust Alternative Fuels Production Capacity
τ^{SL}	Time to Adjust Supply Line
$A^{C}(t)$	Adjustment of Airline Fares to Competition
$A^{LF}(t)$	Adjustment of Airline Fares to Load Factors
$A^{UC}(t)$	Adjustment of Airline Fares to Unit Cost
$AF(t)$	Airline Fares
$AF^{REF}(t)$	Reference Airline Fares
$AFI^{I}(t)$	Alternative Fuels Incentives
$AFP(t)$	Alternative Fuels Price
AFQ	Alternative Fuels Drop-in Quota

Symbol	Expansion
$\mathbf{AFS^{TAR}(t)}$	Alternative Fuels Target Share
$\boldsymbol{AFU^{ANN}(t)}$	Annual Consumption of Alternative Fuels
$\mathbf{AGWP_{CO2,TH}}$	Mass-specific, Absolute Global Warming Potential of Carbon Dioxide
$\boldsymbol{AMC(t)}$	Aircraft Manufacturing Capacity
$\boldsymbol{AME(t)}$	Airline Market Entries/Exits
$\boldsymbol{AS(t)}$	Aircraft in Storage
$\boldsymbol{AU(t)}$	Aircraft in Use
$\boldsymbol{CA(t)}$	Capacity Adjustment
$\boldsymbol{CA^G(t)}$	Capacity Growth Adjustment
$\boldsymbol{CC(t)}$	Alternative Fuels Conversion Costs
$\mathbf{CH_4}$	Methane
CO	Carbon Monoxide
$\mathbf{CO_2}$	Carbon Dioxide
$\boldsymbol{CO_2\ EF}$	CO_2 energy forcing
$\boldsymbol{RF_{CO2}(t)}$	CO_2 radiative forcing
$\mathbf{CO_{2e}\ /\ CO_{2eq}}$	Carbon Dioxide Equivalents
$\boldsymbol{CPI(t)}$	Consumer Price Index
$\boldsymbol{CX(t)}$	Aircraft Cancellation Rate
$\boldsymbol{D(t)}$	Air Travel Demand
$\boldsymbol{D^{REF}}$	Reference Demand per Capita
$\boldsymbol{DAR(t)}$	Desired Acquisition Rate
$\boldsymbol{DC(t)}$	Desired Capacity
$\boldsymbol{DPS}$	Flight Distance per Seat
$\boldsymbol{DR(t)}$	Delivery Rate
$\boldsymbol{DSL(t)}$	Desired Supply Line
$\boldsymbol{E^{AF}(t)}$	Effect of Airline Fares on Air Travel Demand
$\boldsymbol{E^{ANN}(t)}$	Annual Carbon Dioxide Emissions
$\boldsymbol{E^{CG}(t)}$	Effect of System Congestion on Air Travel Demand
$\boldsymbol{E^{GDP}(t)}$	Effect of Gross Domestic Product per Capita on Air Travel Demand
$\boldsymbol{E^{OM}(t)}$	Effect of Operating Margin on Number of Airlines
$\boldsymbol{ED(t)}$	Estimated Demand
$\mathbf{EF_{contrail}}$	Contrail Energy Forcing
$\mathbf{EF_{hydroprocessing}}$	Energy Forcing from Hydroprocessing Emissions
$\mathbf{EF_{net}}$	Net Energy Forcing

Symbol	Expansion
$EGR(t)$	Estimated Growth Rate
EI	Emission Index Conventional Jet Fuels
$\mathbf{EI_n}$	Soot Particle Emissions Number
$FU^{ANN}(t)$	Annual Fuel Consumption
$FU^{FLE}(t)$	Fleetwide Fuel Use per Distance
$FU^{NA}(t)$	Fuel Consumption of New Aircraft
FU^{REF}	Reference Fuel Consumption
GDP^{ref}	Reference Gross Domestic Product
$\mathbf{H_2S}$	Hydrogen Sulfide
$\mathbf{H_2O}$	Water
$IOR(t)$	Indicated Aircraft Order Rate
$IS(t)$	Into Storage rate
LF^{REF}	Load Factor
LF^{REF}	Target Load Factor
$\mathbf{m_{CO2}}$	Mass of Carbon Dioxide emitted by Hydroprocessing
MP	Mitigation Potential of Alternative Fuels
n	Degression Exponent for Scale Effects
$\mathbf{N_2}$	Nitrogen
$NC(t)$	Number of Competitor Airlines
NC^{REF}	Reference Number of Airlines
NO	Nitric Oxide
$\mathbf{NO_2}$	Nitrogen Dioxide
$\mathbf{NO_x}$	Nitrogen Oxide
$\mathbf{O_3}$	Ozone
OH	Hydroxide
$OM(t)$	Operating Margin
$OM^{REF}(t)$	Reference Operating Margin
$OR(t)$	Aircraft Order Rate
$P(t)$	Population Size
$PC(t)$	Production Capacity for Alternative Fuels
$PC^{REF}(t)$	Initial Alternative Fuels Production Capacity
$PC^{TAR}(t)$	Target Alternative Fuels Production Volume
$PCO(t)$	Alternative Fuels Production Costs
$PLF(t)$	Perceived Load Factor
PM	Alternative Fuels Production Margin
PR^{MIN}	Airline Minimum Profitability

Symbol	Expansion
$\boldsymbol{RC(t)}$,	Alternative Fuels Resource Costs
RF'	Radiative Forcing of a Contrail Segment
$\boldsymbol{RS(t)}$	Aircraft Returning into Service
$\boldsymbol{RT(t)}$	Aircraft Retirements
$\boldsymbol{S(t)}$	Factor for Economies of Scale
$\mathbf{S_{earth}}$	Surface Area of the Earth
$\boldsymbol{SLA(t)}$	Supply Line Adjustment
$\boldsymbol{SLA^G(t)}$	Supply Line Adjustment for Growth
$\boldsymbol{SO(t)}$	Aircraft Orders
$\mathbf{SO_2}$	Sulfur Dioxide
$\boldsymbol{TI(t)}$	Technology Improvement Rate
$\boldsymbol{TMC(t)}$	Target Aircraft Manufacturing Capacity
$\boldsymbol{UC(t)}$	Airline Unit Cost
$\boldsymbol{W^G}$	Weighting Factor for Growth Adjustment



1

BACKGROUND

1 Background

This chapter describes the fundamentals of aviation climate impacts (section 1.2) and uses powerfuels (i.e., renewably sourced kerosene from non-biogenic feedstock) as example to discuss the mitigation potential of fuel-related measures in terms of the different climate effect categories (section 1.3). The chapter concludes with a discussion to which extent the climate impacts of aviation could be affected by the introduction of powerfuels as one example of renewably sourced kerosene (1.4).

Climate Impacts of Aviation and the Potential of Aviation Powerfuels towards their Mitigation

Quante, Gunnar; Voigt, Christiane; Kaltschmitt, Martin (2025):
Climate Impacts of Aviation and the Potential of Aviation Powerfuels Toward
Their Mitigation, in POWERFUELS: Status and prospects, [S.l.]:
SPRINGER INTERNATIONAL PU, 2025, pp. 879–904.
Typesetting and formatting are slightly adjusted to ensure consistency within this thesis.

Abstract

The UN Conference of the Parties, representing nearly all UN member states, agreed in the Paris Agreement to "hold the increase in the global average temperature to well below 2 °C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5 °C above pre-industrial levels".

The International Civil Aviation Organization (ICAO) and the International Air Transport Association (IATA) have set a "Net-Zero Carbon Emissions" target by 2050. While the Paris Agreement focuses on limiting global temperature increase, the aviation industry targets primarily address CO_2 emissions. However, aviation's climate impact extends beyond CO_2 to contrails and indirect effects of nitrogen oxide (NO_x) emissions. Research shows that only one-third of aviation's climate impact (in terms of effective radiative forcing, ERF) is due to CO_2, with the remaining two-thirds from the other non-CO_2-related climate impacts. The largest climate impacts of aviation, in order, are contrails, CO_2 emissions, and NO_x effects.

Addressing only CO_2 emissions would overlook a significant portion of aviation's climate impact, making it essential to consider all related climate factors to align aviation industry targets with the Paris Agreement. This chapter first describes aviation's climate effects and then explores how increased use of powerfuels as example for renewably sourced kerosene might influence its overall climate impact.

1.1 Introduction

Manifold human activities affect the earth's weather system in the short-term and the climate system in the longer term. The primary cause of these substantial changes is the combustion of fossil fuel-based energy carriers, resulting mainly in carbon dioxide (CO_2) emissions. In addition, emissions of other climate-effective gases such as methane (CH_4), nitrous oxide and halogenated gases, aerosols and their direct and indirect effects on clouds (e.g., aviation contrails) contribute to anthropogenic climate change (Figure 1.1).

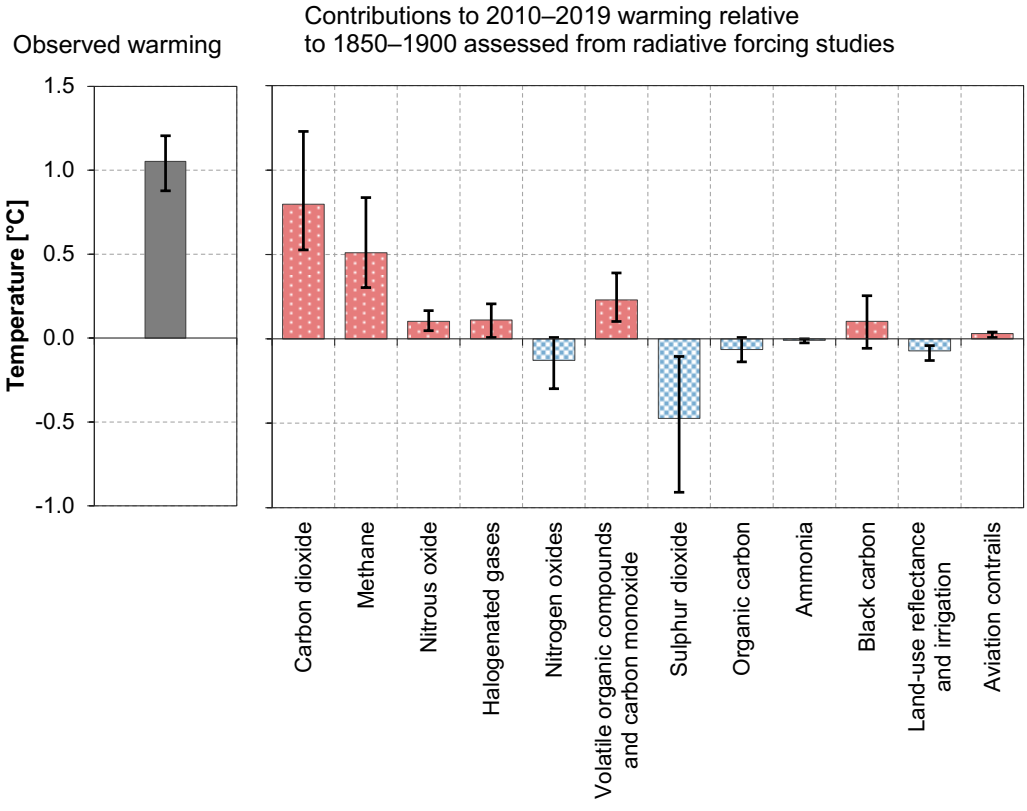


Figure 1.1 Observed global warming (left) and associated drivers (right), adopted from [1]

The influence of human activities on weather and climate results not only in an increase of globally averaged surface temperature levels. Furthermore, global mean sea levels increase, glaciers retreat, extreme weather events such as concurrent heatwaves and heavy precipitation occur more

frequently and climate zones are shifting poleward [1]. These developments are more and more visible; e.g., basically all glaciers within the European alps are rapidly disappearing since a couple of years.

Hence, the UN Conference of the Parties (COP), representing almost all United Nations (UN) member states, agreed within the so-called Paris Agreement to "hold the increase in the global average temperature to well below 2 °C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5 °C above pre-industrial levels" [2].

A central element of this Paris Agreement is the definition of nationally determined contributions, which require each party of the agreement to lay out mitigation measures to constrain anthropogenic climate change to the abovementioned global average temperature increase [2].

The national framework of the nationally determined contributions is difficult to apply to international transport modes, such as aviation and the maritime sector; e.g., the greenhouse gas (GHG) emissions for a flight / ship journey carrying passengers / freight of various nationalities from one country to another, potentially even with an intermediate stop in a third country, can be allocated in manifold ways.

The two international aviation organizations, the International Civil Aviation Organization (ICAO) and the International Air Transport Association (IATA) both defined a "Net-Zero Carbon Emissions" target by 2050 [3, 4]. Both targets focus on the abatement of CO_2 emissions, while the Paris Agreement defines a maximum in globally averaged temperature change. This difference is important because the climate impact of aviation does not only result from "classical" greenhouse gases like CO_2, but also from contrails and indirect effects of nitrogen oxide (NO_x) emissions (among others). The current state of research attributes around one third of aviation's climate impact (in terms of effective radiative forcing (ERF)) to CO_2 emissions and the remaining two thirds to other, so-called "non-CO_2" climate terms [5]. The largest climate effects of aviation are (by decreasing order of magnitude) contrails, CO_2 emissions and indirect effects from NO_x emissions. Mitigating only the climate impact of aviation's CO_2 emissions would omit a significant share of aviation's climate impact. Therefore, a consideration of all aviation-related climate terms is indispensable to align the aviation industries mitigation targets with the Paris Agreement.

The aim of this paper is to describe and characterize the climate effects of aviation and then to discuss the effects of a potentially increased use of

powerfuels[1] onto aviation's overall climate impact. The paper is structured accordingly, while the discussion of the individual climate terms is sorted by their magnitude in terms of effective radiative forcing (ERF).

1.2 Climate Impacts of Aviation

The aviation sector consumed around 300 Mt of fuel (mainly fossil fuel-based kerosene) in the year 2018 resulting in CO_2 emissions of about 1 Gt (2018) [5, 6]. This corresponds to approximately 2.4 % of the worldwide anthropogenic CO_2 emissions and ~0.9 % of the anthropogenic effective radiative forcing due to emissions of greenhouse gases (GHG) [5, 7]. Contrails and indirect effects from NO_x emissions (among others) increase the overall climate impact beyond gaseous emissions. Keeping this in mind, an assessment of aviation's impact on climate available to date estimates a climate impact for the time period between 1940 and 2018 to 101 mW/m² in terms of effective radiative forcing (ERF) [5]. This corresponds to 3.5 % of the overall anthropogenic climate forcing of 2 840 mW/m² (time span 1750 until 2019) [7].

Following Figure 1.2, the most prominent effect of aviation on climate are contrails, in particular contrail-cirrus cluster at night. Compared to that, CO_2 emissions and indirect effects of NO_x emissions contribute less to the effective radiative forcing (ERF). Beside this, water vapor emissions in the stratosphere, aerosol-radiation effects and aerosol-cloud interaction have a still relevant but smaller climate impact than the aforementioned climate terms [5]. Below, those climate terms and their cause-and-effect relationships are described in detail.

1.2.1 Contrails

The climate impact of contrails has been estimated as 57.4 (17 to 98) mW/m² in terms of effective radiative forcing (ERF). This corresponds to ~56 % of the overall aviation-related effective radiative forcing (ERF) until 2018 [5].

[1] In the context of this chapter, the term "powerfuels" refers to fuels produced based on electrical power. "Aviation powerfuels" more specifically denotes powerfuels suitable for the use in aviation turbine engines.

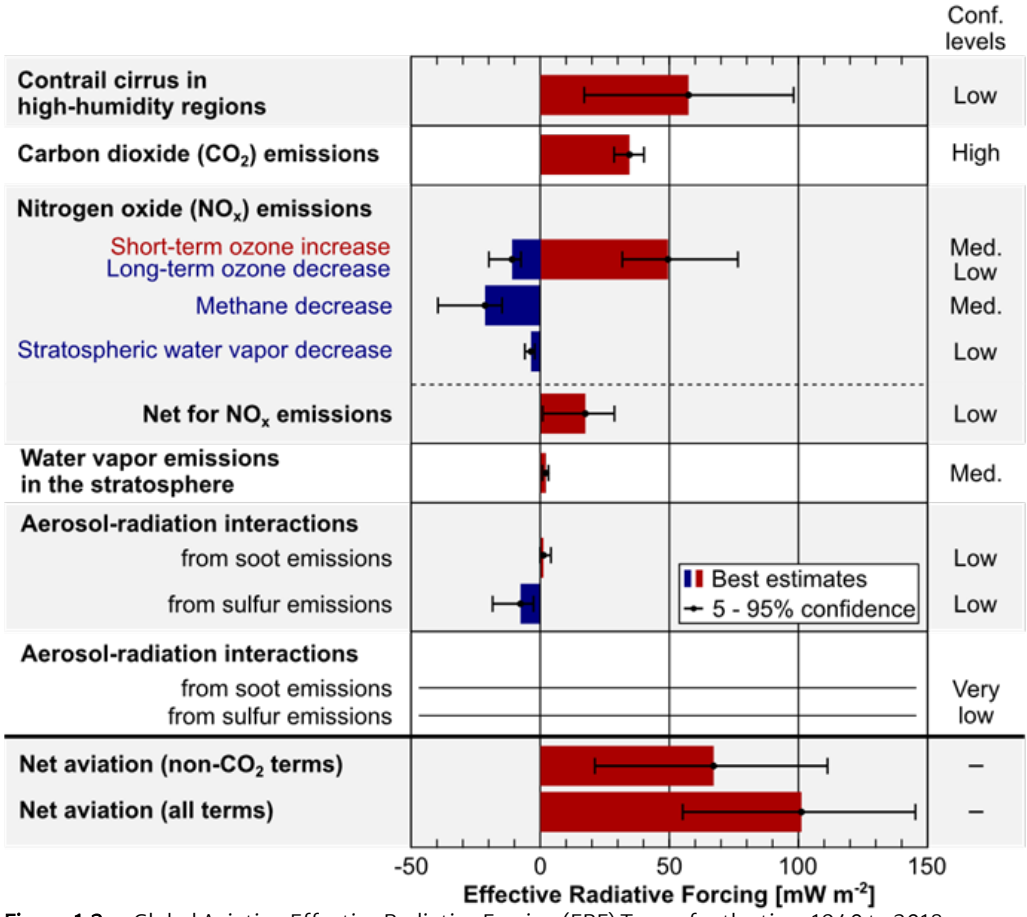


Figure 1.2 Global Aviation Effective Radiative Forcing (ERF) Terms for the time 1940 to 2018, adopted from [5]

The formation of contrails is triggered by particles (soot and aerosols) emitted from aircraft engines. These particles serve as condensation nuclei initiating the condensation of water. When during a flight at the typical cruising altitude of a commercial airplane, the hot engine exhaust mixes with the cool ambient air, rapidly cools down and can reach values above the saturation vapor pressure. In those cases, the water vapor will condense on the nuclei, freeze instantaneously and form a line-shaped condensation trail ("contrail") behind the respective aircraft engine / turbine [8]. These contrails affect the earth's radiative balance by scattering incoming solar radiation (cooling effect) and absorb outgoing terrestrial heat radiation (warming effect). Hence, the climate effect of an individual contrail strongly depends on the time of the day or more precisely the solar zenith angle. In general, around noon contrails tend to have a cooling climate impact, while

they have a clearly warming impact at night, as they do not scatter any solar irradiation, but absorb the outgoing terrestrial heat radiation and reemit it at a colder temperature compared to the ground.

Figure 1.3 shows the cumulative density function for annual energy forcing (EF) by share of contrail forming flights for a global fleet dataset between 2019 and 2021 [9]. Thus, only ~20 % of the flights produce contrails. Most of them are short and medium range flights during the day and are therefore characterized by a slightly cooling effect. Nevertheless, the impact of warming contrails clearly outweighs cooling contrails. As a result, the net impact of aviation contrails on global climate is warming. Simultaneously, the majority of the warming contrail climate impact is caused by less than 5 % of all flights.

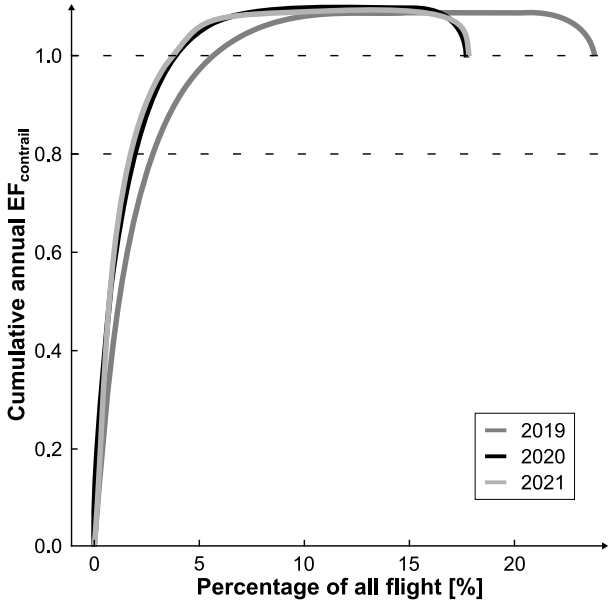


Figure 1.3 Cumulative density function of the annual energy forcing (EF) of the percentage of contrail forming flights (for simplicity, warming contrails are described by EF values > 1 and cooling contrails by EF values < 1) adopted from [9]

The contrail climate impact over the time of the day is shown for flights in the North Atlantic flight corridor for each day in the year 2019 in Figure 1.4 [10]. The distinction between a mainly warming impact at night (red colors) and a predominantly cooling impact during day (green colors) can be seen by the horizontal change in contrail cirrus net radiative forcing (RF). As all investigated flights take place on the Northern hemisphere, a seasonal trend becomes visible by the vertical change in Figure 1.4. On the

Northern hemisphere, days are shorter in winter and accordingly, times with a warming contrail climate impact increase for winter days.

Contrail formation is initiated when the mixture of aircraft engine exhaust and ambient air becomes supersaturated with regard to water under the presence of condensation nuclei. The thermodynamic conditions (temperature, humidity) under which a supersaturation and thus contrail formation occurs, can be determined by the Schmidt-Appleman criterion (SAC) [11, 12]. They depend on the local meteorological situation (pressure and humidity of the surrounding air) and selected aircraft properties (e.g., propulsive efficiency, released combustion heat and water vapor emissions due to fuel combustion) [11, 13, 14].

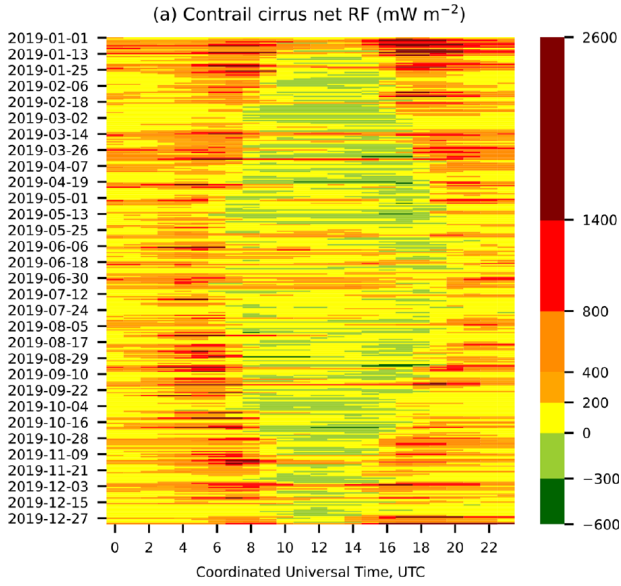


Figure 1.4 Contrail cirrus net radiative forcing (RF) by time of day (x-axis) and calendar day (y-axis), adopted from [10]

Different particles can serve as condensation nuclei for aviation contrails. Aircraft engines emit soot and ultrafine aqueous particles. Additionally, the ambient air contains typically high numbers of aerosols. The amount of soot emissions for a given engine are strongly affected by fuel composition on the fuel side and design aspects as well as the maintenance situation on engine / turbine side. Aviation kerosene typically consists of different hydrocarbon species, such as straight chain alkanes, cycloalkanes and aromatics. Especially aromatics act as an initial soot precursor, due to their molecular

structure, specifically the strong molecular bonds in the aromatic ring. Among different hydrocarbon components contained in jet fuel / kerosene, the soot formation tendency roughly decreases from poly- to monocyclic aromatics via cycloalkanes towards alkanes [15].

The variation of the molecular structure of the hydrocarbon species also affects the mass fraction of hydrogen contained. For example, the alkane Tridecan ($C_{13}H_{28}$) shows a hydrogen content of ~15.2 m-%, cycloalkanes have a hydrogen content of ~14.3 m-%, the mono-aromatic Benzene is characterized by a hydrogen content of ~7.7 m-%, and the bicyclic naphthalene ($C_{10}H_8$) shows even a hydrogen content of ~6.3 m-%. Therefore, for currently used engines / turbines in commercial airplanes, the hydrogen content of a particular kerosene can serve as simplified estimate for its sooting tendency [15–19].

Particulate matter emissions of most modern aircraft engines / turbines range from 10^{14} to 10^{16} particles/kg – fuel (soot-rich regime, Figure 1.5). For these engines / turbines, soot particles are the predominant condensation nuclei. Here, the number of ice crystals formed under the respective weather conditions within the cruising altitude is roughly proportionate to the number of soot particles emitted [17, 20–23].

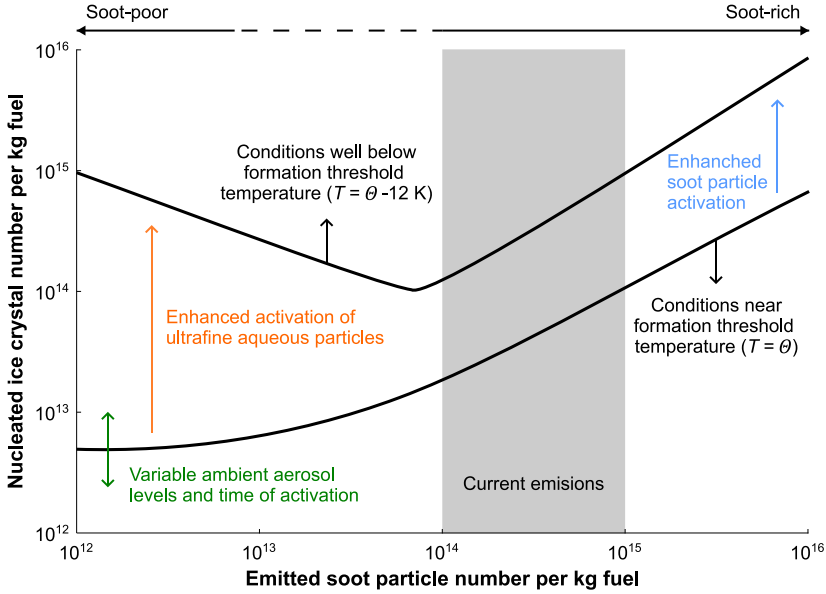


Figure 1.5 Effect of soot particle emissions on nucleated ice crystal numbers, adopted from[8]

Ambitions to further increase engine / turbine efficiency and to improve local air quality around airports have facilitated the development of engines / turbines with substantially reduced soot emissions. Assuming that modern or future engines / turbines can reduce soot emissions substantially below 10^{14} particles/kg of fuel burned, another process would become important for ice nucleation. In this range (soot-poor regime), ice nucleation is primarily initiated by ultrafine aqueous particles and aerosols from ambient air.

The lifetime of a contrail is mainly determined by processes taking place after ice nucleation. If further mixing and cooling of engine / turbine exhaust and ambient air results in sub-saturation, the contrail diminishes relatively fast and its climate impact is small. In some atmospheric regions, however, the relative humidity with respect to ice is greater than 100 % (ice-super-saturated regions). If a contrail is formed under these circumstances, it grows by uptake of water vapor from the ambient air, and can reach a contrail lifetime up to a few hours (so-called persistent contrail). Such persistent contrails typically exist for several hours but usually not longer than one day [24–26]. Thus, this type of contrails can cause a large climate impact, depending on the solar zenith angle and vertical wind shear [10, 27, 28]. Under the influence of vertical wind shear, persistent contrails can lose their linear shape, reach large horizontal extents and form so-called contrail-cirrus or merge into contrail-cirrus cluster. In these cases, the large surface area further increases the contrail's climate impact.

Concluding, the climate impact of contrails is severely influenced by atmospheric and aircraft parameters. The first group is comprised of the ice saturation of the ambient air, potential wind gradients and the solar zenith angle. The latter group depends on the aircraft's propulsive efficiency (a parameter of the Schmidt-Appleman criterion), soot and ultrafine aqueous particle emissions. Atmospheric parameters are externally defined by the prevailing weather situation, hence their impact can only be mitigated by avoiding regions with high contrail formation probability [29, 30]. High propulsive efficiencies are generally preferred for high fuel efficiencies and thus lower CO_2 emissions and operating cost. Another option in the high soot regime of current engine technologies would be to lower soot emissions, either by developing new engine / turbine technology [31] or by using fuels with a lower aromatics content / increased hydrogen content [8, 10, 17, 20]. Further studies are required to investigate the ice nucleation

processes in the low soot regime, when the reduced abundance of soot might lead to the activation of volatile aerosol or background aerosol.

1.2.2 Carbon Dioxide (CO_2)

The climate impact of CO_2 has been estimated as 34.3 (28 to 40) mW/m² in terms of effective radiative forcing (ERF). This corresponds to ~34 % of the overall aviation-related effective radiative forcing (ERF) until the year 2018 [5].

Virtually all aviation kerosene used today consists of hydrocarbons. For the short and medium range fleets, electric propulsion concepts, fuels cells and hydrogen combustion are currently investigated and tested, in order to advance their introduction into the global commercial airplane fleet. Still, especially for long-haul aircraft, due to the long development and use times for such airplanes and engines / turbines as well as their high development cost and associated risks it appears unlikely that a carbon-free fuel or battery-electric solutions can be introduced fleet-wide clearly before 2050 [32].

Despite differences in the exact composition of the various groups of hydrocarbons within aviation kerosene, for a hypothetical ideal combustion the products are always water (H_2O) and carbon dioxide (CO_2). An ideal combustion of fossil-based kerosene would yield ca. 74 g_{CO2}/MJ_{fuel} [33]. In reality, the formation of soot and other products of non-ideal combustion lowers this value slightly; nevertheless, due the fact that the unburned and partly burned fuel components oxidize over time within the atmosphere, it is advisable to stick to the value mentioned above.

Emissions from combustion are commonly referred to as "Tank-to-Wake (TtW)" emissions. Additionally, the provision of kerosene also requires energy and this causes necessarily further CO_{2e} emissions[2], which have to be added to the emission budget calculations in terms of "Well-to-Wake (WtW)" emissions. But in basically all cases, the largest fraction of the "Well-to-Wake (WtW)" emissions are the "Tank-to-Wake (TtW)" emissions.

Crude oil extraction and processing in "classical" refineries and transportation contribute the majority of the so-called "Well-to-Tank (WtT)"

[2] In particular, the provision of fuels may cause the emission of other greenhouse gases (e.g., CH_4). In the following, overall emissions of greenhouse gases are referred to as CO_{2e} emissions and emissions of CO_2 specifically are referred to as CO_2 emissions.

GHG emissions. Figure 1.6 shows sources of CO_{2e} emissions from fossil-based kerosene provision and use in absolute and relative terms.

The largest fraction of the "Well-to-Tank (WtT)" emissions is caused by crude oil refining (Figure 1.6). The upgrading of crude oil towards specification compliant aviation fuels (kerosene type Jet A / A-1) requires hydrogen and heat. In present-day refineries, hydrogen is usually supplied by steam methane reforming (SMR) or petrol coke gasification [34]. Both processes incur GHG emissions, approximately 10 kg_{CO2}/kg_{H2} for steam methane reforming and about 20 kg_{CO2}/kg_{H2} for petrol coke gasification [35–38]. The provision of heat for the various upgrading processes and the catalyst regeneration incurs further CO_{2e} emissions release by conventional refineries to be allocated to kerosene [34]. As fossil resources become increasingly depleted, crude oils tend to become "heavier" (i.e., the density of the crude oil increases) and usually contains higher amounts of sulfur. As a result, upgrading towards specification compliant fuels requires larger amounts of hydrogen as well as thermal energy [39]. If this trend persists, emissions from refining of fossil-based kerosene can be expected to increase in the future [34].

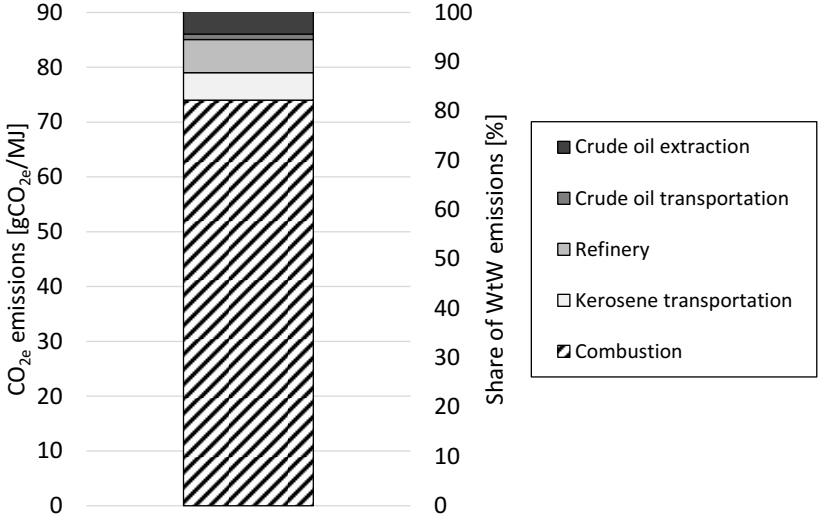


Figure 1.6 CO_{2e} emissions of different steps in the kerosene value chain; based on [33, 40, 41] (values are indicative and will change for different crude oil types and supply chains)

Various modes of transport are available for the transportation of crude oil and aviation kerosene. In general, shorter transport distances and scale effects from larger transport volumes can reduce transport emissions; e.g.,

specific emissions of maritime transport are typically lower than for rail transport, which in most cases still shows lower specific GHG emissions than road transport.

The increasing depletion of fossil resources does not only affect emissions from refinery operations, but also from crude oil extraction. Enhanced oil recovery technologies require additional (thermal) energy usually resulting in increased CO_{2e} emissions. The second major influence on emissions from crude oil extraction are gas flaring practices [42]. If gas from a specific oil field is not economically saleable, it is either flared, vented or reinjected. Flaring refers to the burning of the crude oil gas released from the crude oil due to pressure relief during production (causing mainly CO_2 emissions), while venting refers to directly releasing the gas into the atmosphere. Gas from oil fields typically contains methane, which has a clearly higher mass-specific impact on global climate compared to CO_2. Thus, in most cases the climate impact of flaring is lower than the climate impact of venting. Once released, naturally occurring local and global atmospheric circulations distribute the emitted CO_2 virtually uniformly across the globe.

The atmospheric lifetime of a CO_2 pulse emission is regulated by the fast and the slow carbon cycle.

- The fast carbon cycle encloses land uptake of CO_2 by biomass growth and ocean uptake. It removes about a third up to half of the CO_2 pulse emission.
- The slow carbon cycle encloses the reaction of CO_2 with calcium carbonate and silicate weathering.

The land and ocean uptake of the CO_2 (fast cycle) takes place at timescales up to 100 years, and reactions with calcium carbonate have typical timescales of 1 000 to 10 000 years while silicate weathering rather takes place between 10 000 and millions of years (slow cycle) [43, 44]. The large durations of both cycles yield a thorough mixing of CO_2 across the entire atmosphere and a very slow removal of CO_2 from the atmosphere by natural processes.

In conclusion, CO_2 emissions from aviation are primarily caused by fossil-based kerosene combustion in the engines / turbines and additional emissions arise from the production / provision from crude oil. The removal of CO_2 from the atmosphere by natural processes takes decades to centuries and partly even longer. Thus, a pulse emission of CO_2 – in contrast

to an individual contrail – is characterized by a long-lasting climate impact. This is the reason why CO_2 emissions partially accumulate in the atmosphere over time, provided that the emissions rate is greater than the removal rate, which is clearly the case for present day CO_2 emission levels.

1.2.3 Nitrogen Oxide (NO_x)

The net climate impact of indirect effects from emissions of NO_x has been estimated at ~17.5 (0.6 to 29) mW/m² in terms of effective radiative forcing (ERF), corresponding to 18 % of the overall aviation-related ERF until the year 2018 [5]. The term NO_x commonly refers to nitric oxide (NO) and nitrogen dioxide (NO_2), since most of the nitric oxide (NO) from combustion oxidizes to nitrogen dioxide (NO_2).

As the atmospheric lifetime of NO_x emissions is very short, its direct climate impact is negligibly small. However, NO_x emissions affect the climate by a short-term formation of ozone and a longer term reduction in atmospheric methane [45, 46]. The increase in atmospheric ozone (O_3) has a warming effect (~38 mW/m²), while the methane reduction has a cooling effect (~- 21 mW/m²). Accordingly, the resulting net effect of NO_x emissions from aviation is warming. The ozone production rate and lifetime depend on ambient NO_x and OH concentrations. For global NO_x emissions, the methane lifetime reduction is more pronounced and the ozone production rate is lower compared to the rather specific case of aviation NO_x emissions at aircraft cruise altitudes. Therefore, the net climate impact of global NO_x emissions is most likely cooling, while the net effect of aviation NO_x emissions is clearly warming (Figure 1.1) [47].

NO_x are formed during fuel combustion, when molecular oxygen (O_2) is dissociated to atomic oxygen (O•) and reacts with molecular (N_2) or atomic (N•) nitrogen inside the hottest parts of the combustor of the turbine [48]. The formation of NO_x can be attributed to four different processes: Thermal NO formation, the N_2O mechanism, prompt NO formation and fuel nitric oxide formation [49]. The first three processes describe different reactions for the oxidation of atmospheric N_2 into NO and N_2O, while the latter refers to the formation of NO_x from fuel-bound nitrogen. Aviation kerosene typically contains less than 2 m-% of nitrogen while the atmosphere contains ~75 m-% of nitrogen. Thus, the reaction of fuel-bound nitrogen is of lower

importance for the overall NO_x formation [49]. Nevertheless, the contribution of each formation process largely depends on combustion temperature and equivalence ratio (actual vs. stoichiometric fuel / air-ratio) [31, 49, 50].

In general, an equivalence ratio close to one yields the highest combustion temperature and pressure. This in turn results in increased NO_x emissions (Figure 1.7). For high thrust settings and high fuel efficiency, however, higher combustion chamber temperatures would be desirable [31]. This causes a trade-off between engine / turbine efficiency and NO_x formation. To counteract this trade-off, the design of combustors has become increasingly advanced with the goal to facilitate both, low nitrogen oxide NO_x emissions as well as a high fuel efficiency (e.g., the "Rich-Quench-Lean" (RQL) combustor) [31, 49].

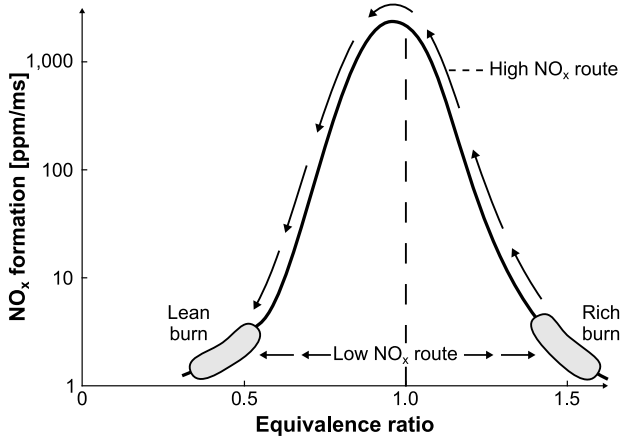


Figure 1.7 Nitrogen oxide (NO_x) formation as function of fuel/air ratio ("equivalence ratio"), adopted from [49]

Once NO_x emissions are emitted from the engine / turbine exhaust, a combination of photochemical and catalytical processes alter the atmospheric composition and thus indirectly its radiative balance. Photochemical reactions with OH yield in an increase in atmospheric O_3 at the expense of NO_x and atmospheric CH_4. Catalytical reactions result in an O_3 decrease. These reactions strongly depend on the background concentration ratio of NO, OH and O_3. For low ratios the O_3 depletion is dominant, while higher ratios favor an O_3 increase [46]. As the NO / O_3 ratio changes geographically, also the effect of nitrogen oxide NO_x emissions on atmospheric ozone (O_3) varies regionally [51]. The CH_4 decrease is less regionally dependent, due to methane's CH_4 comparatively long average atmospheric lifetime of 8 to 9 a, allowing for thorough atmospheric mixing [52].

In conclusion, the climate impact of indirect NO_x effects is to a large extend determined by the engines / turbines thrust setting and combustor design, as well as the flight route. Aviation kerosene properties do not substantially influence overall NO_x emissions, since the amount of NO_x formed from fuel-bound nitrogen contribute only to a (very) small share to the overall NO_x emissions.

1.2.4 Water Vapor (H_2O) in the Stratosphere

The climate impact of water vapor within the stratosphere has been estimated as 2.0 (0.8 to 3.2) mW/m^2 in terms of effective radiative forcing (ERF). This corresponds to ~2 % of the overall aviation-related effective radiative forcing (ERF) until 2018 [5].

Weather phenomena (e.g., wind, clouds and rain) occur in the troposphere, the lowest atmospheric layer. Within this layer, atmospheric circulations cause horizontal and vertical movements of air masses and thus wash out additional water emissions comparatively fast. The boundary between the troposphere and stratosphere (atmospheric layer above the troposphere) is called tropopause. Its height changes with latitude, reaching higher elevations above ground in equatorial (~16 km) than in polar regions (~8 km). Cruise altitudes of present-day aircraft vary between 9 and 13 km height and thus tend to take place in the stratosphere more frequently with increasing latitude [53]. Due to the atmospheric stability of the troposphere, the vertical exchange of air masses between troposphere and stratosphere is quite limited. Once injected into the stratosphere, the lifetime of water vapor increases as it follows the general circulation patterns. For this reason, the lifetime of water vapor emissions is substantially higher in the stratosphere compared to the troposphere. Hence, the climate impact of water vapor emissions becomes significant in the stratosphere. This is particularly relevant for potential supersonic flights, which would usually take place at even higher altitudes than most commercial flights today [54].

1.2.5 Aerosol Effects

Aerosol effects can be distinguished as direct influence of aerosols on radiation and indirect effects from aerosols altering the optical properties of

clouds and thereby affecting the earth's radiative balance. The climate impact of aerosol-radiation effects has been estimated as 0.9 (0.1 to 4.0) mW/m^2 in terms of effective radiative forcing (ERF) for soot emissions and -7.4 (-19 to -2.6) mW/m^2 for sulfur aerosols. Estimates of aerosol-cloud interaction effects exhibit large uncertainties presently preventing the formulation of best estimate values [5].

1.2.5.1 Aerosol–radiation Effects

Emissions of soot and sulfate aerosols have a direct forcing impact by scattering and absorbing radiation. Soot primarily absorbs incoming short-wave radiation and hence has a warming impact. Sulfate aerosols in turn mainly scatter incoming short-wave radiation, less solar radiation reaches the ground and thus they have a cooling impact [5, 55] (for the formation mechanism of soot see section 1.2.1).

Sulfate aerosols are formed by the full oxidation of sulfur components contained within aviation kerosene. Lower levels of sulfur contained in aviation kerosene would directly reduce the emissions of sulfate aerosols as well as the activation of co-emitted soot particles and their associated climate impacts.

1.2.5.2 Aerosol–cloud Interaction

In addition to contrail formation, both, supercooled aqueous solutions (e.g., sulfate aerosol particles) and insoluble ice nuclei particles (e.g., dust particles and soot) can trigger the formation of ice in cirrus clouds and they can modify existing cirrus and low level clouds [56]. They occur in the background atmosphere, and their concentration is affected by aircraft emitting soot and sulfate aerosols. As the processes governing the formation and the modification of clouds from those particles are not yet scientifically well understood, the magnitude and sign of the resulting impact on climate is still unclear. Some studies suggest that their absolute value may be even larger than contrail-related climate effects (warming or cooling) [57–63].

1.2.1 CO_2 and Non-CO_2 Effects

The comparison of aviation CO_2 and Non-CO_2 effects requires careful consideration of their spatiotemporal characteristics. This can be illustrated by an exemplary comparison of CO_2 emissions and contrails.

In temporal terms, contrails exist not longer than one day, but a portion of a CO_2 pulse emission remains in the atmosphere for more than hundred years. For a given point in time, the climate impact of contrails is determined by all contrails existing in this particular moment. But for CO_2, not only current, but also historic emissions need to be considered, even for centuries. In other words, while the climate impact of contrails is primarily determined by the present situation, the climate impact of CO_2 (partially) accumulates over time.

In spatial terms, contrails affect mostly their coverage area resulting in a regionally constrained strong climate impact. Due to the large global variations in air traffic density, the contrail climate impact is regionally very inhomogeneous and concentrated within the flight corridors and in heavily flown areas, where they contribute significantly the anthropogenic radiative forcing (Figure 1.8) (i.e., contrails have a large climate impact regionally). CO_2, however, mixes very well in the atmosphere and thus its regional differences are negligibly small.

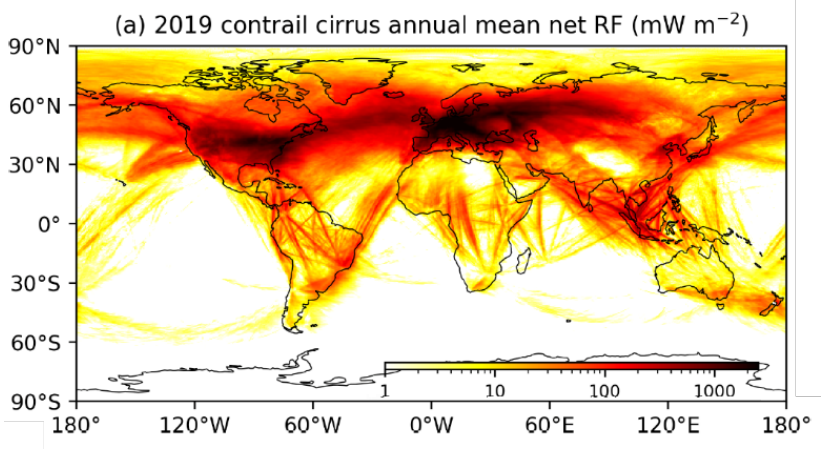


Figure 1.8 Contrail cirrus annual mean net radiative forcing for 2019, adopted from [9]

Different climate metrics can be distinguished following the driver-response-impact chain (Figure 1.9). Uncertainties increase from emissions /

radiative forcing via temperature change estimates which require climate modelling towards socio-economic impacts. However, measures such as welfare loss or other indicators would be desirable from a socio-economic perspective, as these are common targets for political measures instead of physical state variables such as the earth's radiative balance.

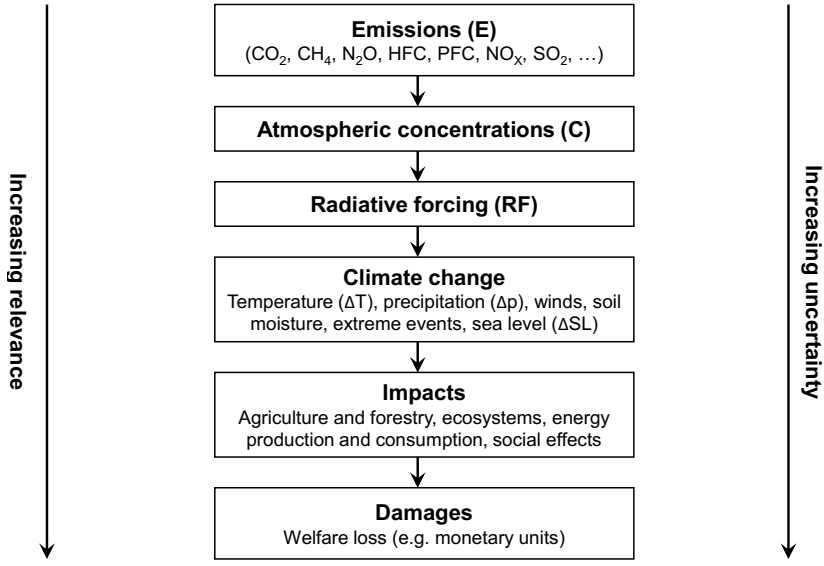


Figure 1.9 Driver–response–impact chain of climate effects from greenhouse-gas (GHG) emissions, adopted from [65]

These aspects complicate a generally valid comparison between different aviation climate terms. At first, the choice of a metric needs to find a balance between low uncertainty and relevance for policy. Secondly, the choice of time horizon has a strong influence on e.g., global warming potentials (GWP) or absolute temperature change potential (ATP) used to compare different climate terms. The time horizon is decisive for the relative weight placed on effects taking place on different time scales. Hence, their choice is rather a value judgement than a physically based selection [64]. Instead, the weighting of short- and long-term effects is rather a political than a scientific decision about how much emphasis should be placed on the situation today versus the mid- to long-term future.

1.3 Climate Impact Mitigation Potentials of Aviation Powerfuels

The average service duration for commercial aircraft is around 20 to 30 years. This results in long delays for the adoption of new technologies. In order to facilitate their timely introduction, renewably-sourced kerosene is often required to be "drop-in capable". This means that they are approved for in-service aircraft and infrastructure without any modifications. To meet this requirement, renewably-sourced kerosene and thus also aviation powerfuels have to fulfill the same specification as fossil-based kerosene plus some additional requirements. But in reality, some characteristic differences between aviation powerfuels and fossil-based kerosene remain.

There are virtually no aromatics in neat aviation powerfuels[3] yielding in a ~1 to 2 m-% higher hydrogen content, resulting in a slightly (< 5 %) increased gravimetric energy content and marginally increased water emissions from combustion. Another difference is that the carbon contained in aviation powerfuels is sourced from recent carbon sources (e.g., the atmosphere, biomass) instead of fossil resources. Aviation powerfuels also contain hardly any molecules contaminated with heteroatoms, such as sulfur or nitrogen.

Against this background, climate relevant properties of aviation powerfuels and their effect on aviation's climate impact are qualitatively discussed below. As there is hardly any effect of aviation kerosene type on aviation NO_x emissions [15, 67], a discussion of the impact of aviation powerfuels on this climate term is omitted. The following aspects are discussed in depth.

- The lack of aromatics in aviation powerfuels can reduce the contrail climate impact (chapter 1.3.1).
- The use of carbon from renewable sources allows for large reductions in lifecycle CO_2 emissions (chapter 1.3.2).

[3] Currently, alternative kerosene are only certified to be used as blend with fossil-based kerosene as per ASTM D7566. But, ASTM is currently developing a standard for unblended alternative aviation fuels (status 2023) [66].

- Water vapor in the atmosphere, aerosol-radiation effects and aerosol-cloud interactions could be affected to some extent. Since their magnitude is most likely far smaller and some of their effects on weather and climate are not yet scientifically well understood, potential effects from using aviation powerfuels on these climate terms are briefly summarized (1.3.3).

1.3.1 Contrails

Figure 1.10 shows the relationship between increasing the aviation kerosene hydrogen content by higher blend ratios of renewably sourced kerosene and the relative change in contrail climate impact relevant parameters. The lower amount of aromatic components in renewably-sourced kerosene (including aviation powerfuels) results in a reduction of soot formation and their higher hydrogen content leads to a slight increase in water emissions from combustion.

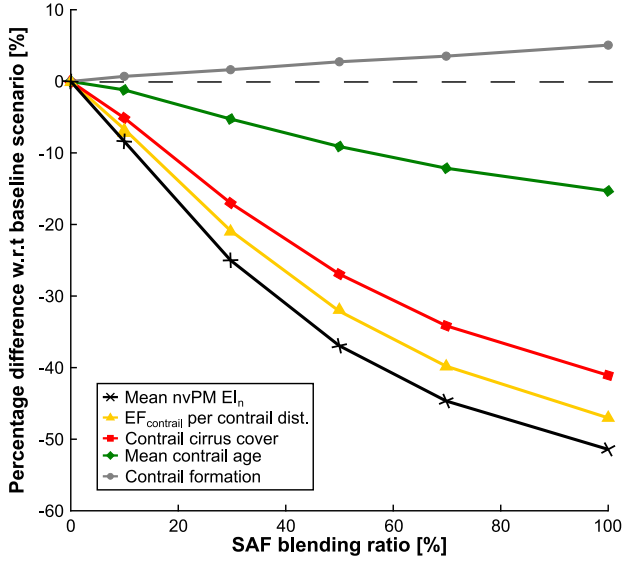


Figure 1.10 Changes in non-volatile soot particle emissions, contrail formation potential, contrail lifetime, contrail cover, and contrail climate impact in terms of radiative forcing and energy forcing per contrail distance when increasing the hydrogen content of aviation kerosene (left), adopted from [10]

Various in-flight measurement campaigns studied engines / turbines emitting in the soot-rich regime and several of them investigated the effect of a reduced content in aromatics and an increased content in hydrogen on the

soot particle emission numbers and ice nucleation [14, 17, 22, 48, 68]. Evidently, ice crystal numbers decrease proportionally with soot particle emissions. Therefore, the optical thickness of the contrail is reduced compared to contrails from fossil-based kerosene. As the water available for ice particle formation remains roughly constant, it condenses on fewer ice particles growing under these circumstances to larger sizes [17, 20]. These heavier ice particles tend to sediment faster into warmer air masses / warmer parts of the atmosphere, where they sublimate by reducing the lifetime of the contrails. Both effects – i.e., the faster sedimentation causing a reduced contrail lifetime and the reduced optical depth reducing the contrail cover – help to reduce the contrail climate impact [28]. For engines / turbines emitting in the soot-poor regime it is not yet clear to which extent this effect diminishes and how ice nucleation on ultrafine volatile particles and low levels of background aerosols affects the climate impact of contrails formed from those engines / turbines [22]. Aviation powerfuels, which typically contain hardly any sulfur, might reduce the ice nucleation on sulfate aerosols.

The increase in water emissions slightly enhances the occurrence of contrails (Figure 1.10) [10]. The exhaust air contains more water from combustion, which increases the likelihood that its mixing with ambient air results (at least temporarily) in supersaturation and subsequent condensation. Also, the higher energy content of the fuel changes the range of atmospheric conditions under which the contrails can form. Even though the use of aviation powerfuels can slightly increase contrail occurrence, modeling studies suggest that this effect is not as pronounced as the reduction in contrail lifetime. Hence, a net reduction in contrail climate impact can be expected from using aviation powerfuels, especially for high blend shares or especially neat aviation powerfuels.

So far, only few studies on the effect of renewably sourced kerosene on the contrail climate impact exist. One uses a global model and finds that a 50 % reduction in ice crystals lowers the contrail climate impact in terms of radiative forcing (RF) by almost 25 % [28]. Another study of the North Atlantic flight corridor finds for a 50 % reduction in soot emissions and ice crystals in contrails a related reduction in radiative forcing from contrails of ~42 % [10].

Current market shares of renewably-sourced aviation kerosene are below 1 %, aviation powerfuels are not even produced at commercial scale

yet [32]. As only a small fraction of all flights causes climate-relevant contrails, the targeted supply of renewably sourced aviation fuels could enable a faster contrail-climate impact reduction [10]. As of now, the implications of infrastructural changes and associated cost are unclear for a targeted use of renewably-sourced kerosene. Hence, aviation powerfuels can substantially reduce the contrail-climate impact of aviation, but the exact extent of this reduction remains uncertain.

1.3.2 Carbon Dioxide (CO_2)

As shown by Figure 1.6, the majority of CO_{2e} emissions from aviation kerosene stems from their combustion in aircraft engines / turbines. A smaller, but still relevant share of CO_{2e} emissions is created during fuel refining, transport and crude oil extraction.

The fundamental approach of renewably-sourced kerosene (including aviation powerfuels) is to replace the carbon of fossil origin contained in fossil-based kerosene by carbon of renewable sources. The carbon of these sources stems more or less directly from atmospheric CO_2 and is bound by various biological and/or thermochemical processes within the powerfuel. In such a way, a closed carbon cycle is established preventing the net increase of atmospheric CO_2 levels. Since the "Tank-to-Wake (TtW)" emissions from combustion remain unaffected and only the net emissions of the fuel's entire lifecycle are reduced, the net effect is often referred to as "lifecycle CO_2 emissions".

However, the closed carbon cycle is a simplification, the fuel needs to be produced and transported also resulting in so-called secondary emissions. These are caused by e.g., energy provision or logistics. Literature indicates that the residual emissions of aviation powerfuels range from 1 to 27 gCO_{2e}/MJ [69–72]. This amounts to less than a third of the ICAO standard emissions value for fossil-based kerosene [33]. Additionally, it is most likely that over time these secondary emissions are more and more reduced because the overall energy system needs to be increasingly defossilized to fulfill the goals of the Paris Agreement and thus e.g., fuel logistics should show less and less GHG emissions.

As Figure 1.11 illustrates, hydrogen production and direct-air-capture (DAC) of CO_2 are the main contributors towards the residual CO_{2e} emissions

of aviation powerfuels. This can be traced back to the provision of renewably sourced electricity in both cases. Hence, the key determinant for the CO_{2e} emissions of aviation powerfuels is the emission factor of the electricity source used. For both conversion routes, the Fischer-Tropsch and the Methanol-to-Jet route, heat integration can cover most of the heat demands [73]. Hence, energy demands (and associated emissions) for the provision of heat can be neglected.

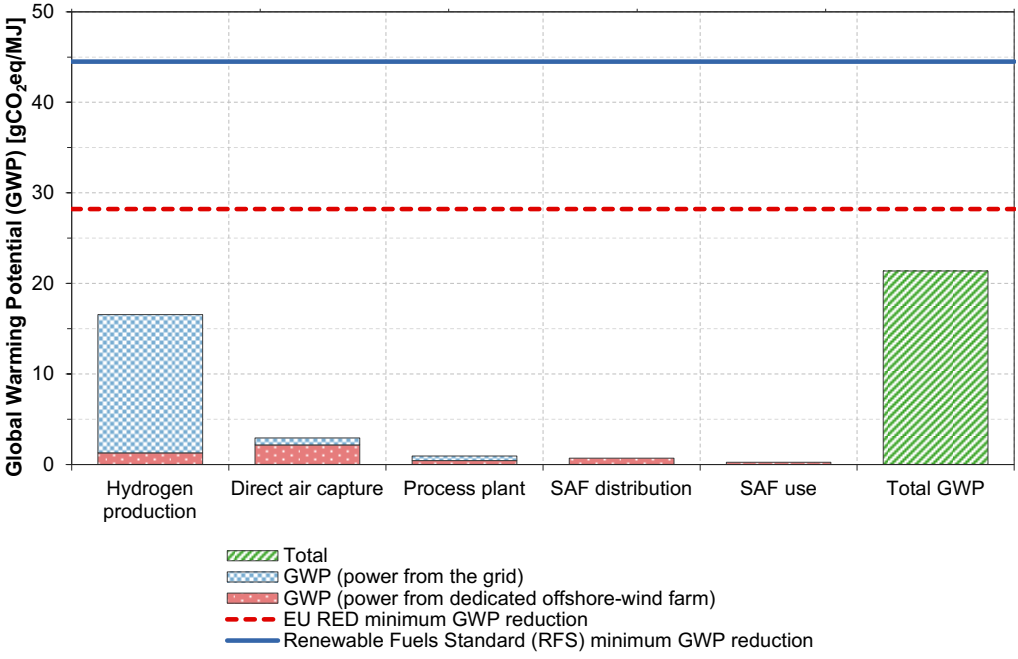


Figure 1.11 Exemplary lifecycle emissions of an aviation powerfuel (FT–SPK using electricity from wind power plants; DAC – Direct-Air-Capture, GWP – Global Warming Potential, SAF – Sustainable Aviation Fuel,), adopted from [72]

Another factor comes into play when comparing fossil-based kerosene and aviation powerfuels. Aviation powerfuels primarily consist of alkanes (chapter 1.2.1), while fossil-based kerosene also contains various cyclic hydrocarbon components. This results in a slightly higher energy and hydrogen content of aviation powerfuels. In comparison with fossil-based kerosene, the increased hydrogen content yields slightly higher water and slightly lower CO_2 emissions assuming a fully stoichiometric combustion.

In terms of "Well-to-Tank (WtT)" emissions, aviation powerfuels provide a further mitigation potential. The provision of such synthetic fuels is realized by the Fischer-Tropsch or Methanol-to-Jet route and thus in theory

powered fully by renewably sourced electricity; thus, the respective GHG emissions on the fossil fuel side can be avoided. The pendant to crude oil refining for aviation powerfuels is the upgrading to specification compliant aviation kerosene. If this step is also powered by renewably sourced electricity and renewably sourced hydrogen is used, CO_{2e} emissions of this step can also be mitigated to a large extent or even fully avoided. Due to the "drop-in" requirement, logistics for aviation powerfuels will most likely be similar to those of fossil-based kerosene. Emissions in this area might decrease, provided that the overall defossilation of the transport sector progresses and "green" fuels are used during the various transport processes.

The emissions factor of the electricity used to produce aviation powerfuels largely determines their lifecycle CO_{2e} emissions. If the power would be supplied from a coal-fired power plant, the powerfuels' life-cycle CO_{2e} emissions would be higher than those of fossil-based kerosene. If power from renewable sources (e.g., wind mills, photovoltaic systems) is used instead, far lower life-cycle CO_{2e} emission values can be achieved. However, it seems questionable to achieve net zero emissions without additional CO_2 sequestration (e.g., to mitigate residual emissions from the construction of wind or photovoltaic power plants) [69–72] on the short-term; on the long term this seems to be possible if defossilation of our overall economy progresses.

1.3.3 Water Vapor and Aerosol Climate Impacts

The increased hydrogen content of aviation powerfuels slightly shifts the stoichiometric ratio between the final oxidation products CO_2 and H_2O towards H_2O. While CO_2 emissions marginally decrease, H_2O emissions increase slightly. For flights within the stratosphere, this would also slightly increase the climate impact of water vapor emission.

The reduction in soot emissions does not only affect contrail formation, but also reduces aerosol-related climate impacts from soot. Aviation powerfuels are virtually free of sulfur, hence also effects of sulfate emissions are reduced or even avoided. In which direction (more warming / more cooling) this changes the net climate impact of direct and indirect aerosol effects still needs to be investigated [54].

1.4 Conclusion

In 2015, a global consensus was reached to limit global warming below 2 °C in order to prevent detrimental effects of anthropogenic climate change. International aviation climate mitigation goals currently focus on the abatement of CO_2 emissions. Aviation powerfuels are considered a key measure to achieve these mitigation goals. However, the climate impact of aviation does not only result from CO_{2e} emissions, but – beside other effects of minor importance – also contrails and indirect NO_x effects contribute substantially to the total climate impact from aviation. Against this background, this chapter quantifies and describes aviation climate terms first. Then, the current knowledge on the effect of aviation powerfuels on the overall climate impact from aviation is summarized.

By decreasing order of magnitude, the individual contributions to the total effective radiative forcing (ERF) from aviation are contrails, emissions of CO_{2e}, indirect effects of NO_x and – to a substantially smaller extent – water vapor in the stratosphere as well as direct and indirect aerosol effects.

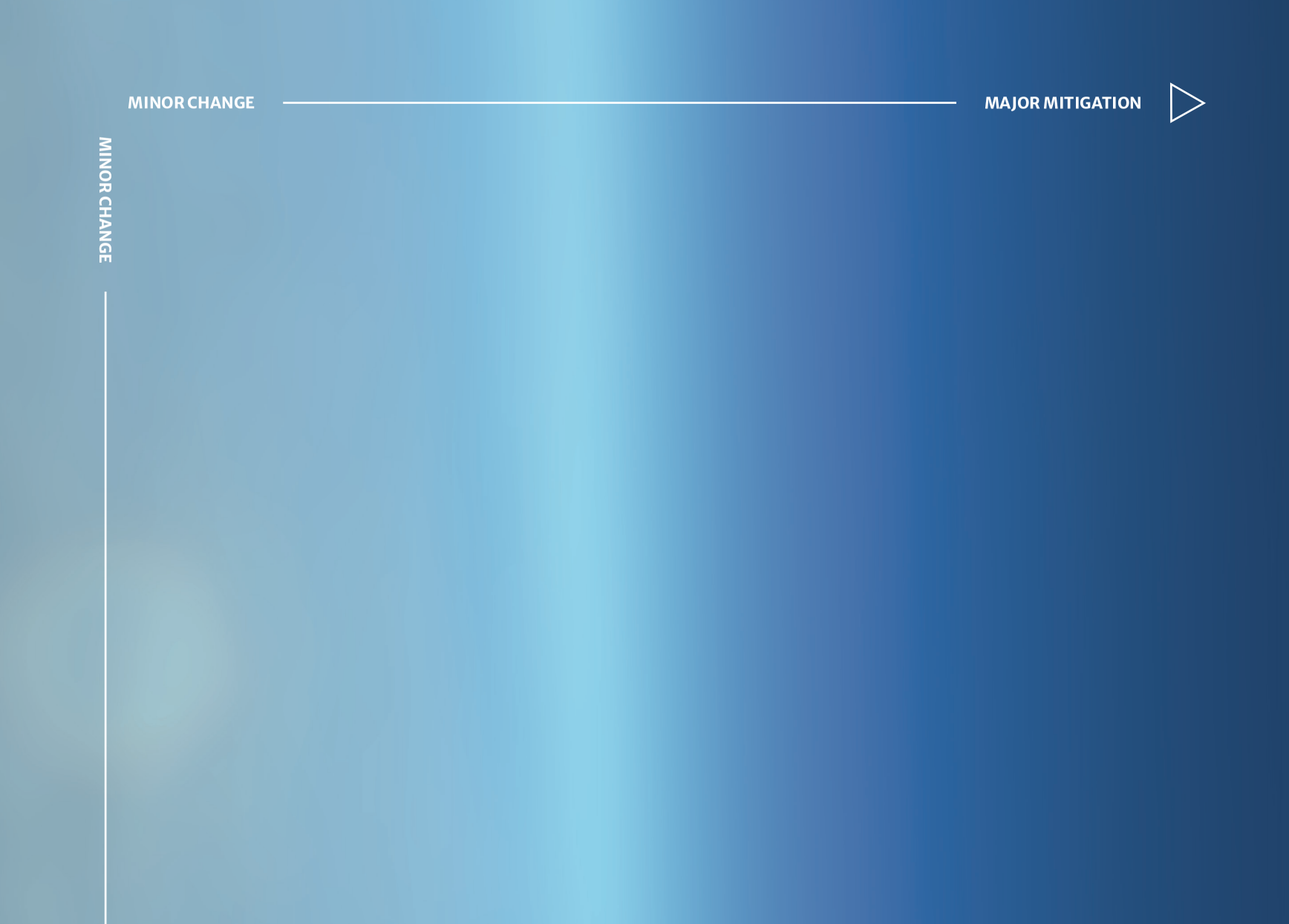
- The climate impact of contrails is determined by atmospheric and aircraft-related parameters. While the first group includes ice saturation of the ambient air, potential wind gradients and the solar zenith angle, the latter primarily depends on the aircraft's propulsive efficiency, fuel and engine / turbine parameters (soot and ultrafine aqueous particle emissions).
- CO_2 emissions from aviation are primarily caused by fuel combustion in the engines / turbines and emissions from crude extraction and refining.
- Indirect NO_x climate effects are to a large extend determined by the engine's / turbines thrust setting and combustor design, as well as the flight route; fuel properties do not substantially influence overall NO_x emissions.
- Emissions of water vapor become climate-relevant for flights in the stratosphere due to the increased atmospheric residence time in this atmospheric layer.
- Direct and indirect aerosol climate effects are caused by soot and sulfate aerosol emissions. They cause warming and cooling climate effects; however, especially in the case of indirect aerosol effects the magnitude of the climate impact is highly uncertain.

The use of aviation powerfuels has significant effects on contrail formation and lifecycle CO_{2e} emissions. For the contrail-related climate impact, aviation powerfuels reduce the emissions of soot particles (at least in the soot emission regimes of most present-day aircraft engines / turbines) and in the end shorten the contrail lifetime and reduce the associated net climate impact of contrails. A quantification of the contrail climate mitigation potential of renewably sourced kerosene is still ongoing, existing studies range between 30 % and 60 %. However, those studies would require market shares of alternative aviation fuels of around 50 % or more, and current market shares are below 1 %. As just a small fraction of all flights causes contrail formation, targeting those flights specifically with renewably sourced kerosene might allow for a faster reduction in aviation's climate impact while their market matures.

In principle, aviation powerfuels can reduce the CO_{2e} emissions of aviation by more than 80 % and in theory on a longer perspective by 100 %. However, this is only realistic if the electricity used for fuel production originates from renewable sources of energy, such as wind power or solar radiation used by wind mills and photovoltaic power plants. Electricity provision with higher CO_{2e} emissions can even result in lifecycle CO_{2e} emissions clearly above the values for fossil-based kerosene.

Other aviation climate terms remain largely unaffected by the use of aviation powerfuels (indirect NO_x effects) or are substantially smaller than the aforementioned climate terms. As contrails and CO_{2e} emissions account for a large share of aviation's climate impact, aviation powerfuels allow for a substantial reduction of aviation's overall climate impact and are not limited to CO_{2e} emissions.

In the future, targeting flight routes with a particularly high contrail-climate impact might enable faster reductions in aviation's climate impact. Further studies and flight experiments are required to improve the understanding of the necessary requirements of a targeted fuel use.


MINOR CHANGE
MAJOR MITIGATION
MINOR CHANGE

2

RESEARCH GAPS, OBJECTIVES AND APPROACH

2 Research Gaps, Objectives & Approach

Chapter 1 describes the physical, societal and economic rationales for mitigating climate forcing globally and also specifically for the commercial air transport system. All climate effects of aviation are at least indirectly related to the combustion of aviation fuel in a jet engine. Two of three main aviation climate terms, contrails and carbon dioxide emissions, can be substantially altered by changing the aviation fuel in use.

For these reasons, the identification and integration of alternatives to the current use of conventional, i.e., crude oil-based, aviation fuel (i.e., kerosene) deserve a profound examination. Therefore, this chapter first identifies gaps in existing research about alternative aviation fuels (section 2.1) and then formulates research objectives (section 2.2) emerging from the aforementioned research gaps. In the end, the approach chosen to derive conclusions for the research objectives is described (section 2.3).

2.1 Research Gaps

To date, extensive research has already been conducted about the use of alternative aviation fuels. The underlying motivation, however, changed from fundamental research (development of first jet engines for aircraft) and resource scarcity (e.g., during the Second World War or the Oil Crises) towards environmental rationales. Already in the years 1936 and 1937, H.-J. Pabst von Ohain drafted a demonstration jet engine using hydrogen as fuel [31]. During the Second World War, about two thirds of the German aviation fuel was supplied by the Fischer-Tropsch process using coal instead of crude oil as feedstock [74]. In principle, this process could also be supplied by feedstock from renewable sources of energy (cf. section 3.3.4). In the year 1957, an American B57 bomber aircraft was modified for the use of hydrogen in one of two engines and several flights were conducted using liquid hydrogen for about 20 min during cruise [75]. Later on, in the year 1988, a Russian airliner, the Tupolev 155, was successfully modified to use hydrogen in one of its three engines [76]. In the early 2000's, the Cryoplane project investigated the development of a commercial airliner fuelled by hydrogen [76]. With the approval of the first alternative pathways for the provision of kerosene in 2009 and 2011, an increasing amount of flights were conducted using kerosene from renewable sources of energy [77]. In 2021, the aircraft manufacturer Airbus announced the goal to build a commercial aircraft using liquid hydrogen to be market-ready until 2035 [78].

At present, the vast majority of aviation fuel in use is conventional kerosene (i.e., kerosene from fossil crude oil). Nevertheless, market shares of renewably sourced kerosene are currently clearly still below 1 % [79]; hydrogen is not used at all for any commercial flight [80]. Apparently, further factors besides the technological availability of an alternative aviation fuel determine the degree to which it is adopted.

For this reason, this thesis examines two aspects. These are on the one side the provision of fuels and on the other their integration into the air transport system. Due to the time-critical nature of climate change, also the temporal availability of any fuel-related climate forcing reduction measure is considered. A short-term (until the year 2030), a medium-term (between the years 2030 and 2050) and a long-term (from the year 2050 onwards) time horizon are considered.

2.1.1 Fuel Provision

The aspect of fuel provision primarily concerns the identification of alternative aviation fuels and an estimation of their effect on aviation's climate forcing. Alternative aviation fuels can be provided either by altering conventional kerosene or by replacing it with a fuel showing similar characteristics as fossil kerosene but being of non-fossil origin. The knowledge documented in existing literature as well as still open research gaps for the aspect of fuel provision are summarized in Figure 2.1.

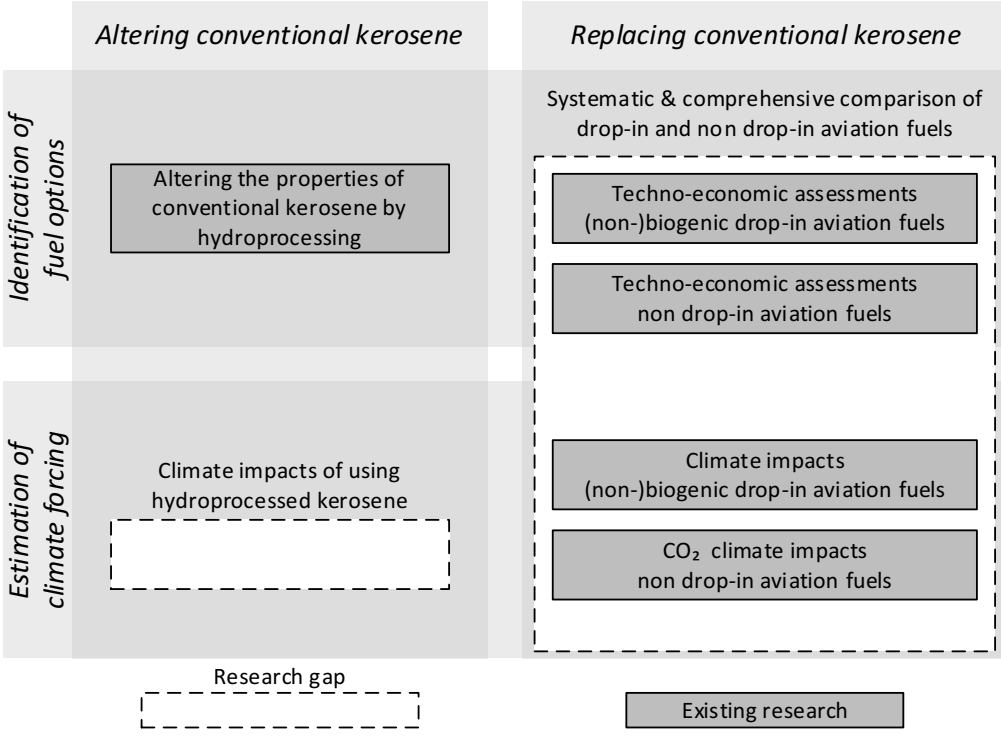


Figure 2.1 Existing knowledge and identified research gaps for the aspect of fuel provision

Altering conventional kerosene can be realized by an additional hydroprocessing step added during the processing of crude oil to kerosene. This process step allows to reduce the kerosene's aromatic content; i.e., it increases its hydrogen content and thus lowers its overall sooting tendency and subsequently reduces the associated contrail climate forcing (cf. section 1.3.1).

Changing the properties of conventional kerosene to reduce aviation's climate forcing has been investigated so far in depth by a few studies only.

Some of them focus on the removal of naphthalene, a bi-cyclic aromatic hydrocarbon [81–83], while others focus more broadly on a reduction of soot precursors, mainly aromatic compounds [84–86].

So far, none of these studies evaluate the change in contrail energy forcing due to hydroprocessing of conventional kerosene. Furthermore, potentially released carbon dioxide emissions from such an additional fuel processing step have not yet been assessed, even though in some cases they may be hardly avoidable, e.g., for the removal of aromatic compounds.

Replacing conventional kerosene could be realized by using fuels produced from renewable sources of energy. Typically, such fuels cause fewer / no carbon dioxide emissions compared to fossil fuel-based kerosene, since they either do not contain carbon or use carbon as feedstock, which has been synthesized by using carbon dioxide from the atmosphere (cf. section 1.3.2, Figure 1.11).

Such fuels have been examined by a broad range of studies already for several years. These studies typically focus on the identification of potential fuel options (1) and / or estimations of the resulting climate forcing of such renewably sourced aviation fuels (2). Commonly, a distinction is made among such alternative aviation fuels between so-called drop-in and non drop-in fuels [87].

1. Drop-in aviation fuels are defined as compliant with the existing aviation kerosene standards and are thus fully compatible with the existing (fuel) infrastructure and aircraft ("drop-in capable", cf. section 4.3).
2. Non drop-in fuels in turn are not compliant with current aviation kerosene standards and as a result their potential use would require the modification of supply infrastructure and / or aircraft.

The state of knowledge of these two options can be summarized as follows.

- Research identifying renewably sourced drop-in aviation fuels based on biogenic feedstock surfaced in the years before the first options were approved for the use in commercial aviation [88–97]. These options were Fischer-Tropsch Synthesized Paraffinic Kerosene (FT-SPK) certified in the year 2009 and Hydroprocessed Esters and Fatty Acids Synthesized Paraffinic Kerosene (HEFA-SPK) certified in the year 2011. By the time, a range of demonstration flights were conducted in order to examine the implications for routine flight operations of using such renewably

sourced kerosene [98]. Increasing societal and political concerns of a potential competition between fuel production and feedstock for food and feed initiated increasing interest in renewably sourced kerosene from non-biogenic feedstock [69, 73, 99–104]. In recent years, further studies also investigated processes combining biogenic and non-biogenic feedstock [105–107] while only very few studies compare biogenic and non-biogenic options against each other [87]. Non drop-in fuels have also been investigated for a long time, whereof noteworthy examples are the use of hydrogen in flight experiments in the years 1957 [75] and 1988 [108]. During the Cryoplane project in the year 2001 [76] and within subsequent research projects, such as Airbus ZEROe study launched in 2021 [78], various studies examined the design of hydrogen-fuelled aircraft [76, 78, 109–114] as well as implications from their use [115–118]. But also other fuel options, such as the direct use of ethanol, have been investigated [119, 120].

- The climate forcing of these alternative fuel options has mostly been estimated for carbon dioxide-related climate impacts [121–128]. Additionally, the influence of renewably sourced drop-in fuels on contrails has been studied extensively by flight experiments and simulation-based studies [15, 17, 18, 20, 28, 68, 129–131]. For non drop-in fuels, far less studies on contrail-related climate impacts are available [132]. Nevertheless, flight experiments to collect data on contrail formation from hydrogen- fuelled gas turbines are presently being conducted [133].

Despite the variety of available studies on replacing conventional kerosene, such studies mostly focus on a set of selected or even individual processes. So far, no studies are available which systematically compare a broad range of drop-in and non drop-in fuel options from biogenic and non-biogenic sources for aviation.

2.1.2 System Integration

The system integration of fuel-related measures to lower aviation's climate forcing is subject to a trade-off between minimizing aviation's climate forcing and the associated efforts for its system integration. Options with a simpler system integration and high mitigation potentials represent particularly promising measures to mitigate aviation's climate forcing. In this thesis, three fields of action, namely the targeted use of alternative kerosene,

current blending requirements and the overall air transport system's dynamics are discussed. The existing state of knowledge documented within literature and the still open research gaps are summarized in Figure 2.2.

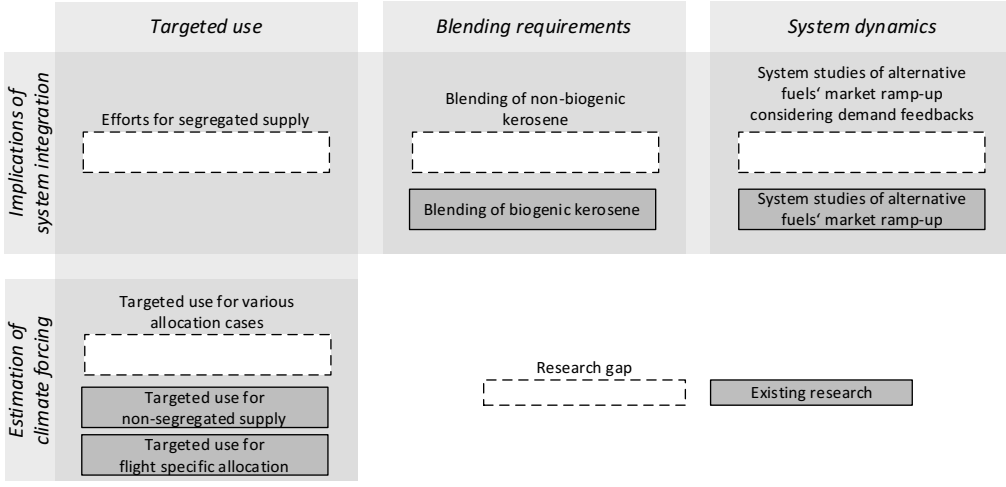


Figure 2.2 Existing knowledge and identified research gaps for the aspect of system integration

The **targeted use of alternative kerosene** refers to using paraffinic kerosene primarily in situations where particularly climate relevant contrails are formed. Since only a fraction of all flights causes warming contrails, such a concept might allow for larger reductions in contrail-related climate forcing compared to uniformly allocating a given amount of paraffinic kerosene to all flights considered (cf. section 1.4).

A recent study for the airspace over the North Atlantic region found that allocating a 50 % blend of paraffinic and crude oil-based kerosene to the most contrail climate-relevant flights reduced overall contrail energy forcing by about 10 %. A uniform allocation would however lower the contrail energy forcing only by 0.6 % [10]. This case would require a segregated fuel supply and thus make its system integration more complex. For this reason, the supply of a 50 % blend of paraffinic and conventional kerosene via the existing fuel system, e.g., at night or in autumn and winter, has been investigated [134].

However, varying degrees of allocation precision, i.e., how accurately the kerosene blend is allocated to contrail-forming conditions, have not yet been compared against each other. Additionally, operational efforts to realize a segregated / targeted kerosene supply have not been analyzed scientifically so far.

Current blending requirements for renewably sourced kerosene (cf. section 1.3) inherently constrain its potential lifecycle carbon dioxide mitigation potential and thus necessarily limit the achievable reduction in contrail energy forcing [10]. Hence, to maximize the mitigation potentials of integrating paraffinic kerosene in the air transport system, the use of ideally neat paraffinic kerosene would be necessary. Various studies discuss current fuel specifications and implications for blending [135–141] and also describe pathways towards higher blend shares to allow for an increased carbon dioxide-related climate forcing reduction [142, 143].

So far, these studies are based on kerosene from biogenic feedstock. Studies about implications from blending renewably sourced kerosene from non-biogenic feedstock are presently not publicly available.

The existing **air transport system's dynamics** are subject to a variety of feedback loops and interdependencies [144–146]. Interventions affecting such systems are prone to unexpected, counterintuitive outcomes such as rebound or backfire effects [145, 147]. For this reason, an in-depth understanding of the air transport system's behavior is required for the successful integration of fuel-related measures to lower the climate forcing of aviation. Such air transport system studies often focus on modelling (parts of) the air transport system [148–154], or the resulting climate forcing from different fleet development scenarios [155–157]. A third focal point are policy measures to incentivize the use of fuel-related mitigation options [30, 45, 46, 158].

However, only few studies include aspects of system dynamics (e.g., demand reductions by higher ticket prices due to higher fuel cost). Additionally, different types of renewably sourced kerosene (e.g., from biogenic and non-biogenic sources) are usually not considered as well.

In summary, for both aspects, fuel provision and system integration, the following research gaps exist.

- Altering the properties of crude oil-based kerosene to reduce contrail-climate forcing by weighing the resulting contrail-related climate forcing reductions against a potential carbon dioxide trade-off due to fuel processing
- A systematic comparison of drop-in and non drop-in aviation fuel options from biogenic and non-biogenic feedstock against each other

- Change in contrail-related climate forcing for varying degrees of allocation precision
- Efforts to integrate a segregated / targeted fuel supply into the air transport system
- Blending implications for renewably sourced kerosene from non-biogenic feedstock
- Studying the dynamics of the air transport system while considering demand feedback-induced effects of introducing different renewably sourced kerosene types

2.2 Research Objectives

In light of these research gaps, the primary goal of this thesis is to contribute towards a better understanding about the role of fuel-related measures to mitigate climate forcing of aviation. Both aspects, fuel provision and system integration are essential for understanding the potential of any fuel-related mitigation measure. Moreover, the urgency of mitigating anthropogenic climate change mandates consideration of the duration to implement any potential mitigation measure. Thus, the following section discusses this overall research goal from both aspects, fuel provision and system integration and derives research questions and objectives from the research gaps identified in section 0.

2.2.1 Fuel Provision

For the aspect of fuel provision, various options exist to either alter the properties of conventional kerosene or to provide aviation fuels from renewable sources of energy. This raises the following questions.

1. *Which processes are available to alter the properties of conventional kerosene or to provide aviation fuels from renewable sources of energy?*
2. *Which are the main influencing factors on the carbon dioxide-related climate forcing of such fuel options?*
3. *Which are the main influencing factors on the contrail-related climate forcing of such fuel options?*

Figure 2.3 shows the research area for fuel provision, differentiated by carbon dioxide and contrail-related climate mitigation potentials. As described in chapter 1, changing aviation fuel primarily affects the contrail- and carbon dioxide-related climate forcing of aviation, while other climate effects such as nitrogen oxide emissions largely remain unaffected. Contrail- and carbon dioxide-related climate effects are studied here individually, since their interrelations with fuel-related mitigation measures differ considerably, contrails and carbon dioxide act on very different timescales on the global climate and the contrail-related climate forcing is still subject to considerable uncertainties.

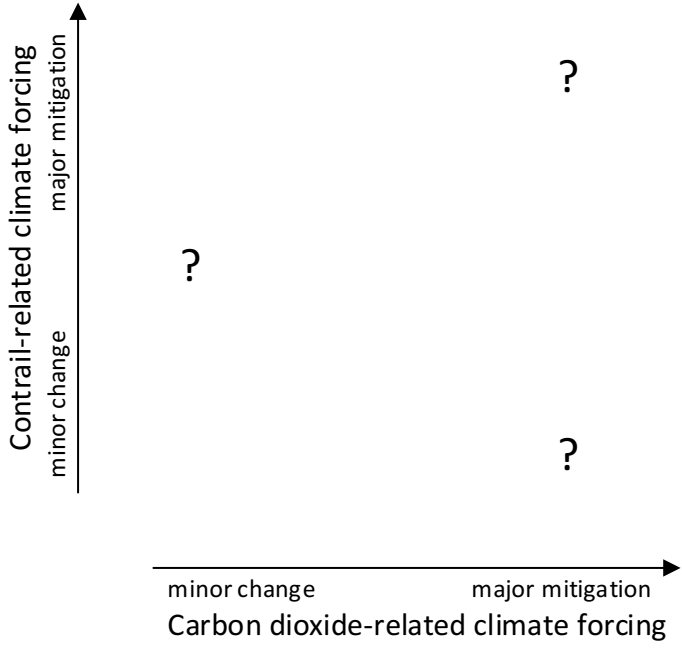


Figure 2.3 Research area concerning the aspect of fuel provision. Both, contrail- and carbon dioxide-related climate effects are considered. Question marks exemplarily indicate potential results for different fuel provision pathways such as a moderate contrail-related climate forcing mitigation, but no change in carbon dioxide-related climate forcing (left), a large mitigation of carbon dioxide-related climate forcing, but hardly any change in contrail-related climate forcing (lower right) or a large mitigation of both climate effects (upper right).

It is very likely that at least a certain (substantial) share of the aviation fuel market will still be supplied by conventional (i.e., crude oil-based) kerosene in the next decade. During this transitional period (i.e., during the time required for the market-ramp up of renewably sourced kerosene) altering the properties of established conventional kerosene might allow for an addi-

tional climate forcing reduction. Hence, the research objective here is to describe options to either alter the properties of conventional kerosene or to provide alternative aviation fuels in order to lower aviation's climate forcing (*Research Question 1*). An additional processing of conventional kerosene could in turn incur additional climate forcing. Hence, the contrail-related climate forcing reduction of additionally processing conventional kerosene (*Research Question 2*) needs to be weighed against potential increases in climate-forcing, e.g., in terms of additional carbon dioxide emissions (*Research Questions 3*).

For replacing conventional kerosene by renewably sourced kerosene options, the objective is to analyze drop-in and non drop-in fuel options from biogenic and non-biogenic feedstock for their potential use as fuel for commercial aviation (*Research Question 1*). This assessment should build upon a comprehensive description of requirements and conversion pathways for such renewably sourced kerosene options and include a set of assessment criteria along the entire fuel provision chain. Among these criteria, the climate forcing mitigation potential will be of central importance (*Research Questions 2 and 3)*.

2.2.2 System Integration

The aspect of integrating fuel-related measures into the air transport system determines the extent to which the fuel-related mitigation measures characterized in section 2.2.1 can be realized. This raises the following research questions.

4. *Which options exist to integrate kerosene with lower climate forcing than conventional kerosene in the air transport system?*
5. *To which extent do these options require changes of / within the air transport system?*
6. *Which are the main influencing factors on the climate forcing of such integration options?*

Figure 2.4 shows the research area weighing their potential climate forcing against their system integration. The simpler the integration of a particular measure within the air transport system, the more likely is its implementation. Thus, the system integration potential for any fuel related measure will be defined by both, its system integration and the resulting change in climate forcing.

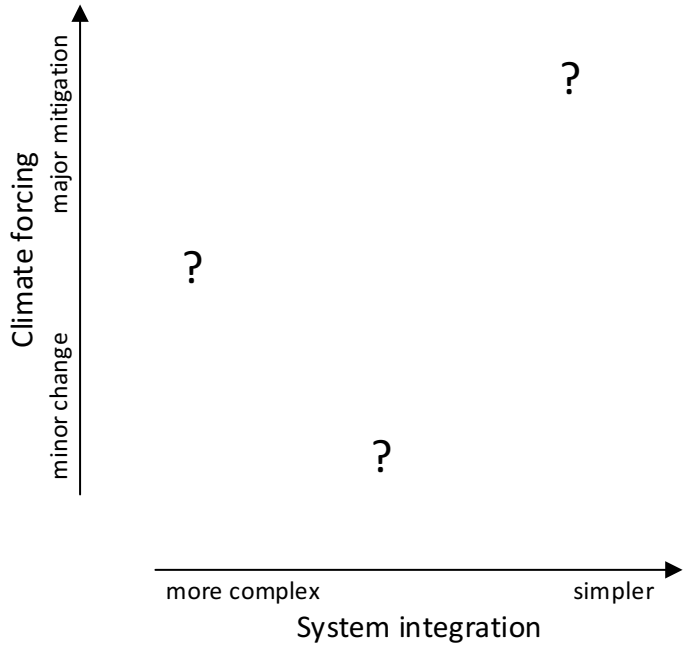


Figure 2.4 Research area concerning the aspect of system integration. Ideally, a large climate forcing mitigation can be achieved with a comparatively simple system integration. Question marks exemplarily indicate potential results for different system integration strategies: Large climate forcing mitigation, but a complex system integration (left), moderate climate forcing mitigation and a moderate system integration (center) or a large climate forcing mitigation with a simple system integration (upper right).

A targeted use of paraffinic kerosene (blends) allows for allocating the currently limited available volumes of such kerosene more precisely towards those flights or flight segments with the highest contrail-related climate forcing and thus also to maximize the associated climate-forcing mitigation potential. Investigating such mitigation potentials for increasing allocation precision embodies a further research objective. At the same time, a higher degree of allocation precision will increase the complexity of its system integration, mainly due to increasingly demanding requirements for the segregated fuel supply and potential aircraft modifications. Hence, the next research objective is to investigate the operational efforts for a segregated paraffinic kerosene supply.

The currently existing fuel specifications limit the use of paraffinic kerosene to blend ratios of 50 m-%, which clearly limits the maximum possible contrail- and carbon dioxide-related climate forcing mitigation. Thus, a further objective is to examine current kerosene specifications, to highlight

properties critical for blending and to discuss potential pathways towards higher blend shares or even neat paraffinic kerosene.

The last research objective aims at the level of the global air transport system. As mentioned above, several economic and infrastructural barriers currently impede the market ramp up of renewably sourced kerosene. This research objective aims at understanding the air transport system's dynamics and identifying levers to efficiently incentivize the ramp up of kerosene with lower climate forcing compared to conventional kerosene.

2.3 Research Approach

In order to derive conclusions about the role fuel-related measures can possibly take to mitigate the climate forcing of aviation, this thesis cumulates different studies evaluating various aspects of the overarching research objective. The following section first describes the thesis' overall structure and how it addresses the research questions raised above (section 2.3.1). Subsequently, the content of the remaining chapters is briefly outlined (sections 2.3.2 to 2.3.4).

2.3.1 Overall Structure

Figure 2.5 shows the overall structure of this thesis. Following the background chapter (chapter 1) and these introductory sections (chapter 2), the aspect of fuel provision is discussed (chapter 3). It begins with an option to alter the properties of conventional kerosene, namely additional hydroprocessing of fossil fuel-based aviation kerosene. Thereafter, renewable fuel options for aviation are broadly investigated (drop-in and non drop-in fuels), followed by a focus on drop-in options ("sustainable aviation fuels"). The results are summarized and discussed in the synthesis for the aspect of fuel provision.

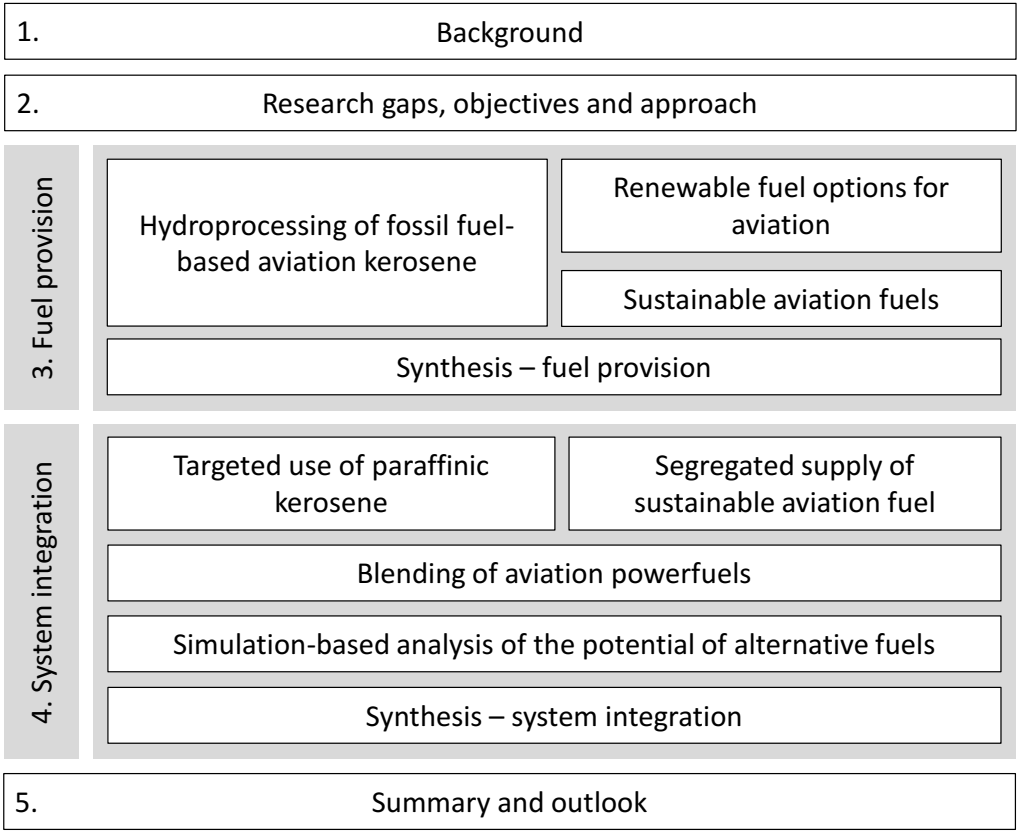


Figure 2.5 Structure of the thesis

Next, the system integration is covered (chapter 4). In this chapter, the targeted use of paraffinic kerosene is studied for different degrees of allocation precision. Then, the system integration of such a segregated fuel supply is investigated based on a real-world demonstration. The last two sections focus on implications from blending and studying the dynamics of the existing air transport system. Again, the results are summarized and discussed subsequently in the synthesis for system integration. At the end, the overarching results are summarized and an outlook on future developments is provided (chapter 5).

This thesis is comprised of five peer-reviewed scientific journal articles, three chapters of scientific books and four sections forming the framework for the research conducted and summarizing and discussing the respective results. The individual chapters address the aforementioned research questions as listed in Table 2.1.

Table 2.1 Thesis structure and addressed research questions; chapter set in bold have been previously published in scientific journals with a strict peer-review process; RQ – research question

Chapter	Title	RQ 1	RQ 2	RQ 3	RQ 4	RQ 5
1	1 Background					
2	Research Gaps, Objectives & Approach					
3.1	**Hydroprocessing of Fossil Fuel-based Aviation Kerosene**	×	×	×		
3.2	**Renewable Fuel Options for Aviation**	×	×	×		
3.2	Sustainable Aviation Fuels	×	×	×		
3.3		×	×			
3.4	Synthesis – Fuel Provision	×	×	×		
4.1	**Targeted Use of Paraffinic Kerosene**				×	
4.2	**Segregated Supply of Sustainable Aviation Fuel**				×	×
4.3	Blending of Aviation Powerfuels					×
4.4	**Simulation-Based Analysis of the Potential of Alternative Fuels**				×	×
4.5	Synthesis – System Integration				×	×
5	Summary and Outlook	×	×	×	×	×

2.3.2 Fuel Provision

This first part addresses the aspect of fuel provision. Following the order of the research objectives derived in section 2.2.1, the following studies are included.

- *Hydroprocessing of Fossil Fuel-based Aviation Kerosene.* The hydroprocessing of fossil fuel-based kerosene for short-term aviation climate forcing mitigation is assessed. This is performed by weighing the change in contrail energy forcing for using hydroprocessed instead of conventional kerosene against the energy forcing of carbon dioxide emissions released by the respective hydroprocessing step within the refinery.
- *Renewable Fuel Options for Aviation.* A wide range of aviation fuel options are investigated for their potential to reduce carbon dioxide-related climate forcing based on nine specific assessment criteria. The fuel options analyzed include blended synthetic kerosene, neat synthetic kerosene,

three alcohols (i.e., methanol, ethanol, butanol) and three gases (i.e., methane, ammonia, hydrogen).

- *Sustainable Aviation Fuels.* Systemic requirements for renewably sourced kerosene from the consumption- and the provision-related perspective are outlined. Based on those requirements, currently approved provision pathways for renewably sourced kerosene are described.
- *Synthesis – Fuel Provision.* This part summarizes the research results regarding the aspect of fuel provision. Provision pathways are outlined first and then the main influential factors on carbon dioxide and contrail-related climate forcing are discussed and compared to conventional kerosene. The respective results are compared against other not fuel-related mitigation measures and future research areas are outlined.

2.3.3 System Integration

Within this part, the aspect of integrating alternative aviation fuels into the air transport system are investigated. The following studies are included, following the order of the research objectives in section 2.2.2.

- *Targeted Use of Paraffinic Kerosene.* A targeted allocation of paraffinic, i.e., aromatic component-free, kerosene is evaluated. The contrail energy forcing of a reference fleet powered by conventional kerosene is compared against a uniform, a flight-specific, and a flight segment-specific approach.
- *Segregated Supply of Sustainable Aviation Fuel.* Here, operational efforts for the segregated supply of low-contrail kerosene to 84 demonstration flights conducted between Stockholm and Copenhagen from 17th January 2023 to 3rd February 2023 are described and an estimation of climate forcing mitigation potentials is provided.
- *Blending of Aviation Powerfuels.* Blending of renewably sourced kerosene from non-biogenic feedstock is investigated by highlighting different fuel properties critical for blending. Furthermore, the influence of these properties on permissible blending ratios is discussed. An outlook on potential pathways towards increasing maximum permissible blend shares of renewably sourced kerosene is additionally provided.

- *Simulation-Based Analysis of the Potential of Alternative Fuels.* Key levers for the market ramp up of renewably sourced kerosene are derived from a system dynamics model of the air transport system. This model is applied to hypothetical incentive schemes to stimulate the use of renewably sourced kerosene.
- *Synthesis – System Integration.* This final part summarizes the research results regarding the integration of alternative aviation fuels within the air transport system. Different options to integrate the fuel-related mitigation measures in the air transport system are described and subsequently discussed against their climate forcing and implications for system integration. Finally, these fuel-related options are compared against other mitigation measures from literature and future research areas are highlighted.

2.3.4 Summary and Outlook

This chapter summarizes the results of the previous chapters. Based hereupon, an outlook is derived for further future research developments concerning the climate forcing mitigation measures discussed in the previous chapters.

3 FUEL PROVISION

3 Fuel Provision

This chapter covers the provision of alternative aviation fuels and a comparison of their climate impact with conventional kerosene. At first, options for altering the properties of fossil-based kerosene to reduce the climate impact of aviation are studied (3.1). Then, replacing conventional kerosene by using renewable drop-in and non drop-in aviation fuel options is evaluated (3.2) and drop-in sustainable aviation fuels are studied in greater detail (3.3). The last section summarizes the results and thus identifies suitable provision pathways for alternative aviation fuels and lists main influential factors on aviation's contrail- and carbon dioxide-related climate impacts (3.4).

3.1 Hydroprocessing of Fossil Fuel-based Aviation Kerosene – Technology Options and Climate Impact Mitigation Potentials

Quante, Gunnar; Voß, Steffen; Bullerdiek, Nils; Voigt, Christiane; Kaltschmitt, Martin (2024): Hydroprocessing of fossil fuel-based aviation kerosene – Technology options and climate impact mitigation potentials. In Atmospheric Environment: X 22, p. 100259.
DOI: 10.1016/j.aeaoa.2024.100259.
Typesetting and formatting are slightly adjusted to ensure consistency within this thesis.

Abstract

Aviation contributes about 4 % of global anthropogenic climate forcing primarily by contrails, CO_2 and NO_x emissions. Renewably sourced aviation kerosene can help to reduce the climate impact from CO_2 and from contrails, but so far, its production capacities are very small. Hence, the climate impact of using fossil fuel-based kerosene with a hydrogen content increased by hydroprocessing as short-term mitigation measure is studied here. Therefore, the change in net energy forcing (ΔEF_{net}) in 2019 is calculated as the sum of the change in contrail energy forcing ($\Delta EF_{contrail}$) and additional CO_2 emissions ($\Delta EF_{hydroprocessing}$) from aviation kerosene hydroprocessing ($\Delta EF_{net} = \Delta EF_{contrail} + \Delta EF_{hydroprocessing}$). The results show that hydroprocessed aviation kerosene can reduce the net energy forcing EF_{net} by about 33 % with $\Delta EF_{hydroprocessing}$ penalty of 5 %-points. Increasing the hydroprocessing severity increases the relative climate benefit, which is only slightly affected by the emissions factor for hydroprocessing or the choice of the time horizon. Data limitations about fuel composition and its effect on contrails and climate cause considerable uncertainties and the fuel's compliance with specification standards needs consideration. This study on the climate effect of hydroprocessed fossil kerosene can help to assess near-term measures to reduce the climate impact from aviation.

3.1.1 Introduction

Today, the contribution of the air transport sector to global anthropogenic climate forcing is estimated to be 3.5–4 %. This climate impact is caused by the release of greenhouse gases (GHG), mainly CO_2, and several other effects not directly related to CO_2. CO_2 presently accounts for roughly one-third of aviation's effective radiative forcing (ERF) [5, 159], the remaining two-thirds consist of contrail effects, indirect effects of NOx emissions, and direct and indirect aerosol effects (by decreasing order of magnitude) [5]. The ERF of contrails has been estimated as 58 (17–98) mW/m^2, corresponding to 57 % of the overall aviation-related ERF until 2018 [5, 159].

In the decades before the Covid-19 pandemic, the global air traffic volume grew by 3–4 %/year. Despite the disruptions due to the pandemic [129], a return to pre-pandemic growth rates is expected in the years to come [160]. Expected growth rates of international commercial air traffic by around 4 %/year do overcompensate reductions of passenger-specific fuel consumption by about 1.3 %/year [156]. As a result, if these rates remain constant, global aviation growth will continue to outpace efficiency gains; i.e., the worldwide commercial aviation kerosene consumption and associated effects on global climate are very likely to increase. Studies expect that the global aviation's CO_2 emissions might more than double within the next 20 years to values clearly above 2 Gt of CO_2 in 2050 [156]. Since non-CO_2 effects are a result of aviation kerosene combustion, they very likely also increase in the future; if no measures for their mitigation are taken [156]. Thus, the air transport sector urgently needs to lower both, its CO_2 and non-CO_2 related climate impact in order to reduce its overall climate impact effectively and promptly.

Initially, contrails form when the exhaust emitted by aviation kerosene combustion cools down and condenses mainly on the particles emitted from the turbines. The droplets formed subsequently freeze into ice crystals if temperatures are sufficiently low. Depending on temperature and humidity of the surrounding atmosphere, contrails can be short lived, but in ice supersaturated air they can persist for several hours [24, 25] and potentially spread over large areas, thereby lose their linear shape and develop into contrail cirrus. Finally, the contrail cirrus dissolves because its ice crystals sublimate [161], e.g., by sedimentation into warmer and dryer air masses.

Whether or not a contrail forms can be determined by the Schmidt- Appleman criterion (SAC). It defines a threshold temperature below which contrail formation occurs [11, 12, 16]. This temperature depends on ambient conditions (pressure, humidity) and aircraft properties [162, 163] including propulsive efficiency, released combustion heat, and water vapor emissions due to aviation kerosene combustion [13]. On a microphysical level, contrail formation is characterized by the condensation of gases (mainly water vapor) onto aerosol particles. Water droplets form on non-volatile and ultrafine aqueous aerosol particles in the cooling engine exhaust. For the soot-rich emission regime of present aircraft (10^{14} to 10^{15} particles/kg_{fuel}), condensation on soot particles is the dominant contrail formation process. In this regime, ice crystal numbers are nearly proportional to the number of emitted soot particles [8, 22, 131]. However, for temperatures close to the SAC criterion only a fraction of soot particles is activated and the aircraft's aerodynamic vortices additionally reduce the fraction of soot particles activated for ice nucleation [22, 163–165]. Various experimental measurements have shown that within the soot-rich regime, a reduction in soot particle emission numbers yields fewer but larger initial ice crystals [16, 17, 20, 68].

Aromatic aviation kerosene components are efficient soot precursors due to their tightly bound ring structure and a lower hydrogen content resulting from conjugated double bonds [18, 68]. Therefore, reducing the aromatic content of aviation kerosene lowers soot emission numbers which in turn causes fewer but larger initial ice crystals [17]. Due to their increased weight they sediment faster into warmer and/or drier air layers [8]. Eventually, this results in faster sublimation, a shorter contrail lifetime, and hence a reduced climate impact [10]. Simultaneously, reducing the aromatics content of a particular fuel increases its overall hydrogen content. The consequence is that the water emissions from combustion are rising and thus slightly increase contrail occurrence [10]. Simultaneously, the increased hydrogen content (and also the reduced sulfur content) increases the fuel's mass-specific energy content and slightly decreases mass-specific CO_2 emissions. Accordingly, reducing the aromatics content of aviation kerosene poses a potential fuel-related measure to lower the contrail climate

impact. Renewably sourced aviation kerosene[4] usually exhibits a much reduced aromatics content compared to fossil fuel-based kerosene. Flight experiments demonstrated that their use reduces soot particle number emissions [15–17, 19, 68] and thus subsequently the contrail climate impact [28, 166]. However, more than 99 % of the global aviation kerosene supply is presently produced from fossil fuel sources. While roughly 311 Mt/year of fossil fuel-based kerosene are consumed, production volumes of renewably sourced kerosene are estimated at around 0.2 Mt/year [167, 168]. Even when considering recent initiatives to ramp up the production of renewably sourced kerosene, most studies indicate significant market shares of renewably sourced kerosene (> 10 %) not before 2030 [144, 169, 170].

For fossil fuel-based kerosene, hydrothermal processing can reduce their aromatics content considerably and the technology is available at industrial scale [82]. Mild hydroprocessing primarily involves the removal of sulfur and (under certain conditions) the saturation of aromatics into cycloalkanes. Harsher process conditions also result in breaking of aromatic rings into acyclic alkanes. In refineries currently operated, the hydrogen required for hydroprocessing is often provided by steam methane reforming (SMR) of natural gas and sometimes via petrol coke gasification [39, 171]. These pathways cause substantial CO_2 emissions, which incur an additional climate impact. Thus, the resulting net effect between reduced contrail climate impact and an increased CO_2 climate impact from aviation kerosene hydroprocessing needs to be evaluated carefully, as it might result in an overall increased climate impact. While few studies exist about hydroprocessed fossil-based kerosene [84], no study could be found which quantifies the associated climate impact mitigation potential.

This paper aims to analyse the net climate-impact of hydroprocessing of aviation kerosene from various types of crude oil with the goal to reduce the climate impact from contrails. Notably, this affects the climate impact from aviation's CO_2 emissions only marginally, but it might provide a fast and feasible option to reduce the overall climate impact from current aviation kerosene use. Only technological options being available in the short-term (up to 5 years) are selected for this assessment, to evaluate and assess a short-term mitigation option. Section 3.1.2.1 examines relevant changes

[4] Such fuels are often referred to as "sustainable aviation fuel" or "SAF". However, this term is not used here, as the fuel's renewable origin does not guarantee the fulfilment of other sustainability aspects (e.g., biodiversity or social criteria).

of aviation kerosene composition by hydroprocessing. The contrail formation process and the cause-and-effect chain for contrail climate impacts and associated methods and data for its estimation are presented in Appendix A.

Based on this, the climate impact reduction potential is analysed and implications on specification compliance are discussed (section 3.1.3.2.2). Finally, the results are summarized and potential further research areas are highlighted.

3.1.2 Methods and Data

This study evaluates aviation kerosene processing strategies differing in processing intensity (Figure 3.1). The central criterion for the assessment is the resulting change in net energy forcing, defined as amount of energy added to the Earth-atmosphere system.

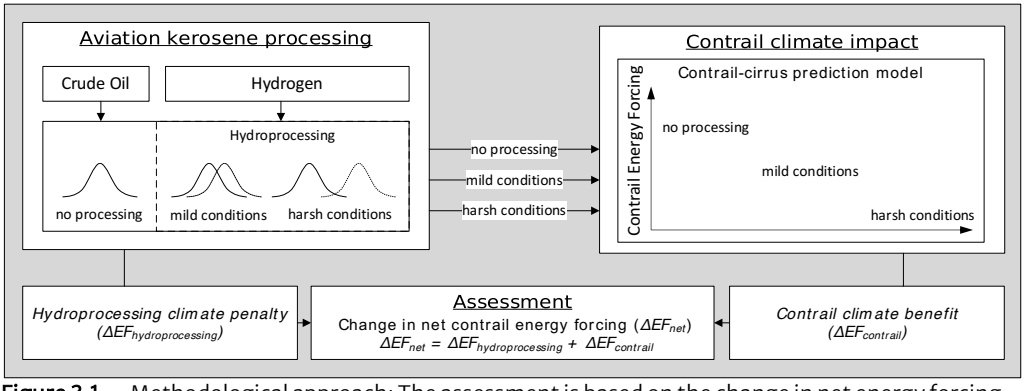


Figure 3.1 Methodological approach: The assessment is based on the change in net energy forcing (ΔEF_{net}), which weighs the climate penalty of additional aviation kerosene hydroprocessing ($\Delta EF_{hydroprocessing}$) with the contrail climate benefit ($\Delta EF_{contrail}$) resulting from an increased fuel hydrogen content.

The choice of any metric to compare the climate impacts of CO_2 emissions and contrails is inherently limited; namely by large uncertainties in the contrail efficacy [5, 9, 172–176], differences in time horizons considered and lacking consensus on a common metric [10]. The choice of energy forcing as climate metric follows previous studies, which also compare a reduction in contrail climate impacts and additional CO_2 emissions [10, 29, 177]. The climate penalty of additional aviation kerosene hydroprocessing ($\Delta EF_{hydroprocessing}$) and the climate benefit of less climate effective contrails are considered ($\Delta EF_{contrail}$). Based hereupon, the net change in energy forcing (ΔEF_{net}) is derived as the sum of the change in energy forcing from additional CO_2

emissions due to mild and harsh hydroprocessing ($\Delta EF_{hydroprocessing}$) and the change in energy forcing from contrails ($\Delta EF_{contrail}$) in 2019.

3.1.2.1 Aviation Kerosene Processing

The contrail climate impact can be reduced by reducing soot precursors in aviation kerosene. The sooting tendency decreases roughly from poly-to mono-cyclic aromatics via cyclo- and iso-alkanes to unbranched alkanes [15, 18]. In this order, the respective hydrogen content of the aviation kerosene components increases. Thus, the hydrogen content is often used as proxy for the sooting tendency of aviation kerosene during combustion in aircraft turbines. Various in-flight and on-ground measurement campaigns support the validity and the limitations of this proxy [15–17]. The hydrogen content of aviation kerosene can be increased by hydroprocessing. This is a commonly used process used for fuel finishing within modern refineries [39]. Hydrogen is added to the fossil straight-run kerosene derived from crude oil under elevated pressure and temperature conditions and reacts with heteroatoms (e.g., sulfur) and – depending on process conditions – saturates aromatics or even cracks cyclic components to alkanes [39, 178].

3.1.2.1.1 Effect on Aviation Kerosene Properties

The composition of crude oil and its aviation kerosene fraction varies greatly, typically depending on the crude oil's respective reservoir. The existing studies on the distribution of hydrogen contents of conventional aviation kerosene [135, 179, 180] indicate a mean hydrogen content of 14.1 m-% with a single standard deviation σ = 0.2 m-% points and a sample size n = 57. Here, only large, international airports are considered. These are typically supplied by pipelines and operate large fuel storage tanks resulting in an averaging tendency for the kerosene properties. The maximum permissible sulfur content of aviation kerosene is 0.3 m-% [181].

Hydroprocessing at comparatively mild processing conditions (typically 270–340 °C, 15 – 30 bar [39], "hydrotreatment") involves the removal of contaminants such as e.g., sulfur and the saturation of unsaturated components, such as alkenes. The saturation of aromatics into cycloalkanes can also be achieved within the upper temperature and pressure range, but typ-

ically aromatics will not be cracked to acyclic alkanes. Reactions by decreasing ease of reaction are heteroatom removal (mainly sulfur), a saturation of olefins, and then saturation of aromatics. Accordingly, for a substantial reduction in aromatics, the majority of the sulfur in the feed will be removed [39]. The hydrogen demand is estimated based on the stoichiometric reactions for removing all sulfur in the feed and a conversion of 50 % of the feed's aromatics content into cycloalkanes. A conversion to acyclic alkanes is rather unlikely due to the mild process conditions during such a hydrotreatment. Based on these assumptions, the hydrogen content of the conventional aviation kerosene can increase by 0.3 m-% points (cf. Appendix A).

In contrast, substantially harsher process conditions (typically 370 – 510 °C, 140 – 170 bar [39], "hydrocracking") even enable cracking of aromatics to acyclic alkanes. Typical reactions for such conditions are (again by decreasing ease of reaction) heteroatom removal, olefin saturation followed by the saturation of rings, cracking of cycloalkanes, and finally, the cracking of acyclic alkanes [182]. It is also assumed that all sulfur is removed and now 80 % of the aromatics in the feed are saturated and broken to acyclic alkanes. Hence, the hydrogen content of the conventional aviation kerosene can increase by about 0.7 m-% points (cf. Appendix A)

Aviation kerosene specifications limit the sulfur content of conventional aviation kerosene to 0.3 m-% [181]. However, studies on distributions of aviation kerosene show that the majority of fossil-fuel based aviation kerosene contains not more than 0.15 m-% sulfur [135, 180]. To indicate the full value range, the sulfur content in this study is varied uniformly from 0.0 to 0.3 m-%. Typically, sulfur occurs in the form of heteroatoms. During hydroprocessing, these heteroatoms are saturated by hydrogen and release sulfur as hydrogen sulfide (H_2S).

3.1.2.1.2 Climate Impacts of Aviation Kerosene Processing

Presently, most hydrogen is produced from steam methane reforming (SMR) and coal / coke / petrol coke gasification (8.2 Exa-Joule (EJ) and 3.2 EJ in 2019, respectively [35]). A minor amount is produced from water electrolysis (less than 0.1 EJ [35]). The first two options result in substantial GHG emissions (about 10 kg CO_2/kg_{H2} for steam methane reforming (SMR) and about 20 kg CO_2/kg_{H2} for petrol coke gasification [36–39]). In case of electrolysis, the lifecycle CO_2 emissions strongly depend on emissions from

the provision of the electricity used for water splitting. In principle, if the entire power for electrolysis is provided from renewable sources, hydrogen from water electrolysis could be produced with almost zero CO_2 emissions. Thus, the emissions factor for hydrogen provision is varied between 0 kg CO_2/kg_{H2} and 20 kg CO_2/kg_{H2}. Hydroprocessing is an exothermic process [39] and thus CO_2 emissions from potential heat demands or benefits from heat integration are not considered.

The energy forcing of the additional CO_2 emissions from hydroprocessing is calculated as a measure for the climate penalty of aviation kerosene processing. The energy forcing is calculated based on the absolute global warming potential (AGWP) of a carbon dioxide (CO_2) pulse emission for time horizons (TH) of 20, 50 and 100 years [10](Eq. 1).

$AGWP_{CO2,TH}$ is the mass-specific, absolute global warming potential of CO_2 (2.39×10^{-14}, 5.35×10^{-14}, 8.8×10^{-14} W yr kg^{-1} m^{-2} for a 20 / 50 / 100 year time horizon [44, 183], respectively). S_{earth} refers to the earth's surface (5.101×10^{14} m^2)[184]. m_{CO2} denotes the mass of CO_2 emitted by the additional hydroprocessing and is calculated as the product of the flight dataset's fuel consumption (cf. section 3.1.2.2, Appendix A), the fuel mass-specific amount of hydrogen required for hydroprocessing and the emissions factor for hydrogen provision. Accordingly, m_{CO2} corresponds to the amount of CO_2, which would have been released if all fuel used in the flight dataset considered here would have been hydroprocessed. The increased hydrogen content results in an increasing gravimetric energy content of the aviation kerosene and thus reduces the flight dataset's fuel consumption. Accordingly, the amount of fuel to be hydroprocessed decreases and also CO_2 emissions from kerosene combustion decrease. While the first effect is taken into account, the reduction in CO_2 emissions from aviation kerosene combustion is not taken into account here. As the reduction in combustion-related CO_2 would (partly) compensate for the additional emissions from hydroprocessing, the change in net energy forcing (ΔEF_{net}) can be considered as conservative estimate (cf. Appendix A). The use of flight data from the year 2019 eliminates uncertainties from air traffic development scenarios as well as uncertainties from assumptions on future meteorological conditions. The inter-annual variability of the simulation results is discussed in section 3.1.3.1.4.

$$CO_2\ EF\ [J] = \int_0^{TH} RF_{CO2}(t)\ dt \times S_{earth} \qquad \text{(Eq. 1)}$$

$$\approx AGWP_{CO2,TH} \times m_{CO2} \times S_{earth}$$

3.1.2.2 Contrail Climate Impact

The contrail climate impact is estimated using the so-called contrail cirrus prediction model (CoCiP) from its open source distribution pycontrails / CoCiP version 48.1 [9, 10, 164, 177, 185, 186]. This model simulates the life cycle of contrail segments formed along individual flight trajectories [164].

In the contrail cirrus prediction (CoCiP) model, when consecutive waypoints meet the Schmidt-Appleman criterion (SAC), contrail formation is assumed. The soot emissions number influences the initial number of ice crystals within the contrail. However, a lower boundary is introduced at 10^{13} kg^{-1} to consider ambient aerosols and organic particles as ice nuclei [8]. Additionally, the ambient temperature affects the initial number of ice crystals, as well as the soot activation rate [16] and the fraction of ice particles that survive the wake vortex phase [164]. Contrail segments enduring the wake vortex phase are simulated in the model using time steps of 1 800 s until they reach their end-of-life conditions; i.e., the contrail ice crystal number decreases below the background ice nuclei concentration ($<10^3$ m^{-3}), the contrail's optical depth $\tau_{contrail}$ is less than 10^{-6}, or the lifetime surpasses a maximum of 24 h [164]. The contrail cirrus prediction (CoCiP) model calculates the local contrail radiative forcing (RF′) for each waypoint, which represents the change in radiative flux over the contrail area [10]. The contrail energy forcing is calculated as the product of the contrail segment RF′, length, and width integrated over the contrail segment's lifetime [14, 177, 186]. The efficacy of the contrail radiative forcing is assumed to be unity, neglecting secondary effects such as the reduction of natural cloudiness as a result of contrail formation [5]. Such secondary effects are beyond the scope of this study, the sensitivity of the results to various efficacies is shown in Appendix A.

The simulations cover 797,602 departing flights from the five largest European airports in the year 2019 by passenger numbers [187], namely London-Heathrow, Paris Charles-de-Gaulle, Amsterdam Schiphol, Frankfurt International and Madrid-Barajas. For the uncertainty assessment, selected months from the years 2018 and 2023 are compared against the same four months related to the year 2019. Flight trajectories are loaded from the OpenSky Automatic Dependent Surveillance Broadcast (ADS-B) database [188]. Aircraft performance is based on the EUROCONTROL Base of

Aircraft Data Family 3.15 [189, 190] and the International Civil Aviation Authority (ICAO) Emission Databank (EDB) [191]. Meteorological data is used from the European Centre for Medium-Range Weather Forecast fifth generation high-resolution reanalysis (ECWMF ERA5) [192] (0.25° × 0.25° horizontal resolution for 37 pressure levels and at a temporal resolution of 1 h). The ERA5 humidity fields are adjusted to in-situ observations using the so-called method of exponential scaling with latitude correction [9]. These datasets and methods have been extensively documented [9, 10, 131, 164, 177, 186, 193]. The average hydrogen content of all fuel supplied to the abovementioned airports is increased gradually in 8 increments from 14.1 m-% up to 14.9 m-% and the fuel's hydrogen content-based soot particle emission index is calculated [10]. The resulting contrail energy forcing is weighted against the energy forcing of the additional CO_2 emissions from additional hydroprocessing of aviation kerosene. The resulting net climate impact is evaluated for a range of hydrogen provision methods (petrol coke gasification, steam methane reforming, water electrolysis) and time horizons (20, 50 and 100 years). By default, the effect of fuel sulfur changes is not considered in the calculation of the contrail energy forcing. Several studies [17, 21, 194–197] suggest that a lower fuel sulfur content might further reduce the ice nucleation efficiency of the soot particles and would subsequently also lower the contrail's energy forcing. Accordingly, the simulations can also be considered conservative in this regard. Furthermore, the emission of sulfate aerosols has a direct and indirect (via aerosol cloud-interaction) climate impact. As both, direct and indirect climate impacts are still associated with large uncertainties [5], robust conclusions on the net climate impact of a kerosene sulfur reduction cannot be drawn so far and this effect is excluded here.

3.1.3 Results and Discussion

3.1.3.1 Results

The measures studied here do not tackle CO_2 emissions from the combustion of fossil fuel-based kerosene. Therefore, from a mid- to long-term perspective, switching towards renewably sourced kerosene will be necessary, particularly because of the long atmospheric lifetime of CO_2. For the timespan while the availability of renewably sourced kerosene is limited,

the climate effects of hydroprocessing fossil fuel-based kerosene are assessed here.

3.1.3.1.1 Variation of Crude Oil

Table 3.1 summarizes hydrogen demand and resulting CO_2 emissions for different aviation kerosene processing strategies and hydrogen sources. Sulfur contents at the specification limit can increase overall hydrogen demand by 2.5–5 %.

Table 3.1 Hydrogen demand of each aviation kerosene processing strategy and estimates for the resulting CO_2 emissions

Type of hydroprocessing	**H_2 demand** [$kg_{H2}/t_{Kerosene}$]			**Additional CO_2 emissions** [$kg_{CO2}/t_{Kerosene}$] ([g_{CO2}/MJ])		
	Total[a]	aromatics conversion[a]	sulfur removal[a]	high[a]	medium[a]	low[a]
Reference case	0	0	0	0 (0)	0 (0)	0 (0)
Mild hydroprocessing	4 – 4.2	4	0 – 0.2	80 – 84 (1.82 – 1.91)	40 – 42 (0.91 – 0.95)	0 (0)
Harsh hydroprocessing	8 – 8.2	8	0 – 0.2	160 – 164 (3.64 – 3.73)	80 – 82 (1.82 – 1.86)	0 (0)

[a]rounded figures

Figure 3.2 compares the energy forcing of CO_2 emissions from hydroprocessing ($EF_{hydroprocessing}$, ◇) with the associated contrail climate impact ($EF_{contrail}$, ○) for each day in the year 2019 assuming hydrogen from steam methane reforming (SMR) and a time horizon of 50 years. Additionally, the mean net energy forcing per day is depicted (EF_{net}, ✕) and Figure 3.3 compares the relative changes.

The daily (intra-annual) variation in contrail energy forcing is shown to indicate the daily variations in $\Delta EF_{contrail}$. $\Delta EF_{contrail}$ ranges from individual days with a cooling climate impact to days with $EF_{contrail}$ being five or more times higher than the mean. The mean EF_{net} per day from contrails is $< 5*10^{16}$ J, while some of the daily variations significantly exceed this value. $EF_{hydroprocessing}$ is significantly smaller, the additional CO_2 emissions due to hydroprocessing reduce the climate benefit from a reduction in energy forcing from contrails non-visibly in this figure representation. The largest changes in EF_{net} are caused by the reduced soot emissions and ice crystal number in contrails from the hydroprocessed fuel. The climate impact of

hydroprocessing increases for harsher process conditions, since they result in an increased hydrogen demand (and thus $EF_{hydroprocessing}$). For the hydrogenation of aromatics to cycloalkanes (mainly mild hydroprocessing), less hydrogen is required than for hydrocracking to acyclic alkanes (mainly harsh hydroprocessing). In principle, higher sulfur contents increase the resulting climate impact, as the removal of sulfur incurs an additional hydrogen demand. However, against the daily variation in contrail energy forcing, this effect is barely noticeable. Due to the large daily variation of the contrail climate impact, in the following sections the annual sums of the hydroprocessing and contrail climate impact for the year 2019 are used and will be compared to other years later on (section 3.1.3.1.4).

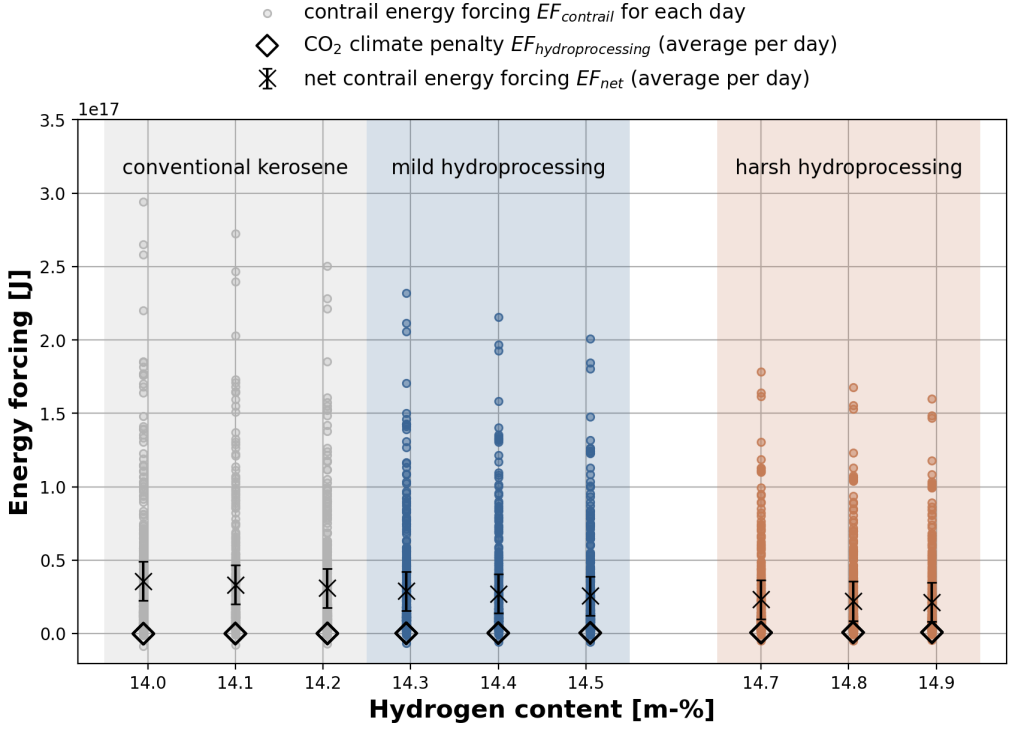


Figure 3.2 Energy forcing of CO_2 emissions from hydroprocessing ($EF_{hydroprocessing}$, ◇) per day, contrail energy forcing for each simulated day ($EF_{contrail}$, ○) and mean net energy forcing per day in 2019 (EF_{net}, ×), for increasing fuel hydrogen content (m-% mass-percentage); error bars indicate the double standard deviation from the mean) assuming medium hydrogen provision emissions and a 50-year time horizon

Figure 3.3 shows the annual change in $\Delta EF_{contrail}$, $\Delta EF_{hydroprocessing}$ and the resulting ΔEF_{net} for increasing hydrogen content by increased hydroprocessing for the flight dataset from the five largest European airports in

2019. The mean hydrogen content of fossil kerosene (cf. section 3.1.2.1.1) of 14.1 m-% is chosen as reference (no relative change in energy forcing).

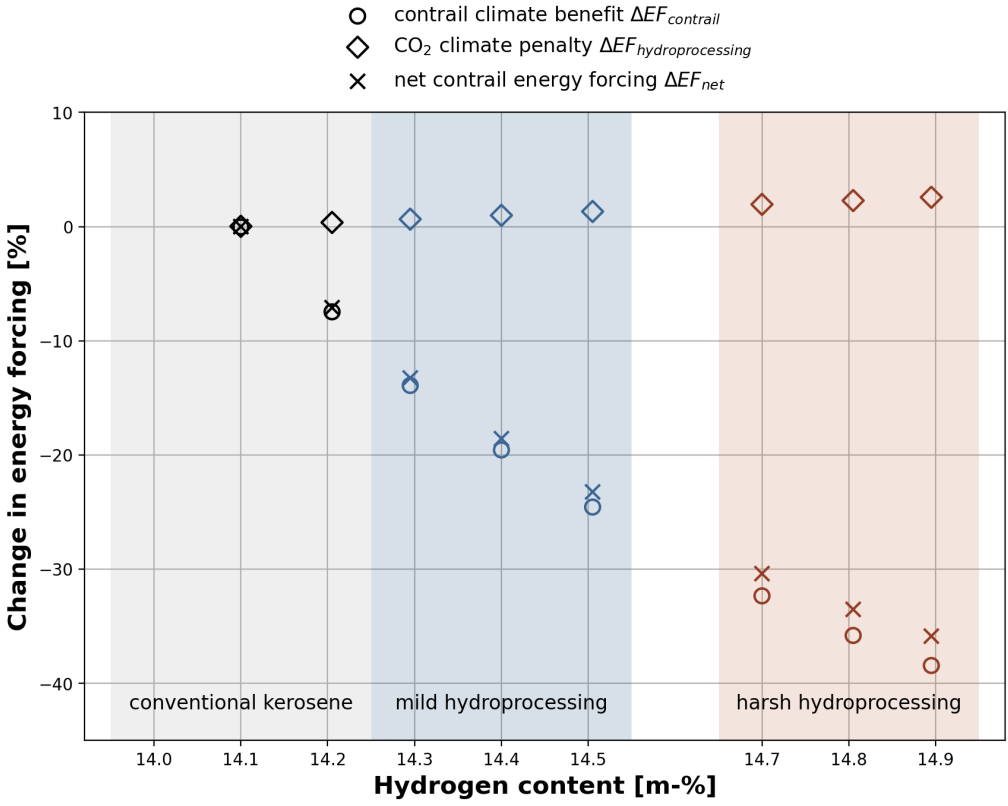


Figure 3.3 Change in energy forcing for increasing kerosene hydrogen content in m-% mass-percentage by CO_2 emissions from hydroprocessing ($\Delta EF_{hydroprocessing}$, ◇), by contrails ($\Delta EF_{contrail}$, ○) and the resulting net effect (ΔEF_{net}, ×) for a 50-year time horizon

In general, the reduction in contrail energy forcing intensifies with increasing hydroprocessing intensity. The climate impact reduction does not increase linearly, but rather weakens in particular for high hydrogen contents, due to the increasing climate penalty of increasingly intense hydroprocessing. Additionally, contrail occurrence slightly increases with increasing hydrogen content [10] and thus further dampens the gain in climate impact reduction. This is shown by a decreased reduction rate of $\Delta EF_{contrail}$ for higher hydrogen contents of the harshly hydroprocessed fuels and the higher $\Delta EF_{hydroprocessing}$ for higher hydroprocessing intensities, both lead to a decrease in the sensitivity of the ΔEF_{net} with higher hydroprocessing intensity. Furthermore, high sulfur contents marginally increase hydroprocessing emissions. Accordingly, kerosene from crude oil with low aromatics

and low sulfur content would be preferable from a climate perspective. The contrail climate benefit $\Delta EF_{contrail}$ increases significantly from mild (~ 20 %) to harsh processing conditions (~ 38 %). The hydroprocessing climate penalty $\Delta EF_{hydroprocessing}$ is small and also increases from mild (~1 %) to harsh conditions (~ 3 %), and leads to a net energy forcing reduction potential of hydroprocessing ΔEF_{net} of about 18 % for mild and about 33 % for harsh processing conditions.

3.1.3.1.2 Variation of Greenhouse Gas (GHG) Emissions Intensity of Hydrogen Provision

Figure 3.4 shows the variation of net energy forcing for different hydrogen provision pathways. The highest reduction potentials (~35 % reduction) are achieved in the case of low hydrogen provision emissions (∇), which could potentially be realized by using renewably sourced hydrogen. Next is the medium emissions factor ($\times$, ~ 33 % reduction), while the lowest potential exists for high specific emissions (Δ , ~ 31 % reduction).

The differences in hydrogen provision pathways can be explained by their different degrees of emission intensity. In case of the (idealized) assumption of hydrogen provision with no CO_2 emissions (e.g., by electrolysis powered by renewable energy sources), the net climate impact reduction ΔEF_{net} corresponds to the reduction in contrail climate impact $\Delta EF_{contrail}$ and increases by about 3 % points compared to a medium emissions factor for hydroprocessing (~10 kg_{CO2}/kg_{H2}). For high emission intensities (~20 kg_{CO2}/kg_{H2}) the climate impact reduction is slightly dampened (~3 %-points) by the CO_2 emissions $\Delta EF_{hydroprocessing}$. Note that a potential climate impact reduction from lower in-flight CO_2 emissions due to an increased gravimetric energy content is excluded in this study (cf. 3.1.2.1.2). Hypothetically, net CO_2 emissions might even decrease when considering both, the increased gravimetric energy content and hydroprocessing with sufficiently low CO_2 emissions.

Consequentially, the lower the CO_2 emissions from hydrogen provision, the greater the climate-impact mitigation potential. However, even the use of hydrogen from processes causing high CO_2 emissions would still enable a reduction in net energy forcing by more than 30 % for harsh hydroprocessing.

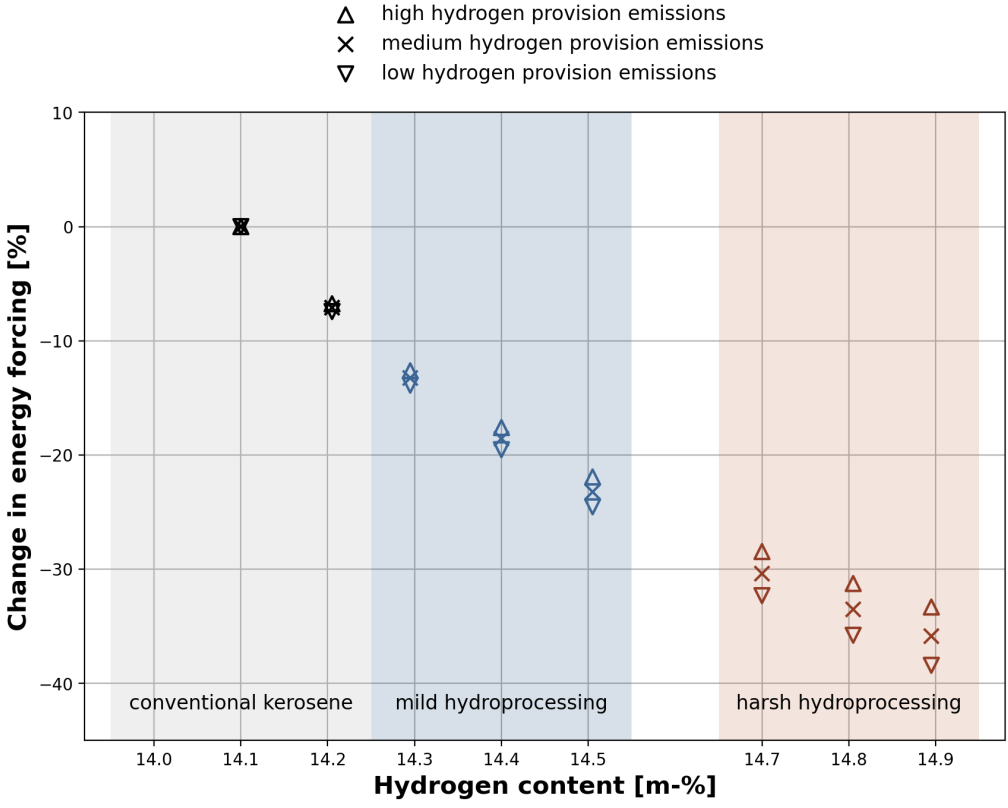


Figure 3.4 Change in energy forcing (ΔEF_{net}) versus hydrogen content (m-% mass-percentage) for hydrogen provided with high ($\triangle$), medium ($\times$) and low CO_2 emissions ($\triangledown$) for a 50-year time horizon

3.1.3.1.3 Variation of the Time Horizon

Figure 3.5 shows the net energy forcing for a time-horizon of 20 years ($\triangledown$), 50 years ($\times$) and 100 years ($\triangle$). A medium emissions intensity of hydrogen provision is assumed (10 kg_{CO2}/kg_{H2}). The net climate impact decreases with increasing processing intensity for all time horizons considered. The reduction potential for a 20 year time horizon is slightly larger than the 50 year and 100 year perspective, but this choice of the time horizon has only a small effect on the relative changes in ΔEF_{net}.

The lifetime of a contrail lies within several hours, which is very short compared to all time-horizons considered. Hence, variations in the contrail-related energy forcing are not altered by the different time horizons. As a long-lived greenhouse-gas, CO_2 has an atmospheric lifetime from decades to centuries. A longer time horizon considers a longer effect duration of CO_2 emissions and thus increases the energy forcing from a CO_2 pulse emission.

Therefore, the time horizon affects the contribution of CO_2 emissions from hydroprocessing towards the net energy forcing. However, since the climate impact of CO_2 emissions from hydroprocessing is quite small compared to the mean contrail climate impact, a large reduction in climate impact can still be observed even for adverse cases with high emission intensities. Thus, Figure 3.5 clearly shows that not only for short-time frames (i.e., 20 years), but also in the longer-term (here 100 years) hydroprocessing of fossil fuel-based kerosene yields additional climate impact reductions, which are most pronounced for harsh processing conditions.

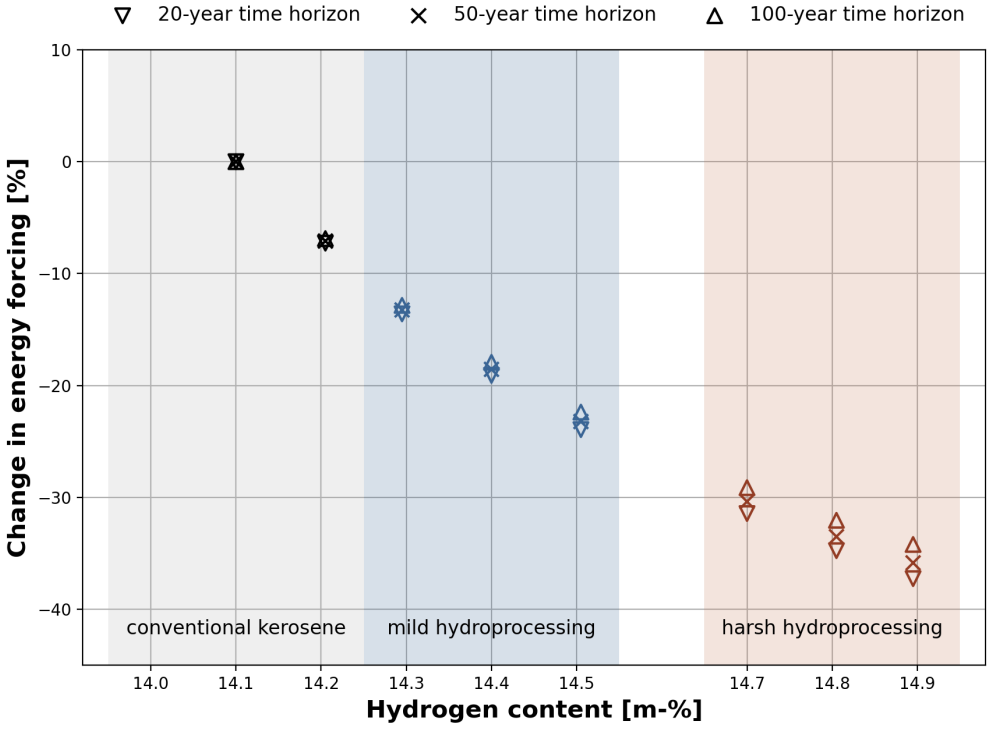


Figure 3.5 Change in energy forcing for a time horizon of 20 years (▽), 50 years (×) and 100 years (△) assuming medium hydrogen provision emissions (m-% mass-percentage)

3.1.3.1.4 Uncertainty Assessment

Figure 3.6 shows net energy forcing per month for the different hydroprocessing strategies for 2018 (⬡), 2019 (▫) and 2023 (◇) to investigate the impact from different weather systems and air traffic volumes. To enhance computational efficiency, January, April, July and October were se-

lected as representative months for each season. Trajectory data for October 2023 were not available in the OpenSky database and are thus not taken into account. In Fig. 6, the left ordinate shows the net energy forcing per month in absolute terms and the right ordinate shows the relative change in net energy forcing.

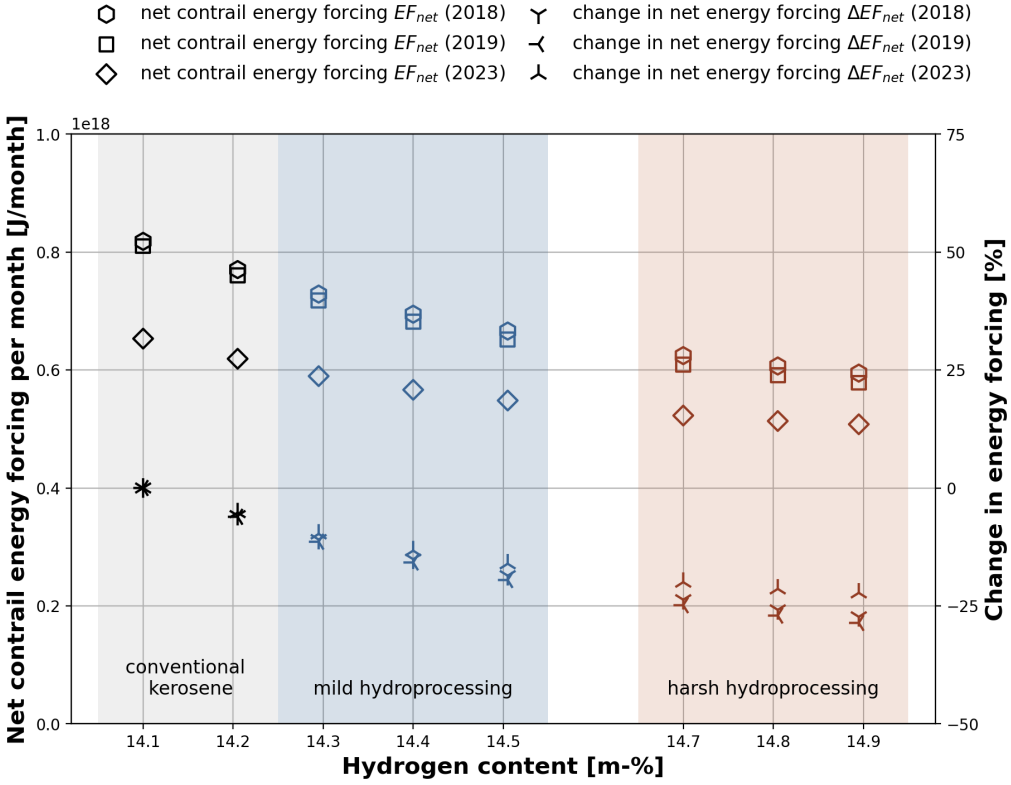


Figure 3.6 Net energy forcing in absolute (left ordinate, empty symbols) and relative terms (right ordinate, star symbols) for January, April, July and October and different years assuming medium hydrogen provision emissions and a 50-year time horizon (m-% mass-percentage)

In absolute terms, the net energy forcing shows a clear inter-annual variability (e.g., ~20 % for 14.1 m-% hydrogen content between 2023 and 2019). Both, inter-annual weather variability and different air traffic volumes contribute to this variation.

In relative terms, however, the inter-annual variability is substantially reduced to a few percentage points. By using the reference case (hydrogen content 14.1 m-%) as baseline, the effects of different air traffic volumes or inter-annual weather variability can largely be excluded.

In conclusion, the absolute reduction in energy forcing for the hydroprocessing intensities varies with the overall climate impact of contrails

among different years. However, the relative potential to mitigate the net contrail climate impact for a particular year appears to be rather consistent inter-annually. It amounts to about 18 % for mild hydroprocessing and about 33 % for harsh hydroprocessing.

3.1.3.2 Discussion

3.1.3.2.1 Climate Impact Reduction Potential

The climate benefits of reducing the contrail energy forcing by means of additional fuel processing outweigh the climate penalty of CO_2 emissions from aviation kerosene hydroprocessing. Based on the taken assumptions, this is not only the case for hydrogen provision with high CO_2 emissions, but also when longer timeframes (up to 100 years) are considered for the climate impacts.

The influential factors on climate impact (fuel hydrogen, and aromatic content, CO_2 emissions from hydrogen provision) could either be influenced by a particularly favourable crude oil (with high hydrogen and thus low aromatics content) and / or hydroprocessing based on hydrogen produced from renewably sourced energy. The development of future crude oil properties is primarily driven by overall crude oil demand for which aviation kerosene demand plays a minor role only. Thus, the future development of overall crude oil demand and its associated properties is difficult to predict [39]. Simultaneously, renewably sourced hydrogen is increasingly considered as an important energy carrier for the future [198, 199]. Accordingly, using hydrogen with low lifecycle CO_2 emissions seems to be more realistic than a dedicated sourcing of favourable crude oils.

Hydroprocessing of aviation kerosene creates several secondary effects, not considered here. The increase in hydrogen content also increases the gravimetric energy density of the “low-contrail” fuel. However, this change in fuel consumption also reduces the CO_2 related climate impact of fuel combustion. This effect would counterbalance the CO_2 climate impact of hydroprocessing. Since this study assumes stoichiometric reactions for fuel processing and a broadly aggregated combustion model, a valid comparison of both effects requires further research. Additionally, the reduced aromatics content results in fewer soot particle emissions, which in turn reduces air pollution and thus improves air quality in particular at airports. The kerosene’s sulfur content does not only affect the hydrogen required

for hydroprocessing but potentially also the number of soot particles activated into ice and hence the contrail climate impact. Various studies [17, 131, 194–197] describe the fuel sulfur content as contributing factor towards soot particle activation. For modern jet turbines with soot emissions in the low-soot regime, the activation of sulfur aerosols might gain importance for contrail formation [131]. In terms of emissions, lower sulfur emissions will improve air quality at airports and reduce the acid rain potential.

Previous studies investigated costs and environmental benefits of removing naphtalenes from aviation kerosene [81, 85] and estimate a smaller impact on reducing soot emissions and thus subsequent climate impact. As these studies only consider the removal of multi-cyclic aromatics, their measures are not as severe as those discussed here.

Some limitations remain inherent to this study, such as a more specific refinery configuration, detailed aviation kerosene composition after hydroprocessing and the influence of individual fuel components (e.g., cycloalkanes) on contrail formation. Due to the limited availability of aviation kerosene properties, the distribution of aviation kerosene hydrogen content is based here on 57 samples from the World Fuel Survey [179]. In light of the strong regional variations of contrail climate impacts, a regionally differentiated study with a larger dataset might allow for more detailed results. Straight-run kerosene differs largely from vacuum-gas oil (the usual feed of a hydrocracker). Hence, it is questionable if both could be processed simultaneously in the same processing unit. A more detailed simulation study of the process would require considering interdependencies with other products and detailed processing flows. Here, the effects of individual aviation kerosene components (e.g., aromatics or cycloalkanes) are aggregated by using their hydrogen content. More detailed combustion chemistry models and measurements of effects on contrail formation are necessary to validate these initial findings.

3.1.3.2.2 Specification Compliance

Standardized fuel specifications define the permissible chemical and physical properties of aviation kerosene. Mainly, these are laid out in the specification ASTM D1655 [181]; other specification standards exist in some countries (e.g., Russia and China). Their requirements, properties, and limitations are – in the case of commercial aviation – similar to those defined by

ASTM [200]. Renewably sourced kerosene must comply with the ASTM-standard D7566, which includes a lower limit of 8 vol-% aromatics content for renewably sourced kerosene. This limit has been introduced because aromatics can play an important role in sealing tightness and fuel quantity measurements among others [135, 137]. Especially legacy aircraft are considered susceptive to a risk of e. g., fuel leakages due to deteriorated seal tightness after prolonged exposition with aromatics free aviation kerosene. For these reasons, compliance with the prescribed aromatics content is a critical issue also for hydroprocessed fossil-based kerosene, even though the specification for fossil-based kerosene, ASTM D1655 does not include a lower limit for the aromatics content.

Table 3.2 shows the change in aromatics content for the different aviation kerosene processing strategies and the resulting net energy forcing reduction (for medium hydrogen provision emissions, 50 year time horizon). Mild hydroprocessing achieves an aromatics content in the range of the ASTM-standard D7566 lower limit and in turn a reduction in net energy forcing by about 18 %. Harsher process conditions would remove aromatics beyond the minimum content, but also allow for a larger net energy forcing reduction of about 33 %.

Table 3.2 Hydrogen and aromatics content and associated energy forcing reduction (medium hydrogen provision emissions, 50 year time horizon)

Processing case	Hydrogen content [m-%]	Aromatics [m-%] (incl. Napthalene)	Net energy forcing reduction [%]
Reference case	~14.1	~16.0	0
Mild hydroprocessing	~14.4	~8.0	~18
Harsh hydroprocessing	~14.8	~3.2	~33

Based on these values, mild hydroprocessing appears rather unproblematic from a specification compliance perspective. Harsh hydroprocessing at global scale would thus most likely require additional developments of the current fuel specifications [142].

Thus, in the short-term, the aromatics content of aviation kerosene could be reduced within the current limits, i.e., down to 8 vol-%. This aviation kerosene could be used in all aircraft, even in older legacy aircraft with sensitive sealing materials. The drawback of this option is a limited net energy forcing reduction at about 18 % (Table 3.2). As most present-day refineries already use mild hydroprocessing ("hydrotreatment"), e.g., for road

transport fuel desulfurization, this option might even incur comparatively low refinery modifications.

The climate mitigation potentials of harsh hydroprocessing would most likely require additional measures to ensure safe operation also for legacy aircraft. These measures could involve the development of an additional fuel standard for low contrail kerosene. Newly produced aircraft could potentially be certified for this standard. Some of the currently used aircraft could potentially be modified, e.g., by replacing particular fuel sealings or sensors with components compatible with such a low contrail kerosene. Moreover, it should be evaluated which legacy aircraft cannot be modified and would not be compatible with such a new fuel standard.

The increased hydrogen content due to fuel processing strategies content of the aviation kerosene produced (e.g., density). However, the relationships between aviation kerosene composition and resulting properties are very complex [201, 202], hence a comprehensive study of all specification-related aviation kerosene properties would be required to ensure safe operation of air transport. This would most likely involve the analysis of physical volumes of hydroprocessed fossil-fuel based kerosene and is thus far beyond the scope of this study [142, 201].

Additionally, a reduced aromatics content of fossil-based kerosene might incur challenges for its blending with renewably sourced kerosene, since the latter typically does barely contain any aromatics. As soon as the aromatics content of the blend decreases below 8 %, it would fall out of the limits of the current specification. The adjustment of both specifications, ASTM D1655 and ASTM D7566 as described above and an increasing fleet penetration of modern aircraft might alleviate this constraint.

3.1.3.3 Conclusion

Based on these results, increasing the hydrogen content of aviation kerosene, and thus reducing sulfur and aromatics content, allows for a short-term reduction in aviation's contrail-climate impact. Increased hydroprocessing intensity improves the mitigation potential but also raises associated uncertainties. The results discussed above show a reduction in net energy forcing between about 18 % (mild conditions) and about 33 % (harsh conditions) seems achievable by hydroprocessing for the case of medium emissions from hydrogen provision. The climate impact reduction potential

is influenced by the unprocessed kerosene fraction's hydrogen and aromatics content and the CO_2 emissions intensity of hydrogen provision. The use of hydrogen with a low emissions intensity (e.g., from renewable sources) seems to be a promising option to further reduce the climate penalty of fuel processing.

A potential future option to balance the climate impact reduction and additional CO_2 emissions more efficiently would be to use such a "low-contrail" fuel only on flights where contrails form with a warming climate impact. As only a small percentage of the flights are responsible for a large share of the contrail climate impact, this might reduce the required amount of aviation kerosene to be treated [10, 185, 186]; e.g., for the North Atlantic flight corridor, around 3–12 % of the flights cause around 80 % of the contrail climate impact [186]. Supplying low-contrail kerosene (regardless of its fossil/renewable origin) specifically to the most climate-relevant flights would necessitate to segregate logistics infrastructures to accommodate for two different aviation kerosene types. Associated costs and emissions and their trade-off with additional climate benefits could be another area for further research.

The extent to which the benefits estimated in this analysis are further constrained, e.g., by the effects of individual aviation kerosene components on contrail formation or constraints from aviation kerosene specifications, is yet to be determined.

While this study provides a first insight into the potential of hydroprocessing of fossil-based kerosene to reduce aviation's climate impact, given the above-mentioned uncertainties, many open questions remain and provide potential for surprises. Therefore, before additional hydroprocessing of kerosene can be implemented as climate mitigation measure, specific uncertainties inherent to this study need to be reduced.

For instance, more precise hydroprocessing models might provide more detailed data on the resulting aviation kerosene composition and thus on specification compliance. For harsh hydroprocessing, compliance with current fuel specifications appears to be a critical issue especially for legacy aircraft. The abovementioned safety concerns have to be addressed and fuel specifications need to evolve accordingly. Moreover, comprehensive experimental data and detailed studies on the emission properties of such a hydroprocessed, "low-contrail" fuel would be required to provide insights into

potential aircraft and infrastructure modifications, as well as on the magnitude of the climate impact reduction. More detailed combustion models and an extended suite of ground and cruise measurements of the effects of the hydroprocessed, "low-contrail" fuel on contrail formation are required to evaluate these initial findings. Additionally, a study of the associated cost of hydroprocessing, e.g., by increased hydrogen demand and switching to renewably sourced hydrogen would be interesting from an economic perspective. This particularly holds true for the cost as function of hydrogen content, since presumably cost are over-proportionately higher for removing all aromatics compared to a partial reduction in aromatics content by milder hydroprocessing. Based on this relationship, marginal abatement cost for hydroprocessing of fossil-based kerosene could be determined and allow for a comparison with other aviation climate impact mitigation measures.

3.2 Renewable Fuel Options For Aviation – A System-wide Comparison Of Drop-in And Non Drop-in Fuel Options

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Typesetting and formatting are slightly adjusted to ensure consistency within this thesis.

Abstract

The air transport sector's contribution to anthropogenic climate forcing is estimated at around 4 %. In this respect, alternative fuels are considered as a key measure to reduce greenhouse gas emissions within the air transport system and thus to reduce the contribution of commercial aviation to anthropogenic climate change. Nevertheless, so far, the usage-shares of alternative fuels are below 1 %. Thus, the goal of this paper is to analyse a broad selection of aviation fuel options for their greenhouse gas reduction potential based on a set of nine assessment criteria. The fuel options studied are blended synthetic kerosene and neat synthetic kerosene fuels, three alcohols (methanol, ethanol and butanol) and three gases (methane, ammonia and hydrogen). For these fuels a multi-criteria assessment based on a five-step ordinal scale is performed. The assessment results show that the availability of some biogenic feedstock is not sufficient to replace the present overall energy demand of aviation; while the availability of non-biogenic fuels might increase in the near- to mid-term. In general, alternative kerosene-like fuel options are mainly constrained by lacking production capacities, while alcohols and gases considered are constrained by aircraft modifications or development of new aircraft types. All discussed fuel options have the potential to mitigate greenhouse gas emissions of commercial aviation substantially also from a life cycle perspective. Within the next decade, especially alternative kerosene-like options with (intermediate) products experiencing demand from other sectors, such as FT-SPK or AtJ-SPK, show a high development potential. The same holds for hydrogen provided that a hydrogen fueled aircraft will be brought successfully to the market.

3.2.1 Introduction

The air transport sector emitted about 1 Gt of CO_2 globally in 2018 corresponding to approximately 2.4 % of the world wide anthropogenic CO_2 emissions [5]. With regards to overall anthropogenic climate forcing, recent studies estimate the air transport sector's contribution at around 4 % by taking non CO_2 effects additionally into consideration [8]. Also, air traffic volumes grew by ca. 4 %/an in the past decades and despite a sharp decrease due to the Covid-19 pandemic in 2020, a return to pre-pandemic levels is expected and based on current developments most likely [160]. In the longer term, the air transport sector will continue to grow – like in the past – with a high probability at average growth rates of approximately 4 %/a [156]. In contrast, technological and operational measures to increase fuel efficiency reduced the passenger-specific fuel consumption of air-travel by about 1.3 %/a [156]. Assuming for the years to come the outlined air traffic growth is constant and the named fuel efficiency improvements can be sustained, aviation's emissions could rise to above 2 Gt of CO_2 in 2050 [156].

In view of these circumstances, the commercial aviation sector is required to lower its climate impact effectively and swiftly. In 2021, the International Air Travel Association (IATA) raised previous GHG reduction emission targets for the air transport sector to a net-carbon neutral GHG emission level in 2050. Also, the International Civil Aviation Organization (ICAO) presently develops a "long-term aspirational goal" in addition to its present aim of a carbon-neutral growth from 2020 onwards [3, 203]. One of the key measures to achieve these goals is the use of "green" aviation fuels (i.e., fuel derived from renewable energy; often-called sustainable aviation fuels (SAF)). This means, currently used aviation fuels almost exclusively produced from fossil crude oil ("fossil kerosene") will have to be gradually replaced by fuels provided from renewable sources. In this respect, primarily kerosene-based fuel alternatives have been pursued so far. These fuels can be summarised as "synthetic" kerosene[5].

[5] In some cases this term is used to refer to fuels of non-biogenic renewable origin only or to distinguish among different fuel options within aviation fuel specifications [204]. The use of "synthetic" in this study includes both, options of biogenic and non-biogenic feedstock. Additionally, alternative aviation fuels are often referred to as "sustainable aviation fuel" or "SAF". However, this term will not be used here, as the fuel's renewable origin does not guarantee the fulfilment of other sustainability aspects (e.g., biodiversity or social criteria).

To produce synthetic kerosene, the ASTM D7566 specification is applicable. This specification presently requires the neat synthetic kerosene to be blended with fossil kerosene [137]. After a specification compliant blending procedure, the blend must meet the requirements of ASTM D1655, which is the same specification as for fossil kerosene. This blend can be used within the existing kerosene infrastructure and aircraft without any further technical modifications. Also, the blend can be seamlessly commingled with other kerosene types being in the fuel infrastructure. Therefore, such blends are referred to as "drop-in" aviation fuels [135].

Presently, most of the aviation fuel in use is produced from fossil crude oil. To a minor extent, kerosene is also produced from coal or natural gas (cf. Appendix B). Although various synthetic kerosene options of a "green" origin have been extensively discussed and tested for nearly 15 years [200], the usage-share of such synthetic kerosene is globally still at approximately 0.1 % related to the overall kerosene use [167, 205, 206]. The statistically recorded production volume of kerosene of renewable origin is at around 200 kt/a compared to around 300 Mt/a of fossil kerosene [167]. Higher production costs of synthetic kerosene compared to fossil kerosene, a lack of production facilities as well as missing regulatory frameworks to foster a synthetic kerosene usage are often stated as major reasons for the missing market ramp up [87, 125, 144, 158].

Additionally, other mobility and industrial sectors claim access to the feedstock needed to produce synthetic kerosene and are possibly willing to pay higher prices compared to the aviation sector. This could limit the availability and cost-effective supply of feedstock for the production of synthetic kerosene options. Simultaneously, the development and use of other fuel options (e.g., hydrogen or methanol), receive increasing interest in other sectors or within the overall energy system [35, 117, 207]. Hydrogen, for example, can be produced in relatively few process steps and – in contrast to synthetic kerosene – without the provision of a sustainable carbon source. Therefore, hydrogen has become increasingly relevant recently as a fuel option for aviation applications [78]. Clearly, such fuels are not drop-in capable in contrast to blended synthetic kerosene.

Additionally, the scientific understanding of non-CO_2 related effects (e.g., radiative forcing from aircraft-induced clouds or aerosol emissions) for the assessment of the overall climate impact of aviation is increasing [5,

8]. Studies show that using synthetic kerosene can also reduce those effects (but most likely not entirely rule out) [17, 27].

In view of this diverse mix of fuel options and an increasing need for climate protection in the air transport sector, the question of how to classify and assess the various "drop-in" options among the "non drop-in" options is becoming increasingly important. Against this background, the goal of this paper is to analyse both drop-in and non drop-in fuel options for their potential use as a fuel for commercial aviation. This assessment uses nine assessment criteria including technological and system-related aspects to compare each fuel option's suitability as an aviation fuel option.

To achieve this goal, the selected fuel options are described in section 3.2.2. The assessment methodology and selection of fuel options is presented in section 3.2.3, while in section 3.2.4 their assessment is conducted. Section 3.2.5 contains the results as well as the respective discussion and section 3.2.6 provides a brief summary and a final consideration.

3.2.2 Background

The distinction between drop-in and non drop-in fuel options is based on whether or not a fuel option complies with the standardized fuel specification. For the majority of the various kerosene options, this specification is defined by the American Society for Testing Materials (ASTM) developing the fuel standards for global civil aviation [142].

- **Drop-in.** The term "drop-in" fuel refers to all specification compliant aviation fuels according to the ASTM D1655 specification. This includes synthetic kerosene produced in accordance with ASTM D7566 and properly blended as well as fuels produced according to ASTM D1655 by a common processing of specific renewable feedstock (e.g., used cooking oil) or specific synthetic crude oils and fossil crude oil in conventional refining processes (Co-Processing). Drop-in fuels can be used within the existing fuelling infrastructure and the commercial aircraft fleet in operation without any technical modifications as a blend with fossil kerosene up to a specific blending limit [208].
- **Non drop-in.** The term "non drop-in" fuel refers to all fuel options, which do not fulfil the ASTM D1655 requirements. Hence, this comprises also synthetic kerosene produced in accordance with ASTM D7566 used above the blending limit or even without any blending procedure [137].

Based on these definitions, below the aviation fuel options selected for the further assessment are presented and described with respect to their main production pathways and future applications.

3.2.2.1 Selection

Today, a wide spectrum of different fuels are used for various mobility sectors. Typical examples are diesel and gasoline, methane, liquefied petroleum gas (LPG), bioethanol, fatty-acid-methyl-ester (FAME), or even butanol. Also, e.g., the chemical industry uses several of them as a bulk chemical to be further processed to high-value products. Additionally, hydrogen is also often added as an important future fuel option for the transport sector [35]. From this broad variety, here such fuels are selected, which seemingly have a high potential for a system-wide implementation within the commercial aviation industry. This selection is based on three main criteria.

1. A fuel option is already in use as a renewable fuel option in the air transport system or another specific sector (e.g., bioethanol).
2. A fuel option is considered as an integral part for defossilation of the overall energy system.
3. The potential aviation fuel is liquid or gaseous under standard conditions (i.e., battery-electric aircraft concepts are excluded as well as solid fuels).

Based on these criteria, three alcohol fuel options (methanol, ethanol, butanol, i.e. n-butanol and its isomers) as well as three gases (ammonia, methane, hydrogen) are taken into account. For kerosene-based options, blended and neat drop-in synthetic kerosene options are considered. Table 3.3 distinguishes the investigated fuel options as (non) drop-in fuel options. Additionally, the considered production pathways, the present production and the present / the future use possibilities are listed. Table 3.3 can be summarized as follows.

- Methanol and butanol are selected due to their role as platform chemicals [209]. Not only energy provision, but also the defossilation of the chemical industry could be a good reason for their production from feedstock of renewable origin (criterion 2). So far, ethanol is already produced to a significant share from feedstock of renewable origin (criterion 1).

- Ammonia, methane and hydrogen are all considered as options for storage and transport of renewably sourced energy (criterion 2) [210].
- The kerosene-based options take into account all conversion pathways being presently certified by ASTM D7566 (criterion 1). Additionally, an unblended use as neat synthetic kerosene is also discussed.

Table 3.3 Drop-in and non drop-in fuel options considered for the assessment (A with aromatics; ABE Acetone, Butanol, Ethanol; AtJ Alcohol-to-Jet; Cat Category; CH Catalytic Hydrothermolysis; FT Fischer-Tropsch; HC Hydroprocessed Hydrocarbons; HEFA Hydroprocessed Esters and Fatty Acids; HFS-SIP Hydrofermented Sugars Synthesized Isoparaffins; N/A not applicable; Ref Reference; SK Synthesized Kerosene; SPK Synthetic Paraffinic Kerosene)

Cat		Fuel option	Production pathway considered	Present production (fossil origin renewable origin)	Ref	Present use	Future use
Synthetic Kerosene	Drop-in	Blended Synthetic Kerosene	FT-SPK HEFA-SPK HFS-SIP FT-SPK/A AtJ-SPK CH-SK HC-HEFA-SPK	0.4 Mt/a[6] < 0.2 Mt/a	[167, 211]	aviation fuel	
	Non drop-in	Neat Synthetic Kerosene					
Alcohols	Non drop-in	Methanol	Methanol synthesis	90-100 Mt/a < 1 Mt/a	[212]	platform chemical, fuel	
		Ethanol	Fermentation	N/A 100 Mt/a	[213]	fuel (additive), potable alcohol, chemical and pharmaceutical applications	
		Butanol	ABE-fermentation	3.7 Mt/a N/A	[56]	platform chemical	platform chemical, fuel
Gases		Ammonia	Haber-Bosch conversion	180 Mt/a N/A	[214]	fertilizer for agriculture, chemical and pharmaceutical industry	fertilizer for agriculture, chemical and pharmaceutical industry, energy storage and fuel
		Methane	Fermentation Methane synthesis	2,671 Mt/a 0.1 Mt/a	[210]	heat and power generation, production of syngas for chemical industry	heat and power generation, production of syngas for chemical industry, fuel
		Hydrogen	Electrolysis	70 Mt/a N/A	[215]	chemical industry, refineries	chemical industry, refineries, heat and power generation, steel production, fuel, energy storage

[6] This value resembles the global production of FT-fuels (e.g., naphtha, gasoline, kerosene) from coal and gas.

3.2.2.2 Fuel Options

Kerosene based fuels. Here, kerosene based fuels are considered either as a specification-compliant blend of a fossil and a synthetic kerosene component or neat synthetic kerosene. Both usually consist of a range of hydrocarbons with a typical chain length of 8 to 16 carbon atoms. The most prominent hydrocarbon types in aviation fuels are n- and iso-alkanes, cycloalkanes and aromatics [137]. Seven conversion and two co-processing options are approved for the provision of synthetic kerosene by ASTM D7566 and ASTM D1655. From these options only the production pathways considered in the assessment are discussed here [87, 92, 94, 102, 123] (cf. Appendix B).

Conversion pathways based on Fischer-Tropsch synthesis (FT-SPK) thermo-catalytically convert a synthesis gas ("syngas") into long-chain hydrocarbons ("syncrude"). Syngas can be provided from lignocellulosic biomass (e.g., forestry or agricultural residues) or non-biogenic feedstock[7] (i.e., electricity from renewable energy, water and sustainable CO_2). If syngas is produced exclusively based on "green" electricity, these fuels are often referred to as "power-to-liquid" (PtL) fuel [94, 216, 217]. The "Hydroprocessed Esters and Fatty Acids" (HEFA-SPK) pathway or catalytic hydrothermolysis (CH-SK) are suitable conversion processes for lipid feedstock. Both utilize a thermochemical conversion of lipids into long-chain hydrocarbons. Another conversion pathway is the Alcohol-to-Jet (AtJ-SPK) process; here, alcohols are converted into long-chain hydrocarbons including the jet fuel range. Suitable feedstock for this pathway are sugar and starch and potentially also lignocelluloses. Presently ethanol and iso-butanol are certified for the production of AtJ-SPK [204]. This pathway shows a promising potential for two reasons: Ethanol is already being produced from renewable feedstock at large scale (s. Table 3.3) and in contrast to their direct use, the conversion of alcohols to AtJ-SPK does not require modifications at the infrastructure or aircraft technology (s. 3.2.4.3). Methanol as intermediate for AtJ-SPK is not yet certified but announcements indicate the start of the certification process for the begin of 2023 [218]. Hydroprocessed Fermented Sugars – Synthesized Iso-paraffins (HFS-SIP) denotes a conversion path-

[7] A production of syngas based on fossil feedstock (e.g., via coal gasification or methane reforming) is also possible. Due to the fossil origin of the feedstock, this pathway is not included here.

way, where a sugary solution is converted via biocatalysts into hydrocarbons. As co-processing pathways contain a large share of feedstock of fossil origin, they are not considered here.

Due to a (slightly) different chemical composition of neat synthetic kerosene (depending on the specific conversion pathway), compliance with ASTM D1655 requires additional adaptations, e.g. the addition of aromatics. Several production pathways do not yield aromatics (e.g., HEFA- or FT-SPK) or show a different distillation curve gradient (e.g., HFS-SIP) [142]. Theoretically, the same production pathways as described for synthetic kerosene blends can be used for neat synthetic kerosene production. To which extent all conversion pathways allow an unblended use has not yet been determined.

Alcohols (Methanol, Ethanol, Butanol). Methanol is also produced from syngas (above and Appendix B) [219]. The origin of methanol (i.e., fossil or renewable) is thus primarily determined by the used syngas. The majority of the present methanol production utilizes fossil-based syngas. Compared to that, the major production pathway for ethanol is an anaerobic fermentation of a sugar solution produced from naturally available sugar or converted from starch. Ethanol is basically the only alcohol that is currently produced from renewable feedstock at industrial scale [220, 221].

"Green" butanol is produced via the Acetone, Butanol, Ethanol (ABE-) fermentation realised by bacteria. As different products (acetone, butanol, ethanol) are provided, there is a need to separate this product spectrum afterwards [220, 222]. In principle, the products of the ABE-fermentation could be used as a blend. However, this option is excluded from this study to limit the number of fuel options, as other combinations of fuel options might also appear advantageous (e.g. blending a small amount of ethanol with fossil kerosene). Other production pathways for butanol do exist, such as the acetaldehyde pathway or fermentation utilizing genetically engineered biocatalysts. In contrast to ABE fermentation, these technologies are at a relatively low degree of technological maturity and thus not included in this study [223–225].

Gases (Ammonia, Methane, Hydrogen). The current ammonia production is based on the Haber-Bosch process converting hydrogen and nitrogen into ammonia. Before that, nitrogen is extracted from ambient air by an air separation process. Currently, hydrogen for such an ammonia production is provided from natural gas via steam methane reforming. This

provision pathway could be replaced by hydrogen provided by water electrolysis using "green" electricity [118].

To produce "green" methane, biomass-based as well as electricity-based supply pathways are possible [210, 220, 226]. These provision pathways either consist of biomass degradation by anaerobic digestion or methane synthesis [219].

Hydrogen of renewable origin can be produced by water electrolysis. If the electricity for such a water electrolysis is provided exclusively from sustainable, renewable sources (e.g., from photovoltaic and / or wind power plants), "green" hydrogen can be provided [35, 207, 227]. At standard conditions, gases have a comparatively low volumetric energy density, which can substantially be increased by liquefaction. However, this comes at the cost of energy requirements and higher losses ("boil-off") [198]. Therefore, the present study assumes that the large scale infrastructure for fuel distribution uses compressed gases, liquefaction takes place at the airport and subsequently aircraft are being fuelled by liquefied gas.

3.2.3 Methodology

This assessment (Figure 3.7) considers nine criteria covering various aspects across the entire fuel value chain. The following section first describes the methodological approach of the assessment performed and then specifies the selection of assessment criteria.

For the considered fuel options, the requirements and implications as aviation fuels are ranked according to a set of nine assessment criteria. A five-stage uniform ordinal ranking is applied for each assessment criterion, as considerable uncertainties exist for several of the criteria. For every assessment criterion, each fuel option is ranked from 1 ("very disadvantageous") to 5 ("very advantageous"). The decision of the respective ranking is based on an extensive assessment of literature data and other public available information. All values mentioned reflect present-day (2022) techno-economic parameters based on a global view. Additionally, the trend most likely becoming visible within the next decade is discussed based on the expected developments.

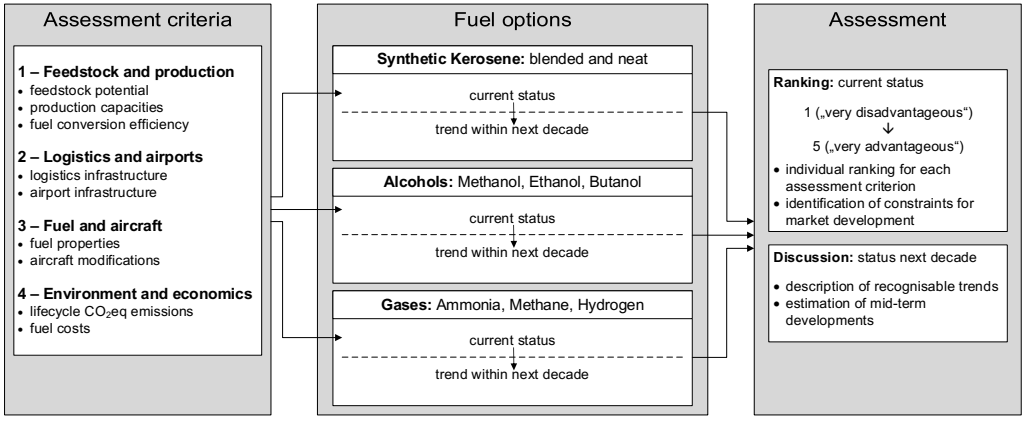


Figure 3.7 Methodological approach

The different criteria are not weighted against each other as they fall into very different categories. Thus, they can only be compared with each other to a very limited extent in a robust, fair, and consistent manner. Additionally, the rankings are not aggregated into a single value as this assessment rather aims at illustrating the complex interplay of implications for the use of a fuel option as an alternative aviation fuel instead of finding one "ideal fuel option".

Table 3.4 lists the assessment criteria to compare the different fuel options. They are grouped into three categories across an aviation fuels physical value chain and one related to overarching aspects.

Table 3.4 Assessment criteria considered for the fuel option assessment

#	Assessment criterion	Definition
1	Feedstock potential	Availability of a particular feedstock
2	Fuel conversion efficiency	Energy (feedstock) required to produce a defined amount of energy per mass unit of a respective fuel option
3	Production capacities	Extent to which production capacities are available or other production infrastructure could be utilized
4	Logistics infrastructure	Extent to which transport infrastructure is available or other transport infrastructure could be used to deliver the fuel from production to the airport
5	Airport infrastructure	Extent to which airport infrastructure is available for fuel storage and handling
6	Fuel properties	Chemical fuel properties and their implication for aviation use
7	Aircraft modifications	Required technological changes and their technology readiness level (TRL) to facilitate the use of non drop-in fuels
8	Lifecycle CO_2 emissions	CO_2-related climate impact of using the respective fuel option
9	Fuel cost	Production costs bandwidth of a respective fuel option

- The first category comprises three criteria: feedstock potential, production capacities, and fuel conversion efficiency.

- Logistics and airports are evaluated by an assessment of logistics, infrastructure, as well as fuelling and storing capabilities at airports.
- Fuel and aircraft technology is studied by investigating operational fuel properties and aircraft modifications.
- The overarching category, environment and economics is discussed using the criteria life cycle greenhouse gas emissions and fuel costs.

Following this assessment criteria-based analysis, potential constraints for a market development at commercial scale are discussed. Such constraints often depend on exogenous influences, such as the development of a global production system for hydrogen of renewable origin. Hence, the constraints outlined below rather serve as an indication for existing bottlenecks from a time perspective than as a reliable quantitative estimate.

Such a procedure shows clear limitations. One limiting factor is the always incomplete data availability related to one assessment time period; additionally, most of the assessment criteria involve parameter difficult to convert or transform to the same system boundaries. The varying degrees of technological maturity of various processes induce further uncertainties about key process parameter (e.g., conversion efficiency, fuel costs). Beside this, the future trajectory of the fuel options' potential largely depends on the further progress of the entire energy system and thus the further development of the global energy system. One example is the development of hydrogen as a possible energy carrier for a large-scale defossilation of various industrial sectors. Thus, interdependencies with and developments of other sectors significantly effects the air transport system's energy provision as well as the respective economic development. Also, costs and efforts for the deployment of infrastructure are critical factors for the likelihood of the market introduction of alcohols and gases as aviation fuels; a clearly uncertain setting of the political frame conditions add up to this. Nevertheless, based on such an assessment robust conclusions can be drawn.

3.2.3.1 Category 1 – Feedstock and Production

Feedstock potential. A limited feedstock availability limits production possibilities of a fuel option. This is underlined by the fact that primary (renewable) energy sources as well as (sustainable) raw materials are demanded by various sectors being part of our overall economy – and not only by commercial aviation. Within the five-stage ordinal ranking, a feedstock

potential being at least two orders of magnitude greater than aviation's energy demand is rated as "very advantageous" (5), a feedstock potential comparable to aviation's energy demand is seen "neutral" (3) and a substantially lower feedstock potential is rated as "very disadvantageous" (1) (Table 3.5).

Production capacities. As the duration to ramp up production capacities can significantly delay the deployment and large-scale use of a corresponding fuel option, this criterion describes the current (2022) availability of existing fuel production capacities. The usability of an existing production infrastructure is rated as "very advantageous" (5), first industrial plants as "neutral" (3) and the complete lack of a corresponding production infrastructure as "very disadvantageous" (1) (Table 3.5). Additionally, the technology readiness level (TRL) [228] is discussed in this section.

Fuel conversion efficiency. Due to a (still) limited availability of "green" energy as well as the respective other (sustainable) resources, a specific conversion route to provide a certain fuel is particularly favourable based on high conversion efficiencies. This criterion is defined as the ratio of energy content of produced jet fuel to the required secondary renewable energy to produce the same mass of fuel (Figure 3.8).

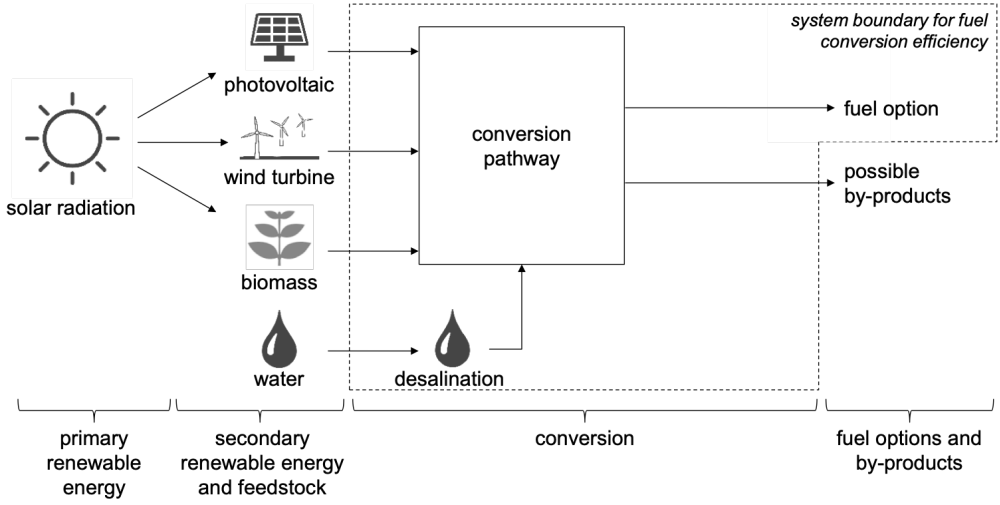


Figure 3.8 System boundaries for the selection of literature values estimating aviation fuel conversion efficiency

The values for the ranking are based on the median of estimates of present (2022) technology. Figure 3.8 shows the system boundaries used for this

assessment. The energy content of other by-products is not taken into account. The kerosene yield can be altered significantly by thermochemical post-conversion processes such as hydroprocessing, thus the final kerosene fraction is not necessarily a characteristic of a particular conversion pathway. Therefore a 70 % kerosene fraction is assumed for all synthetic kerosene conversion pathways, to ensure comparability. A median lower than 20 % is ranked as "very disadvantageous" (1), between 40 % and 60 % as "neutral" (3) and above 80 % as "very advantageous" (5) (Table 3.5).

3.2.3.2 Category 2 – Logistics and Airports

Logistics infrastructure. The extent to which logistics and transport infrastructures are currently available for the respective fuels determines the practicability for a global deployment of these fuel options. If an existing logistics infrastructure is available for fuel transportation to airports, this ranks "very advantageous" (5). The possibility to modify infrastructure ranks "neutral" (3) and no existing usable infrastructure is considered "very disadvantageous" (1) (Table 3.5).

Airport infrastructure. Safety and operational implications create considerable differences between fuel logistics to and at the airport. This criterion assesses, to which extent storage and fueling infrastructure at airports would need to be modified / adapted / newly developed for the use of the fuel options discussed. Similar as for logistics infrastructure, if existing storage and fueling infrastructure can be used for a particular fuel option, this ranks "very advantageous" (5). The need for modifications of infrastructure ranks "neutral" (3) and no existing usable infrastructure is considered "very disadvantageous" (1) (Table 3.5).

3.2.3.3 Category 3 – Fuel and Aircraft

Operational fuel properties. Fuel properties might have significant effects on the flight performance and flight profiles of an aircraft. Thus, this criterion evaluates chemical-physical properties of fuel options (e.g., energy and storage density). Favourable operational range improvements (storage density > 5 % above fossil kerosene average of 43.25 MJ/kg [135]) are considered as "very advantageous" (5), small range improvements / losses (storage density ± 1 % 43.25 MJ/kg [135]) as "neutral" (3) and a significant

reduction in aircraft range (storage density > 50 % below 43.25 MJ/kg [135]) as "very disadvantageous" (1) (Table 3.5).

Aircraft design/modifications. Due to high technological and regulatory safety requirements in aviation, the design of a new aircraft as well as aircraft modifications due to another fuel can be associated with high technological efforts, economic risks and considerable time requirements [229]. This criterion compares technological modification requirements of currently certified aircraft technology to enable the use of an alternative fuel option. A "new" fuel option is rated as "very advantageous" (5) if there is no need for modification compared to today's overall aircraft configuration. Minor modifications are rated "neutral" (3) and a need for a new aircraft design and associated certification is ranked as "very disadvantageous" (1) (Table 3.5).

3.2.3.4 Category 4 – Environment and Economics

Lifecycle CO_{2eq} emissions. This criterion evaluates the life cycle greenhouse gas emissions of the fuel options. CO_{2eq} emissions below 25 g CO_{2eq}/MJ are considered to be "very advantageous" (5), 50 to 75 g CO_{2eq}/MJ as being "neutral" (3) and CO_2-emissions in a similar range compared to fossil kerosene (at or above 95 g CO_{2eq}/MJ [230]) as "very disadvantageous" (1) (Table 3.5). All emission estimates consider the present state of technology.

But, a significant part of aviation's climate effect does not linearly depend on fuel burn [5]. As hardly any data exists describing the magnitude of such non-CO_2-effects for non-kerosene fuel types (e.g., ethanol or ammonia), these effects are not included in the ranking [5, 231].

Fuel cost. The provision costs of each fuel option are a key determinant of airline economic performance[8] [232]. The median of published values from techno-economic analyses of different fuel conversion technologies is used to rank the various fuel options. All cost estimates use real, present

[8] The use of several of the considered fuel options would require the design of a new aircraft. This is usually associated with high development cost for such an aircraft and engine manufacturer and high investment cost for airlines. However, results of existing design studies differ significantly with regard to the magnitude of these cost [76, 111]. Therefore, they are not taken into account in the ranking.

day (ca. 2020/22) costs. Costs below 20 €/GJ are considered "very advantageous" (5), between 40 and 60 €/GJ are ranked "neutral" (3) and costs above 80 €/GJ "very disadvantageous" (1) (Table 3.5).

Table 3.5 Ranges for the ranking of each assessment criterion

#	Assessment criterion	1	2	3	4	5
1	Feedstock potential	Feedstock potential significantly below energy demand of aviation	Feedstock potential below aviation energy demand	Feedstock potential up to one order of magnitude greater than aviation energy demand	Feedstock potential more than one order of magnitude greater than aviation energy demand	Feedstock potential more than two orders of magnitude greater than aviation energy demand
2	Production capacities	No existing production infrastructure	< 5 plants at demonstration scale	First industrial plants	Current renewable production amounts to < 5 % of 2019 global aviation energy demand	Current renewable production amounts to > 5 % of 2019 aviation energy demand
3	Fuel conversion efficiency	< 20 %	20 - 40 %	40 - 60 %	60 - 80 %	> 80 %
4	Logistics infrastructure	No existing logistics infrastructure	Major modifications of existing infrastructure required or regionally limited infrastructure	Existing logistics infrastructure can be modified	Minor modifications of existing infrastructure or widespread infrastructure	Usable logistics infrastructure exists for long-range transport
5	Airport infrastructure	No existing airport infrastructure	Major modifications of existing infrastructure required	Modifications of airport infrastructure necessary	Minor modifications of existing infrastructure	Usable airport infrastructure exists
6	Fuel properties	Significant reduction in aircraft range (storage density > 50 % below 43.25 MJ/kg)	Noticeable reduction in aircraft range (storage density < 50 % but > 1 % below 43.25 MJ/kg)	Negligible reduction in aircraft range (storage density ± 1 % of 43.25 MJ/kg)	No effect on range (storage density < 5 % but > 1 % above 43.25 MJ/kg)	Range improvements (storage density > 5 % above 43.25 MJ/kg)
7	Aircraft modifications	New design and certification required	Major modifications required	Minor modifications required	Modification of only a few components	No need for modifications
8	Life cycle greenhouse gas emissions	≥ 95 gCO_2eq/MJ (reference value for fossil kerosene)	< 95 gCO_2eq/MJ and ≥ 75 gCO_2eq/MJ	< 75 gCO_2eq/MJ and ≥ 50 gCO_2eq/MJ	< 50 gCO_2eq/MJ and ≥ 25 gCO_2eq/MJ	< 25 gCO_2eq/MJ
9	Fuel cost	> 80 €/GJ	60 - 80 €/GJ	40 - 60 €/GJ	20 - 40 €/GJ	< 20 €/GJ

3.2.4 Assessment of Aviation Fuel Options

This section covers the assessment of each fuel option along the value chain of an aviation fuel according to the criteria defined above. The main characteristics related to each assessment criterion are given and the assessment results are presented.

3.2.4.1 Feedstock and Production

Feedstock Potential. Feedstock of renewable origin can be clustered into feedstock of biogenic (i.e., various types of biomass) and non-biogenic origin (i.e., electricity from renewable origin together with sustainably provided carbon / CO_2) [220]. A renewable provision of non-biogenic carbon / CO_2 can be achieved in principle by capturing atmospheric CO_2 being theoretically available in abundance. But the present technology shows high energy requirements and significant material (and space) demands [233]. Water for electrolysis can be provided basically unlimited by sea water desalination; here the main limitation is its energy requirement [234]. Accordingly, the potential for non-biogenic feedstock is ultimately determined predominantly by the availability of "green" electricity. Therefore, for the availability estimation of non-biogenic feedstock, the assessment is based on its availability instead of the availability of water or atmospheric CO_2. The use of carbon point sources, e.g. from industrial food processing, is not taken into account by assuming that there are abundant carbon resources from this sector to cover the demand for commercial aviation. Figure 3.9 summarizes the ranking.

Biomass feedstock can be distinguished by four main categories: lipid, sugar, starch and lignocelluloses [220]. Sugar and starch from biomass is not considered for this assessment, as present legal definitions for sustainable aviation fuels increasingly exclude feedstock being in competition with the food and fodder market [235, 236]. Remaining and eligible biomass feedstock are mainly non-edible crops and / or organic waste, residues and / or by-products (e.g., sawmill residues, sewage sludge, used cooking oil (UCO)).

The potential for lipid containing, non-edible biomass and waste lipids is estimated to be around 125 to 330 Mt/a corresponding to roughly 4.6 to 12.2 EJ/a [125, 167, 237] excluding edible vegetable oils (e.g., palm oil). The potential of lignocelluloses-biomass (non-edible), organic waste,

residues and by-products is estimated to 2,660 Mt/a corresponding to approximately 46.5 EJ/a [167]. Other estimations state a potential of 125 EJ/a for lignocelluloses-biomass [237]. For comparison, the final energy consumption of aviation fuel in global commercial air transport was about 290 Mt/a fossil kerosene or 12.4 EJ/a in 2019 [238].

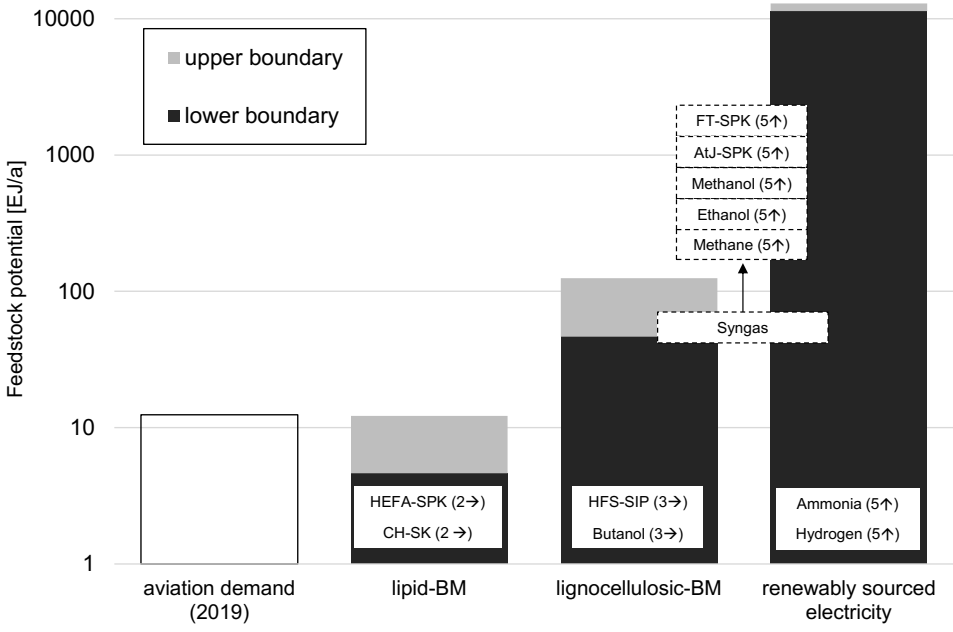


Figure 3.9 Comparison of potential energy provided by each feedstock category for the corresponding conversion pathways (numbers in brackets indicate each fuel option's ranking) (AtJ Alcohol-to-Jet; BM Biomass; CH Catalytic Hydrothermolysis; FT Fischer-Tropsch; HEFA Hydroprocessed Esters and Fatty Acids; HFS-SIP Hydrofermented Sugars Synthesized Isoparaffins; SK Synthesized Kerosene; SPK Synthetic Paraffinic Kerosene; ranking: 1 – "very disadvantageous"; 2 – "disadvantageous"; 3 – "neutral"; 4 – "advantageous; 5 – "very advantageous"; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear)

These figures clearly illustrate the limited availability of lipids and thus their limited ability as the only feedstock option to provide synthetic kerosene. This is especially true since conversion losses or an extra-sectoral demand is not taken into account in Figure 3.9 ("disadvantageous", 2). Some conversion pathways based on lignocelluloses do not utilize syngas ("neutral", 3). As syngas can be provided based on lignocelluloses-biomass or renewably sourced electricity and / or a combination of both, pathways based on syngas show an even higher feedstock potential ("very advantageous", 5). AtJ-SPK and Methane cannot only be produced via syngas but also directly from lignocellulose ("very advantageous", 5). The potential for

the utilization of renewably sourced electricity is very high ("very advantageous", 5). However, it is currently limited by capacities to convert e.g. solar energy to electricity. Even though a strong ramp up of "green" electricity is most likely in many regions of the world, the present use does by far not match its potential [239]. For this assessment criterion, limitations by lacking production capacities are not taken into account as the availability of production capacities is discussed in the following section.

Trend within next decade. Due to their characteristic as waste and / or residue, the availability of lipid-based feedstock keeps most likely constant in the decade to come. Substituting lipid-based fuels in road transport by battery-powered vehicles might improve their availability for aviation.

Similarly, the availability of lignocelluloses waste and residues will not change substantially. An extension of the feedstock bases may be realized if lignocelluloses-biomass is cultivated with agricultural methods and / or the existing potentials are more extensively used. Assuming that non-biogenic renewable energy sources are utilized more intensively, their availability can increase drastically. Bearing in mind increasing global ambitions to fulfil the legally defined greenhouse gas reduction goals, such a development appears at least possible [169]. However, it remains uncertain, to which extent increasing demand from other sectors outbalances the increased availability of non-biogenic feedstock.

Production Capacities. There are hardly any production capacities for the synthetic kerosene options assessed (less than 0.3 Mt/a, ca. 0.013 EJ/a) [240]. For FT-SPK based on renewable feedstock presently only demonstration facilities exist (TRL 7) [87, 95]. However, the fact that large commercial FT-plants for fossil feedstock exist in South Africa (coal), Qatar (natural gas) and Malaysia (coal) [74], might potentially ease the transition of renewable FT-SPK from TRL towards commercial scale. A few commercial plants produce HEFA-SPK ("neutral", 3); but most of them focus on the production of renewable diesel. This is also the pathway with the highest TRL (8 to 9) [87, 216]. For AtJ-SPK and HFS-SIP the conversion of sugar / starch is more developed (TRL 7 to 8) compared to the feedstock lignocelluloses (TRL 5 to 6) [87]. CH-SK is still in the demonstration stage (TRL 3 to 4) [87, 216].

Almost the entire global methanol production (90 to 100 Mt/a, ca. 2 EJ/a) is based on (fossil-based) syngas. But the provision of syngas from renewable resources is still not implemented [46]. Similar to FT-SPK,

these (fossil-based) production capacities might ease the transition of methanol from renewably sourced syngas towards commercial scale. For "direct" "green" methanol synthesis only a few, small-scale plants are under operation ("neutral", 3; TRL 8) [212, 219, 226].

Most of the global ethanol production (100 Mt/a, ca. 3 EJ/a) is currently renewably sourced ("very advantageous", 5), but mostly based on sugar and / or starch (TRL 9) [213]. As these types of feedstock are increasingly excluded for fuel production due to legal sustainability criteria, lignocelluloses-biomass would need to be converted to ensure long-term compliance (TRL 6) [221, 235, 236, 241]. To provide sugar for fermentation from lignocelluloses-biomass pretreatment steps for saccharification are additionally required, such as comminuting and subsequent hydrolysis or steam explosion [220]. Globally, 3.7 Mt/a (ca. 0.1 EJ/a) of fossil-fuel based butanol is produced being clearly less compared to methanol or ethanol [119, 242]. Production capacities for renewably sourced butanol are hardly available so far, because existing ABE-fermentation capacities have been shut down due to economic reasons in recent years (TRL 6 to 7) [222]. Currently, no production capacities for "green" butanol greater than a demonstration scale exist ("disadvantageous", 2) [243].

Table 3.6 Existing production capacities and resulting ranking (AtJ Alcohol-to-Jet; BM Biomass; BtL Biomass-to-Liquid; CH Catalytic Hydrothermolysis; FT Fischer-Tropsch; HEFA Hydroprocessed Esters and Fatty Acids; HFS-SIP Hydrofermented Sugars Synthesized Isoparaffins; LC Lignocellulosic; S Sugar/Starch; SK Synthesized Kerosene; SPK Synthetic Paraffinic Kerosene; PtL Power-to-Liquid; ranking: 1 – "very disadvantageous"; 2 – "disadvantageous"; 3 – "neutral"; 4 – "advantageous; 5 – "very advantageous"; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear)

#	Fuel option		Production capacities	Ranking	Trend	TRL
1	Blended Synthetic Kerosene and Neat Synthetic Kerosene	FT-SPK (BtL)	First industrial plants	3	→	7
2		FT-SPK (PtL)			↑	7
		HEFA-SPK			→	8-9
		AtJ-SPK			↑	7-8
		HFS-SIP			→	7-8
		CH-SK			→	3-4
3	Methanol		First industrial plants	3	↑	8
4	Ethanol		Current renewable production > 5 % of global aviation demand	5	→	9 (S-BM) 6 (LC-BM)
5	Butanol		< 5 plants at demonstration scale	2	→	6-7
6	Ammonia		< 5 plants at demonstration scale	2	?	8-9
7	Methane		First industrial plants	3	?	8-9
8	Hydrogen		First industrial plants	3	↑	8

Ammonia production exists at industrial, global scale (180 Mt/a, ca. 3 EJ/a) [214]. If renewably sourced hydrogen and "green" electricity would be used, these capacities could produce "renewable" ammonia. However, this is currently not realised at scales larger than demonstration scale ("disadvantageous", 2; TRL 8 to 9) [214].

The major share of the current methane use originates from the consumption of natural gas [210]. Only a few methane production plants (biogas plants) based on biomass exist (< 0.2 EJ/a). Even though this production of so-called "biomethane" is technologically well-developed (TRL 9), it seems unrealistic for them to fulfil aviation's energy demands ("neutral", 3). For electricity based methane no industrial scale plants exist (TRL 6) [210, 226].

Annually, about 70 Mt/a of hydrogen are produced worldwide, but only a minor share via electrolysis of water (approximately 0.1 %, ca. 0.01 EJ/a; "disadvantageous", 2) [244]. However, the technology to produce hydrogen via electrolysis is well-developed (TRL 8) [35, 227]. Additionally, a significant increase in renewably sourced hydrogen production is politically envisioned.

Trend within next decade. The demand for aviation fuel is small compared to other sectors such as road transport or the chemical industry. Therefore, the development of production capacities for synthetic kerosene is strongly influenced by the further development of liquid fuel / bulk chemical production capacities for the overall energy system / for the industrial sector. Here an increasing demand seems particularly likely for applications, where electrification is technologically difficult (e.g., shipping) and/or where industry needs hydrocarbons for the respective production process [169]. Particularly synthetic kerosene options including (intermediate) products / side products with specific application fields outside the "classical" aviation sector would benefit (FT-SPK or AtJ-SPK).

Similar to synthetic kerosene, increasing demand for "green" methanol from other sectors being significantly larger than the demand from aviation (e.g., chemical industry) would support the ramp up of production capacities on a global scale. This is likely due to the prominent role of methanol as bulk chemical used already within the chemical industry globally. As most ethanol is produced based on renewable resources already today, a steep increase in production capacities is unlikely due to existing limitations in fertile land. However, current land / road transport can be substituted to a

certain extent by electric vehicles and thus existing bioethanol production could shift towards aviation and/or other sectors. Increasing interest from the chemical industry for bioethanol as a "green" bulk chemical would most likely further stimulate demand. As butanol is of minor importance compared to methanol or ethanol, a mid-term increase in "green" butanol production capacities seems rather unlikely.

"Green" ammonia could be used in the mid-term future for fertilizer production and as a potential energy (or hydrogen) carrier, which might cause a significant ramp up of renewable production capacities. If "green" methane takes a central role as energy carrier in the future, production capacities would increase substantially (similar to synthetic kerosene and methanol). But, a fast development of hydrogen production capacities receives significantly greater interest and investment compared to biomethane production [169]. Taking the ramp up of renewably sourced electricity into account, increasing production capacities for hydrogen seem to be most likely, while the development of a possible ramp up of "green" methane or "green" ammonia remains unclear for the time being.

Fuel Conversion Efficiency. Figure 3.10 compares fuel conversion efficiencies and Table 3.7 summarizes the corresponding references and ranking. Here it becomes obvious that the variation of the conversion efficiency estimates can largely be attributed to the feedstock energy content and the energy demand for feedstock provision. In general, high feedstock energy densities and/or low energy requirements for the conversion positively affect the fuel conversion efficiency. Simultaneously, large uncertainties exist as to the differing technological maturity of the conversion pathways.

FT-SPK shows significant variation in the conversion efficiencies justified by different types of feedstock. Typically, FT-SPK (BtL) conversion efficiencies increase with the feedstock energy content (e.g., higher values for black liquor). For FT-SPK (PtL), low conversion efficiencies result from the high-energy requirements of atmospheric CO_2 capture. HEFA-SPK is the technologically most mature pathway and its feedstock (lipids) is characterized naturally by a relative high energy density. Thus, its conversion efficiency with a median of 0.62 is clearly the highest among the synthetic kerosene options assessed here. The conversion efficiencies for AtJ-SPK include the conversion of biomass to alcohols, resulting in similar feedstock energy densities for all pathways using sugar as intermediate feedstock.

Low values of AtJ-SPK conversion efficiencies relate to the conversion of lignocelluloses and higher values to converting sugar or starch. As no study for AtJ-SPK provision based on butanol from ABE-fermentation was available, the lower end of AtJ-SPK does only take into account the conversion of ethanol. If AtJ-SPK were to be provided by butanol from ABE-fermentation, even lower conversion efficiencies would be possible. Other butanol production pathways might yield higher conversion efficiencies (s. below). The median of HFS-SIP is considerably lower than the median of CH-SK (0.32 compared to 0.42).

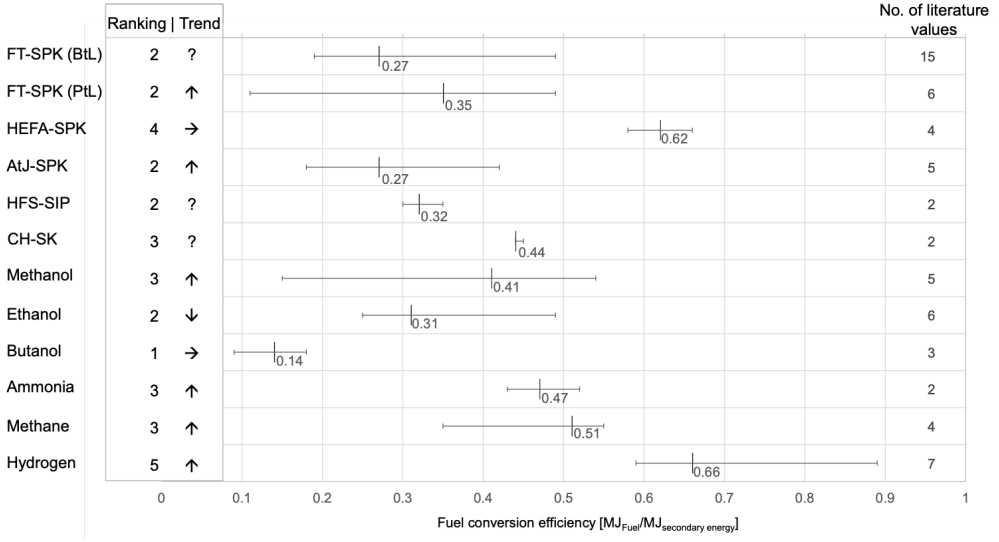


Figure 3.10 Median and range of aviation fuel conversion efficiencies; error bars indicate the lowest/highest values considered (AtJ Alcohol-to-Jet; BtL Biomass-to-Liquid; CH Catalytic Hydrothermolysis; FT Fischer-Tropsch; HEFA Hydroprocessed Esters and Fatty Acids; HFS-SIP Hydrofermented Sugars Synthesized Isoparaffins; SK Synthesized Kerosene; SPK Synthetic Paraffinic Kerosene; PtL Power-to-Liquid; ranking: 1 – "very disadvantageous"; 2 – "disadvantageous"; 3 – "neutral"; 4 – "advantageous; 5 – "very advantageous"; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear)

Values for methanol relate to different syngas feedstock. For syngas based on biogenic feedstock, the conversion efficiency increases with increasing energy content of the feedstock. For non-biogenic feedstock, the used carbon source and the associated energy requirements influence the pathway's conversion efficiency clearly. The conversion pathway to ethanol indicates a lower median in comparison to methanol (0.31 and 0.41) as well as low variations. Lower conversion efficiencies occur for ethanol production from lignocelluloses, while higher efficiencies are given for sugar or starch. The conversion efficiency estimates for butanol are considerably lower than for

the other alcohols due to the limited butanol yield of the ABE-fermentation [222, 224]. This can be attributed to the fact that only the butanol (and not ethanol or acetone) from this process is taken into account. Additionally, other pathways such as fermentation by genetically engineered biocatalysts, might yield higher efficiencies but were excluded a priori due to their low technological maturity (s. 3.2.2.2).

Table 3.7 Fuel conversion efficiency and resulting ranking (AtJ Alcohol-to-Jet; BtL Biomass-to-Liquid; CH Catalytic Hydrothermolysis; FT Fischer-Tropsch; HEFA Hydroprocessed Esters and Fatty Acids; HFS-SIP Hydrofermented Sugars Synthesized Isoparaffins; SK Synthesized Kerosene; SPK Synthetic Paraffinic Kerosene; PtL Power-to-Liquid; ranking: 1 – "very disadvantageous"; 2 – "disadvantageous"; 3 – "neutral"; 4 – "advantageous; 5 – "very advantageous"; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear)

#	Fuel option		Conversion efficiency [$MJ_{fuel}/MJ_{secondary\ energy}$]			Ranking	Trend
			Median	Min-Max	References		
1	Blended Synthetic Kerosene and Neat Synthetic Kerosene	FT-SPK (BtL)	0.27	0.19-0.49	[73, 91, 99, 122, 216, 219, 245–247]	2	?
		FT-SPK (PtL)	0.35	0.11-0.49		2	↑
		HEFA-SPK	0.62	0.58-0.66		4	→
2		AtJ-SPK	0.27	0.18-0.42		2	↑
		HFS-SIP	0.32	0.30-0.35		2	?
		CH-SK	0.44	0.44-0.45		3	?
3	Methanol		0.41	0.15-0.54	[219, 245]	3	↑
4	Ethanol		0.31	0.25-0.49	[91, 248, 249]	2	↓
5	Butanol		0.14	0.9-0.18	[224]	1	↑
6	Ammonia		0.47	0.43–0.52	[214]	3	↑
7	Methane		0.51	0.35-0.55	[219, 221, 245]	3	↑ (except Biomethane)
8	Hydrogen		0.66	0.59–0.89	[214, 219, 245, 250]	5	↑

For the gaseous fuel options, energy requirements for liquefaction are not taken into account. This is due to large uncertainties regarding boil off losses during handling and fueling of cryogenic fuels. As presently aircraft are not fueled with cryogenic fuels, their magnitude is difficult to estimate, even though they might be significant especially for hydrogen [76]. Hydrogen conversion efficiencies are the highest (median of 0.66) among the gaseous fuel options. This is ultimately limited by the electrolyser technology considered and potential energy requirements from liquefaction [198, 219].

For methane, values based on fermentation are mostly higher (above 0.5) than for a thermo-chemical synthesis. Methane provided from hydrogen and CO_2 as well as ammonia using hydrogen as an intermediate product show necessarily lower conversion efficiencies than hydrogen used as a

pure substance (approximately 0.5 compared to 0.7). As methane and ammonia have higher boiling points than hydrogen, their energy requirements for liquefaction and losses by handling and fueling are potentially lower than for hydrogen.

Trend within next decade. For synthetic kerosene based on non-biogenic feedstock (e.g., FT-SPK (PtL)), ongoing improvements for hydrogen and carbon provision (electrolyser technology, direct air capture) might increase overall fuel conversion efficiencies. In contrast, the conversion efficiency of HEFA-SPK has already reached industrial scale at high conversion efficiencies and is thus unlikely to yield further substantial improvements. The inclusion of further feedstock, e.g. methanol, for AtJ-SPK might result in higher jet fuel yields and resulting higher conversion efficiencies.

Methanol based on synthesis of non-biogenic feedstock would also benefit from improvements in non-biogenic hydrogen and carbon provision. Nevertheless, the saccharification step required for the use of lignocelluloses as a feedstock for ethanol will incur necessarily lower conversion efficiencies compared to using sugar / starch. The conversion efficiency of butanol is likely to improve provided that in the mid- to long-term other pathways than ABE-fermentation reach commercial scale.

In the light of globally increasing hydrogen production, conversion efficiencies for all gases considered might improve. A particularly high potential is the development of clearly more efficient electrolysis systems. As the provision of biomethane from fermentation already has a high conversion efficiency (even from less promising organic feedstock) and technological maturity, further improvements seem unlikely.

3.2.4.2 Logistics and Airports

Below, the assessment of infrastructure for fuel logistics and airport infrastructure is conducted. The first of the two criteria ("logistics") covers transportation from the place of production to airports in general, while the second criterion ("airports") discusses peculiarities of handling the fuel options at an airport. Both criteria are summarized in Table 3.8.

Table 3.8 Available infrastructure for logistics to and at airports and the resulting ranking (ranking: 1 – "very disadvantageous"; 2 – "disadvantageous"; 3 – "neutral"; 4 – "advantageous; 5 – "very advantageous"; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear)

#	Fuel option	Logistics	Ranking	Trend	Airports	Ranking	Trend
1	Blended Synthetic Kerosene	Usable logistics infrastructure exists	5	→	Usable logistics infrastructure exists	5	→
2	Neat Synthetic Kerosene	Minor modifications of infrastructure required	4	↑	Minor modifications of infrastructure required	4	↑
3	Methanol	Existing logistics infrastructure can be modified	3	?	Modifications of airport infrastructure necessary	3	→
4	Ethanol						
5	Butanol						
6	Ammonia	Minor modifications of existing infrastructure or widespread infrastructure	4	? ↑	Major modifications of airport infrastructure necessary	1	→
7	Methane						
8	Hydrogen	No existing logistics infrastructure	1	↑	Major modifications of airport infrastructure necessary	1	↑

Logistics Infrastructure. Due to their drop-in characteristic, the existing infrastructure used to supply fossil kerosene can be used without any modifications for specification compliant blends containing synthetic kerosene. Basically, all major modes of transport can be applied (e.g., pipelines, tanker ships, tank wagons) depending on the overall fuel demand at a particular airport ("very advantageous", 5) [251]. Regulatory requirements to account for the use of synthetic kerosene may require separate logistics [208]. From a technological point of view, also neat synthetic kerosene can be transported within the existing infrastructure. But, as long as they are specified as non drop-in options, they would need to be physically separated from fossil kerosene due to legal reasons ("advantageous", 4).

For all alcohols considered here, infrastructures at global scale exist, even though they usually lack connection to airports. But the existing logistics infrastructure could be easily extended for the supply of airports because the technology is basically there ("advantageous", 4).

For ammonia and methane, logistics infrastructures exist at a global scale (in particular ships and pipelines, respectively). For the transport of compressed methane, the natural gas pipeline system could be utilized ("advantageous", 4) [214, 226]. Ammonia transportation via ship is being performed at industrial scale already but the use of existing pipeline systems might require additional efforts due to the toxicity of ammonia ("advantageous", 4) [214]. Still, most of the airports would need a connection to the

existing infrastructure. For hydrogen, a global distribution infrastructure is not in place yet and due to its chemical properties (e.g. the lower volumetric energy density compared to methane) it appears unlikely that an existing system such as the natural gas pipeline system could be modified ("very disadvantageous, 1) [110, 117].

Trend within next decade. For synthetic kerosene blends, no changes in logistics infrastructure are required in the years to come. The use of neat synthetic kerosene is presently investigated and will most likely be possible by the end of this decade as hardly any technical changes are necessary [142]. If "green" alcohols will be used at a large scale, also their transport infrastructure might grow. To which extent this development materializes, remains questionable due to the limited importance of these fuels for the time being. The same is true for ammonia. Logistics infrastructures for "green" methane do already exist, while the envisioned ramp up for hydrogen could incentivize the development of transport infrastructure at large scale.

Airport Infrastructure. Again, the drop-in characteristic of synthetic kerosene blends allows for a seamless integration into the existing storage and fuelling infrastructure at airports ("very advantageous", 5). However, for neat synthetic kerosene regulatory requirements or other reasons might (partially) require separate infrastructure at the airport ("advantageous", 4). This requirement might be eased in the mid-term [142].

The use of methanol, ethanol or butanol as aviation fuel would require at least significant modifications of aircraft, if not an entirely new design. This, in turn would raise the need for a separate fuel handling system at airports [251, 252]. If the existing airport infrastructure is to be used (e.g., aboveground storage tanks), this would most likely require a rededication to the use of alcohols and further modifications. An alternating use of infrastructure for alcohols and kerosene is practically unfeasible. For example, fuel storage would need to be modified to take into account e.g. the greater risk of corrosion and the water adsorption ("neutral", 3) [253]. As long as no clear indication is visible to use alcohols as an aviation fuel, a change of this situation is highly unlikely.

For ammonia, methane, and hydrogen fuel storage and handling at the airport would require entirely new (different) storage and refuelling systems. Foremost, facilities to liquefy the fuels would be required. The storage of cryogenic hydrogen is particularly technologically challenging [215].

Boil-off losses during storage and handling need to be minimized while managing / distributing such gases at very low temperatures within a liquid state. Based on the higher condensation temperature of ammonia, it ranks somewhat better than methane and hydrogen ("disadvantageous", 2 compared to "very disadvantageous", 1) (with the disadvantage of being toxic). As for alcohols, strong changes in the airport infrastructure would be realized only if a clear trend towards using these fuels is apparent.

Trend within next decade. At airports for synthetic kerosene blends no changes in infrastructure are required and the use of neat synthetic kerosene will most likely be possible by the end of this decade [142]. Due to high investment costs and interdependencies with fuel supply at other airports, the provision of non drop-in fuel will be constrained to an option with broad industry consensus for its use. Presently, this is only – if at all – recognizable for hydrogen.

3.2.4.3 Fuel and Aircraft

Fuel Properties. A variety of fuel properties have been defined to be relevant for a fuel to be used for commercial aviation purposes. These are for example the energy and storage density as determinants of range, the freezing point as the lower limit for the fuel temperature within the aircraft fuel tanks and the flash point as an important safety measure [137, 254]. Here, energy and storage density are chosen due to their significant influence on aircraft design and flight envelope [209].

Figure 3.11 shows the energy densities (volumetric vs. gravimetric) and estimated storage densities for the fuel options considered [109, 115–117, 209, 255, 256]. While the energy density only takes the energy of a certain volume / mass of the fuel option into account, the storage density includes an estimate for volume and mass requirements by the overall fuel system (e.g., insulation for cryogenic storage).

The higher the storage density of a fuel option, the less mass / volume is required for fuel storage on board of an aircraft (i.e., the higher the fuel's storage density, the more payload can be carried for a given aircraft design). Figure 3.11 clearly underlines the advantage of synthetic kerosene options due to their high gravimetric storage density, which is not only higher compared to alcohols but also ca. 2 % higher than fossil kerosene ("advantageous", 4) [135, 136]. Butanol, ethanol and methanol show lower gravimet-

ric storage densities (Butanol and ethanol (73 % and 55 % of fossil kerosene average) “disadvantageous”, 2 and methanol (39 % of fossil kerosene average) “very disadvantageous”, 1). To achieve the same range with a similar aircraft design, a reduction in payload has to be accepted. The storage systems incur a moderate loss.

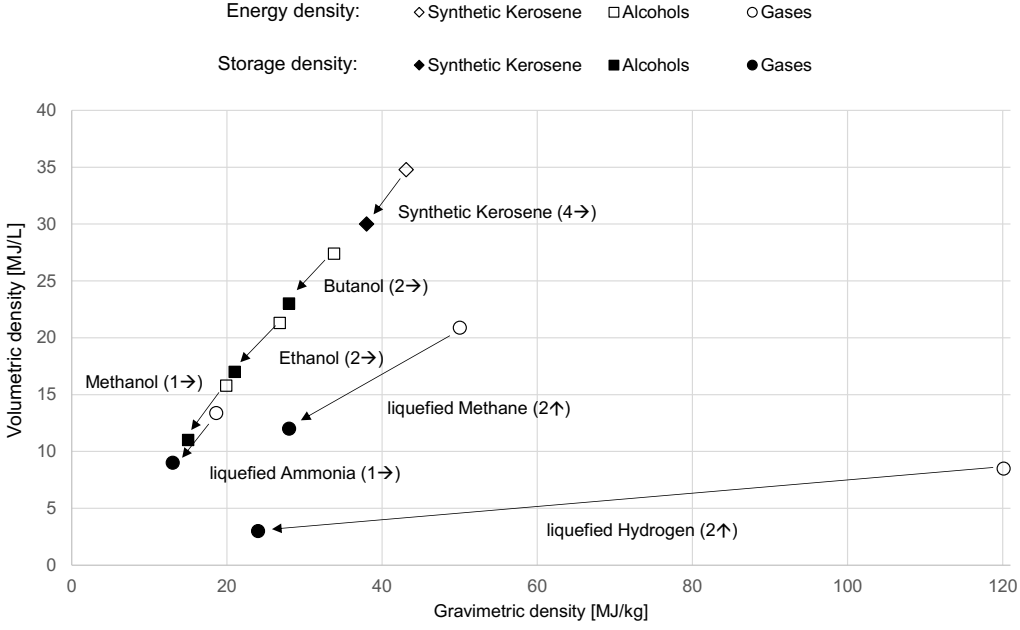


Figure 3.11 Gravimetric vs. volumetric energy and estimated storage densities (based on lower heating value) for the fuel options considered; arrows indicate the relation between storage (full symbols) and energy density (empty symbols); (ranking: 1 – “very disadvantageous”; 2 – “disadvantageous”; 3 – “neutral”; 4 – “advantageous; 5 – “very advantageous”; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear) [109, 115–117, 209, 255, 256]

A similar situation can be observed for ammonia (34 % of fossil kerosene average, “very disadvantageous”, 1) and methane (73 % of fossil kerosene average, “disadvantageous”, 2). Ammonia has a lower storage density (volumetric and gravimetric) than methane, but both are lower than synthetic kerosene. Losses due to the storage of liquid fuels are moderate for ammonia, but more significant for methane, due to its lower freezing point and the corresponding insulation and cooling requirements. Liquid hydrogen has a lower volumetric storage density but a significantly greater gravimetric storage density than synthetic kerosene. In principle, the same amount of energy carried in form of liquid hydrogen instead of synthetic kerosene would require a greater volume, but less weight. This effect is substantially reduced by the large toll of the storage system for hydrogen in a liquid state

at -253 °C (63 % of fossil kerosene average, “disadvantageous”, 2). The increased volume requirement might be constrained by aircraft design limitations, which would in turn incur range limitations of hydrogen fuelled aircraft [110]. Table 3.9 summarizes the associated ranking.

Trend within next decade. For all liquid fuel options and ammonia, the difference between energy and storage density is rather low. In case of methane and hydrogen, their large scale implementation is likely to positively affect storage technology which again yield improvements for their storage on board of an aircraft [110, 117].

Table 3.9 Operational fuel properties and the resulting ranking (ranking: 1 – “very disadvantageous”; 2 – “disadvantageous”; 3 – “neutral”; 4 – “advantageous; 5 – “very advantageous”; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear)

#	Fuel option	Operational fuel properties	Ranking	Trend
1	Blended Synthetic Kerosene	No effect on range	4	→
2	Neat Synthetic Kerosene	No effect on range	4	→
3	Methanol	Significant reduction in aircraft range	1	→
4	Ethanol	Noticeable reduction in aircraft range	2	→
5	Butanol	Noticeable reduction in aircraft range	2	→
6	Ammonia	Significant reduction in aircraft range	1	→
7	Methane	Noticeable reduction in aircraft range	2	↑
8	Hydrogen	Noticeable reduction in aircraft range	2	↑

Aircraft Modifications. The use of fuel options with an energy density lower than kerosene in existing aircraft designs would result in a significant loss in flight range. From an airline’s perspective this incurs significant disadvantages as some destinations might be out of range [90, 229]. Such a range reduction also decreases the degree of flexibility on which routes the aircraft can be used. As airline operations largely depend on the ability to shift aircraft according to demand fluctuations and other operational factors, such a loss in flexibility would be disadvantageous [229].

Neat and blended synthetic kerosene have similar energy densities and storage properties as fossil kerosene. The energy density of neat synthetic kerosene is slightly higher than for blended synthetic kerosene [136]. Thus, no technical adjustment would be required to maintain similar, if not even improved payload-range properties. However, besides energy densities, other chemical properties of neat synthetic kerosene types may vary to a considerable extent amongst different synthetic kerosene options and compared to fossil kerosene; this might require modifications for the use of unblended synthetic kerosene [9]. For example, most production processes for synthetic kerosene provide a fuel being virtually free of aromatics and of

higher energy density compared to fossil kerosene [135]. However, minimum and maximum levels for aromatics are specified for drop-in kerosene with synthetic components [135]. The lower limit (defined within ASTM D7566, does not apply for fossil kerosene) aims to ensure the tightness of sealing components and the upper limit (ASTM D1655) to constrain soot emissions [17, 137]. From an environmental perspective, it would be desirable to reduce the fuel's aromatics content as far as technically possible. Modern aircraft use elastomers being less sensitive to the fuel aromatics content (i.e., fluorocarbons and fluorosilicone) [142]. For some legacy aircraft, a replacement of the sealing components might be a prerequisite to allow for the use of neat synthetic kerosene ("advantageous", 4), but not for blended synthetic kerosene ("very advantageous", 5). An exchange of the concerned fuel system components seems comparatively simple compared to implications resulting from the use of e.g. neat alcohols.

The lower energy density (and the resulting storage density) of the alcohols considered, implies a loss in range. Various components of the fueling system (e.g., pumps, heat exchangers) would need to exchanged. Preventive measures need to be taken to avoid corrosion, microbial contamination or freezing of water dissolved in the alcohols [253]. Injectors and heat exchangers need to be replaced to facilitate the different volume flows and chemical properties (e.g. surface tension). Similar requirements apply to the combustion chamber design. Therefore, at least the fueling system and engines of an alcohol-fueled aircraft would need a new design and a time-consuming certification process ("disadvantageous", 2). The loss in range could be avoided by designing a new aircraft at the expense of even longer development times [229, 232].

Among the gaseous fuel options, the implications from cryogenic storage and reduced storage densities would require an entirely new design and certification ("very disadvantageous", 1). Aircraft designs utilizing hydrogen as fuel are discussed in a variety of studies [76, 110, 117, 255, 257]. Cryogenic hydrogen storage is usually preferred due to increased energy density. This requires significant technological developments for lightweight storage and fuelling systems [255]. All gaseous fuel options considered would also require the design of a gas turbine specifically designed for the combustion of the respective gaseous fuel [100]. A modification of existing aircraft designs does not seem feasible for any of the discussed gaseous fuels. Accordingly, aircraft using one of the considered gases would rather

be available in the long-term. Table 3.10 summarizes the associated ranking.

Trend within next decade. Due to its relative simplicity compared with e.g., hydrogen, using neat synthetic kerosene in existing aircraft seems feasible within the decade to come. Again, the use of any of the alcohols and gases is strictly constrained by the required industry consensus for the corresponding option. For the time being, this appears only realistic for hydrogen characterized simultaneously by the highest technological barriers. Whether or not a hydrogen fuelled commercial aircraft will be available in the mid- or long-term is still an open question.

Table 3.10 Aircraft modifications and the resulting ranking (ranking: 1 – "very disadvantageous"; 2 – "disadvantageous"; 3 – "neutral"; 4 – "advantageous; 5 – "very advantageous"; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear)

#	Fuel option	Aircraft Modifications	Ranking	Trend
1	Blended Synthetic Kerosene	No need for modifications	5	→
2	Neat Synthetic Kerosene	Modification of only a few components	4	↑
3	Methanol	Minor modifications required	2	→
4	Ethanol	Minor modifications required	2	→
5	Butanol	Major modifications required	2	→
6	Ammonia	Major modifications required	1	→
7	Methane	Major modifications required	1	→
8	Hydrogen	New design and certification required	1	?

3.2.4.4 Environment and Economics

Life cycle greenhouse gas emissions. Combusting 1 kg of fossil kerosene emits approximately 3.16 kg CO_2, 1.2 kg water vapour, 1.5 g (0.0015 kg) NO_x, 1.2 g (0.0012 kg) sulfur (SO_2) and 0.03 g (0.00003 kg) soot. All of these affect the earth's radiative balance through a cascade of interrelationships and influence the air quality around airports. Related to climate-effects, a distinction is commonly made between CO_2 and non-CO_2 related climate effects [5].

Figure 3.12 illustrates the broad range of potential life-cycle CO_{2eq} emissions for many of the examined fuel options. The feedstock used and the provision of energy needed for feedstock conversion influence the resulting greenhouse gas emissions substantially.

In terms of the synthetic kerosene options, FT-SPK shows the lowest median ("very advantageous", 5). Values below zero refer to a partial removal of the carbon captured into waste streams. High emission cases for

FT-SPK conversion processes often relate to either energy intensive processing of biomass conversion (e.g., due to (indirect) land-use change) or indirect emissions caused by the provision of renewably sourced energy (e.g., manufacturing processes). The medians of greenhouse gas emission values for HEFA-SPK, AtJ-SPK and HFS-SIP (all "advantageous", 4) are slightly higher compared to FT-SPK. These processes are generally based on biomass; especially the extraction of lipids from biomass or the saccharification of lignocelluloses for AtJ-SPK or HFS-SIP is energy intensive. The narrow bandwidth of emission estimates for CH-SK ("very advantageous", 5) is most likely related to a low amount of accessible data. However, for synthetic kerosene blends a maximum emission reduction of 50 % compared to neat synthetic kerosene is possible due to the legal blending requirement of maximum 50 vol.-%. The development of a certification for neat synthetic kerosene is ongoing [142], accordingly the limit to lifecycle CO_2 reduction by blended synthetic kerosene might diminish in the near future.

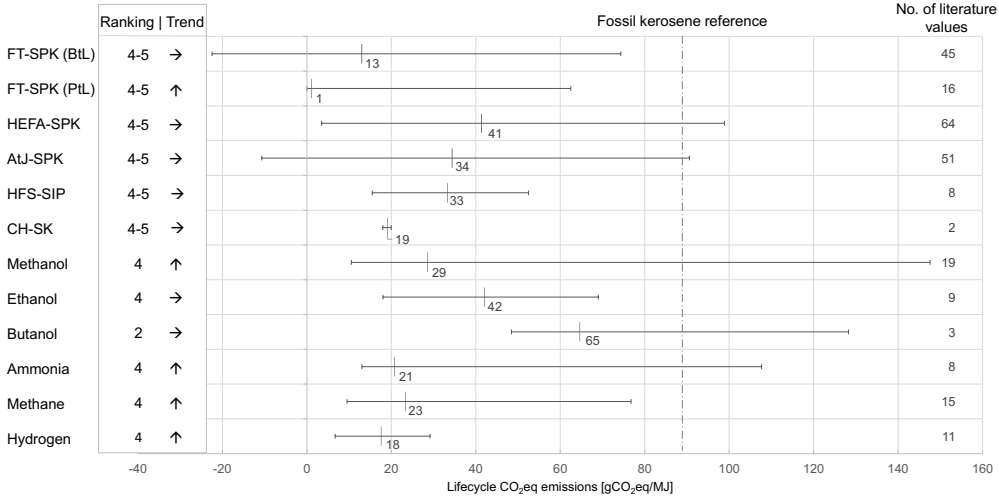


Figure 3.12 Median and range of values for each fuel options life-cycle CO_2eq emissions. Error bars indicate the lowest/highest values considered (AtJ Alcohol-to-Jet; BtL Biomass-to-Liquid; CH Catalytic Hydrothermolysis; FT Fischer-Tropsch; HEFA Hydroprocessed Esters and Fatty Acids; HFS-SIP Hydrofermented Sugars Synthesized Isoparaffins; SK Synthesized Kerosene; SPK Synthetic Paraffinic Kerosene; PtL Power-to-Liquid; ranking: 1 – "very disadvantageous"; 2 – "disadvantageous"; 3 – "neutral"; 4 – "advantageous; 5 – "very advantageous"; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear)

Methanol shows the greatest variety in lifecycle greenhouse gas emissions for all fuel options considered. As this process is based on the use of syngas, again the type of feedstock is a central determinant of the respective life

cycle emissions. Low emissions can be attributed to lignocelluloses waste streams, while higher emissions stem from the use of electricity provided by photovoltaics ("advantageous", 4). For ethanol, only fermentation of biogenic feedstock is considered; in this case, the use of lignocelluloses is associated with higher life cycle emissions compared to sugar-rich biomass ("advantageous", 4). As ABE-fermentation is presently not used at an industrial scale, a limited amount of data is available. Among these, the extent to which emissions from production are allocated to the various products of such an ABE-fermentation (acetone, ethanol) influences clearly the lifecycle emissions attributed to butanol ("disadvantageous", 2).

In general, the median lifecycle emissions of the gases considered are lower compared to the liquid fuel options ("very advantageous", 5), mostly influenced by the type of energy provision for water electrolysis. In the case of ammonia, the broad range of different data result from the technology to retrieve nitrogen from ambient air (e.g., cryogenic distillation, pressure-swing adsorption) and the hydrogen provision process (low or high temperature electrolysis). For the greenhouse gas emissions by methane provision either via synthesis or fermentation, no clear distinction can be made. In case of synthesis, the choice of renewable electricity provision (wind on-/offshore, photovoltaics) shows a substantial influence and for biomass-based fermentation the type of feedstock (organic waste or cash crops) largely explains the variation.

Concluding, life cycle greenhouse gas emissions of biomass-based fuels are clearly influenced by the chosen feedstock. Additionally, for fuel options based on "green" electricity, indirect emissions of energy provision have a substantial effect. The potential of "negative" life cycle emissions seems rather limited. Table 3.11 depicts a summary of the resulting ranking.

Trend within next decade. For synthetic kerosene options, the improvements will mostly be the approval to use neat synthetic kerosene. For non-biogenic feedstock, increasing shares in renewable electricity and increasing hydrogen provision will further lower lifecycle emissions. For fuels based on biogenic feedstock, the influence of feedstock choice will remain the most significant aspect and thus improvements seem unlikely. Advancing technology for methanol provision based on non-biogenic feedstock can reduce corresponding lifecycle greenhouse gas emissions. For ethanol and butanol, no change can be expected, as the increased use of lignocelluloses as preferred feedstock for ethanol and butanol lowers conversion efficiency

and raises material and energy demands. Increasing production of "green" hydrogen and corresponding improvements in electrolyser technology do not only lower lifecycle greenhouse gas emissions of hydrogen but also of ammonia and methane.

Table 3.11 Life-cycle CO_2eq emissions and resulting ranking (AtJ Alcohol-to-Jet; BtL Biomass-to-Liquid; CH Catalytic Hydrothermolysis; FT Fischer-Tropsch; HEFA Hydroprocessed Esters and Fatty Acids; HFS-SIP Hydro-fermented Sugars Synthesized Isoparaffins; SK Synthesized Kerosene; SPK Synthetic Paraffinic Kerosene; PtL Power-to-Liquid; ranking: 1 – "very disadvantageous"; 2 – "disadvantageous"; 3 – "neutral"; 4 – "advantageous; 5 – "very advantageous"; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear)

#	Fuel option		Lifecycle CO_2eq [g CO_2eq/MJ]			Ranking	Trend
			Median	Min-Max	References		
	Fossil kerosene reference		89	N/A	[258]	N/A	N/A
1	Blended Synthetic Kerosene and Neat Synthetic Kerosene	FT-SPK (BtL)	13	-22-74	[69, 88, 94, 98, 123, 155, 235, 257, 259–262]	5	→ (biogenic)
2		FT-SPK (PtL)	1	0-62		5	
		HEFA-SPK	41	3-99		4	
		AtJ-SPK	34	-11-91		4	↑ (non-biogenic)
		HFS-SIP	33	15-52		4	
		CH-SK	19	18-20		5	
3	Methanol		29	11-148	[219]	4	↑
4	Ethanol		42	18-69	[263]	4	→
5	Butanol		65	48-128	[264]	2	→
6	Ammonia		21	13-108	[265]	5	↑
7	Methane		23	10-77	[219]	5	↑
8	Hydrogen		18	7-29	[219, 266, 267]	5	↑

Fuel Cost. The production costs of each fuel option outlined below are related to their specific energy content (based on the lower heating value), in order to take into account differences in energy density. In general, all investigated fuel options show higher production costs compared to average market prices for fossil kerosene. The majority of the cost variations presented in Figure 3.13 can be attributed to the influence of costs for the feedstock, the needed energy, as well as the effort needed for the conversion. Table 3.12 indicates the corresponding ranking.

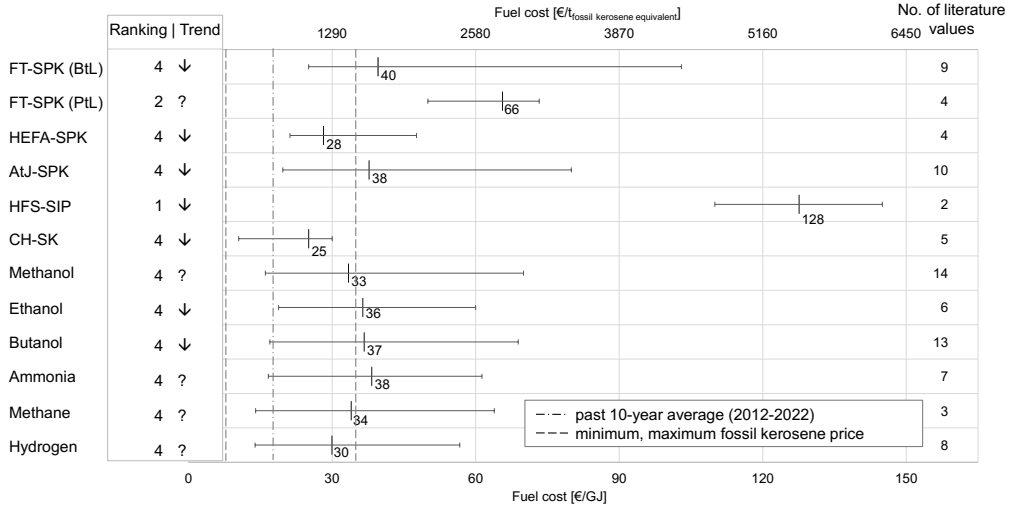


Figure 3.13 Present fuel costs of the considered fuel options, error bars indicate the lowest/highest values taken into account. The solid line depicts the average price of fossil kerosene, the dashed lines the corresponding lowest/highest price of the past 10 years as of July 2022 (AtJ Alcohol-to-Jet; BtL Biomass-to-Liquid; CH Catalytic Hydrothermolysis; FT Fischer-Tropsch; HEFA Hydroprocessed Esters and Fatty Acids; HFS-SIP Hydrofermented Sugars Synthesized Isoparaffins; SK Synthesized Kerosene; SPK Synthetic Paraffinic Kerosene; PtL Power-to-Liquid; ranking: 1 – "very disadvantageous"; 2 – "disadvantageous"; 3 – "neutral"; 4 – "advantageous; 5 – "very advantageous"; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear)

Among the synthetic kerosene options, costs for FT-SPK based on "Power-to-liquid" feedstock are considerably higher ("disadvantageous", 2) than those for biogenic feedstock ("advantageous", 4). This is caused by high demands for renewable electricity for the earlier [103]. The lower values for HEFA-SPK ("advantageous", 4) correspond to relatively low-cost feedstock (e.g., waste animal fat), while higher values relate to the cultivation of non-edible oils (e.g., Jatropha plants) [91, 94]. The cost estimates for AtJ-SPK show a slightly higher median ("advantageous", 4). Lower values are based on studies considering sugar / starch (corn grain, maize) for ethanol production [267], while higher costs are associated with lignocelluloses [91]. The analysis for the HFS-SIP process considers lignocelluloses-based feedstock with saccharification. The process' relatively low degree of technological maturity might explain its high cost estimates. CH-SK is associated with the lowest cost estimates ("advantageous", 4) due to the specific low-cost feedstock options usually considered for CH-SK analyses (e.g., sewage sludge, manure). However, a relatively low technological maturity of this process yields uncertainties in comparison with other processes.

Table 3.12 Fuel costs and resulting ranking. Fossil kerosene is shown for comparison (AtJ Alcohol-to-Jet; BtL Biomass-to-Liquid; CH Catalytic Hydrothermolysis; FT Fischer-Tropsch; HEFA Hydroprocessed Esters and Fatty Acids; HFS-SIP Hydrofermented Sugars Synthesized Isoparaffins; N/A not applicable; SIP Hydrofermented Sugars Synthesized Isoparaffins; SK Synthesized Kerosene; SPK Synthetic Paraffinic Kerosene; PtL Power-to-Liquid; ranking: 1 – "very disadvantageous"; 2 – "disadvantageous"; 3 – "neutral"; 4 – "advantageous; 5 – "very advantageous"; trend: ↑ – improvement; ↓ – deterioration; → – no change; ? – unclear)

#	Fuel option		Cost range [€/GJ]			Ranking	Trend
			Median	Min-Max	References		
	Fossil Kerosene		12.9	3.9-20.9	[268]	N/A	N/A
1	Blended Synthetic Kerosene and Neat Synthetic Kerosene	FT-SPK (BtL)	39.5	25.1-103.0	[91, 93, 94, 103, 167, 219, 267]	4	?
		FT-SPK (PtL)	65.5	50.0-73.3		2	
2		HEFA-SPK	28.1	21.2-47.6		4	
		AtJ-SPK	37.6	19.7-80.0		4	↓
		HFS-SIP	127.5	110.0-145.0		1	
		CH-SK	25.0	10.5-30.0		4	
3	Methanol		33.3	16.0-70.0	[103, 209, 212, 219, 269]	4	?
4	Ethanol		36.3	18.8-60.0	[93, 103, 269]	4	↓
5	Butanol		36.6	17.0-68.9	[103, 224, 243]	4	↓
6	Ammonia		38.2	16.7-61.3	[35, 209, 270, 271]	4	?
7	Methane		33.9	14.0-63.9	[35, 209, 219, 270]	4	?
8	Hydrogen		29.9	13.9-56.7	[35, 209, 219, 250, 270]	4	?

Despite significantly different conversion processes, the estimates for alcohols are in a similar range (all "advantageous", 4). On an energy-specific basis, they show costs comparable to HEFA-SPK or FT-SPK based on biogenic feedstock. Again, most of the variations can be explained by varying assumptions for feedstock costs. Similar to the kerosene-based options, cost improvements could mostly be expected for feedstock types requiring further technological developments, such as lignocelluloses for fermentation or non-biogenic feedstock for methanol synthesis.

Values for ammonia and methane (both "advantageous", 4) are slightly higher than for hydrogen ("advantageous", 4), since both options can be produced within pathways with hydrogen as a key component. Production pathways for methane based on fermentation of biomass residues show very low cost estimates (ca. 14 to 25 €/GJ) indicating a low-cost option. The variability in cost estimates for hydrogen can largely be attributed to different methods of renewably sourced electricity provision [35, 209, 219].

Trend within next decade. The costs of synthetic kerosene based on non-biogenic feedstock is mostly influenced by the costs of renewably sourced electricity. Whether or not the development of electricity from renewable sources outpaces increasing demand and thus lowers prices is uncertain. Cost for biogenic waste as feedstock for synthetic kerosene are likely to rise

with increasing demand as supply is limited (section 3.2.4.1). This also applies to ethanol and butanol, as their production is also based on biogenic feedstock. The cost development for methanol is uncertain for non-biogenic feedstock and – like biogenic synthetic kerosene – will most likely increase for biogenic feedstock. Cost for all gases are driven by hydrogen provision costs (except biomethane). Thus, low cost renewable electricity and substantial improvements in electrolysis technology are necessary. The latter seems likely due to industry-wide interest in electrolyser technology.

3.2.4.5 Market Development

Based on the previous assessment of the value chains for the different fuel options, in this section key constraints are discussed when and to which extent the various fuel options could be available for aviation. The fuel's value chain is subdivided into four stages: production, logistics, airport and aircraft. Table 3.13 summarizes the constraints along each of them.

Table 3.13 Key constraints for the market development of the investigated fuel options.

#	Fuel option	Production	Logistics	Airport	Aircraft
1	Blended Synthetic Kerosene	Development of production capacities	None	none	none
2	Neat Synthetic Kerosene			Potentially minor modifications due to different chemical properties	Potentially modifications of components due to different chemical properties
3	Methanol	Switch to renewably sourced syngas	None	Modification of storage and fuelling infrastructure necessary	Modification of existing aircraft necessary
4	Ethanol	none			
5	Butanol	Development of plants, e.g. for ABE-fermentation			
6	Ammonia	Provision of renewably sourced hydrogen and electricity	None	Development and construction of storage and fuelling infrastructure required	Development and certification of new aircraft design
7	Methane	Provision of renewably sourced hydrogen, carbon and electricity			
8	Hydrogen	Provision of renewably sourced electricity	Development of large-scale transport systems (e.g., pipelines, ships)		

The development of production capacities poses a significant constraint for synthetic kerosene fuel options. Several processes are technologically mature (e.g., HEFA-SPK), but for commercial reasons existing production capacities are scarce (section 3.2.4.1). Due to their drop-in characteristic, transportation, storage and fueling would not require any changes of the existing system. The introduction of neat synthetic kerosene is further constrained by the necessity to accommodate a greater variety in fuel properties. This might imply minor modifications of the respective aircraft. In small amounts, synthetic kerosene is available today.

The only alcohol presently produced at large scale from renewable resources is ethanol. The provision of methanol via synthesis would require the provision of a renewably sourced syngas. For butanol production, ABE-fermentation (or another fermentation process) at large scale would be required. In principle, the existing logistics and airport infrastructure is capable of transporting liquids. Still, due to high investment cost and network interdependencies among airports, broad consensus for a particular non drop-in fuel option would be required. Additionally, infrastructure modifications might become necessary to facilitate larger volumes due to the alcohol's lower energy densities, to ensure material compatibility and / or to prevent microbial contamination. For all alcohols, present aircraft would at least need to be modified to accommodate different volume flows (e.g., fuel pumps, heat exchangers) and to be equipped with newly developed jet engines suitable for alcohol combustion[64]. For both, infrastructures and aircraft, the compatibility of materials presently in use with the respective alcohols will need to be evaluated and components might need to be replaced. The time to develop and develop a jet engine for alcohol combustion appears to be the strictest constraint.

For gaseous fuel options all value chain elements need further technological developments and – similar to alcohols – consensus for a particular option due to the high effort to establish the necessary fuel provision infrastructure. Capacities for a production from renewable resources are technologically available but not installed at industrial scale so far. For methane, it seems likely that the existing network to transport natural gas could be re-used. To which extent this is feasible for ammonia and hydrogen is questionable so far. Additionally, a new fueling infrastructure (trucks, hydrant systems) needs to be built at airports. However, the most prominent barrier is the development and certification of new aircraft and engine types [229].

Hence, for synthetic kerosene options the central temporal constraint is the development of production capacities and technologies. The use of the considered alcohols as aviation fuel is predominantly limited by aircraft modifications and certification as well as by the required development of production capacities (except for ethanol). The greatest temporal barriers exist for the gaseous fuel options. With a development of production capacities, transport and airport infrastructure, and the development of entirely new aircraft designs, each element of the value chain is substantially affected. Concluding, synthetic kerosene seems like a short-term feasible option, while the other investigated fuel options could only become available in a mid- to long-term timeframe.

3.2.5 Overall Results

Current status. A summarised comparison of all assessment criteria and fuel options shows Table 3.14. Synthetic kerosene options achieve the most advantageous rankings for logistic and airport infrastructure, fuel properties and aircraft modifications.

Compared to the amount of other sectors (e.g., road transport, industrial production), the feedstock demand to cover overall aviation fuel demand is relatively small. It appears unlikely that the demand for aviation fuel alone is sufficient to incentivize the use of a particular feedstock and / or conversion process. Rather, pathways for (intermediate) products seem more likely to develop at an industrial scale, if they can defossilize several industrial sectors and / or can cover a higher demand. This is for example the case for FT-SPK or AtJ-SPK with syncrude or methanol / ethanol / butanol respectively as intermediate feedstock.

Even though neat synthetic kerosene options are not drop-in fuels by present specification / legal constraints, enabling their use in existing infrastructure and aircraft requires substantially less technological adaptations than for other non drop-in fuel options. Conversion efficiency and costs of the synthetic kerosene options varies significantly due to different production processes and various types of feedstock. Overall, while post-production value chain steps of the synthetic kerosene options appear advantageous, the lack of production capacities is disadvantageous.

For alcohols, feedstock potentials and in case of ethanol also production capacities rank highest. If edible feedstock which compete with food and

fodder purposes are to be avoided for fuel production (e.g., by using lignocelluloses) further developments of feedstock conversion technologies are required. All alcohols considered are already used as bulk chemicals, especially methanol and ethanol in large amounts. If these are converted to AtJ-SPK, they can become available comparatively soon without any further technological constraints after production. The business model of airlines currently relies to a great extent on the ability to schedule aircraft flexibly in order to adapt to demand fluctuations, (un-)scheduled maintenance events and other factors [229]. Additionally, airport infrastructure is used by a variety of stakeholders more or less simultaneously. If various, incompatible fuels would be offered at different airports, these advantages would not exist anymore. Consensus of the air transport industry for using a particular fuel is a prerequisite to introduce any non drop-in fuel option and to avoid the aforementioned loss of flexibility. As of now, such an industry-wide consensus is not recognizable. Hence, the need for aircraft modifications and / or a new aircraft design and production poses a significant barrier for their use as aviation fuel.

The gaseous fuel options appear particularly advantageous in the area of feedstock and production. Fuel conversion efficiency is highest for hydrogen among the gases considered. Most of the conversion pathways currently under discussion are technologically more or less mature. Yet, the requirements to adopt logistics and airport infrastructures as well as fuel system and aircraft in general are clearly higher than those for alcohols. For this group of fuel options, the development of new aircraft designs will be necessary and an even greater barrier than for alcohols. The development of logistics infrastructures is in particular necessary for hydrogen. The existing natural gas logistics might be used by "green" methane or potentially ammonia, at least from a technological perspective. The gaseous fuel options – especially hydrogen – will be required for the defossilation of several industrial sectors, e.g., the chemical industry. This might incentivize increasing production capacities and supply.

Overall, the global potential for feedstock with a rather high energy content (i.e., lipid biomass / waste) is significantly restricted. Fuels from non-biogenic feedstock have a greater overall availability, but less production capacities are established for their conversion and provision yet and the conversion technology is less mature. Key determinants for fuel conversion efficiency are the feedstock's energy content and the technological maturity

of the conversion process or the respective conversion concept. The need for technological modification on both the fuel infrastructure and aircraft side to use gaseous fuels (and also alcohols) can prevent their timely market introduction. The key determinants for fuel costs are feedstock and energy costs.

Drop-in options are constrained by provision steps of the value chain, such as production capacities and (partial) technological maturity of the respective conversion processes. In contrast, most of the non drop-in options are constrained by post-production steps, i.e. the development / design of aircraft certified to use non drop-in fuels and the implementation of infrastructure to provide them.

A reduction of greenhouse gas emissions can be achieved by all fuel options, assuming a favourable combination of feedstock and energy provision. The certification of neat synthetic kerosene would allow for greater greenhouse gas emission reductions of these fuel options at rather low post-production efforts compared with e.g., the gaseous fuel options considered.

Status next decade. Table 3.14 also indicates the trends for the next decade. For synthetic kerosene options, the availability of lipid-biomass and lignocelluloses-biomass will remain restricted. The ranking of production capacities for FT-SPK and AtJ-SPK from non-biogenic feedstock might improve within the next decade, specifically by a potential certification of methanol for AtJ-SPK and in general due to interest from several sectors for their (intermediate) products. Enabling the use of neat synthetic kerosene will reduce logistical efforts to and at airports and – most importantly – lower life-cycle greenhouse gas emissions. To which extent the ramp up of energy from renewable sources and increasing fuel production capacities can yield price reductions remains uncertain. This is due to the strong influence of extra-sectoral demand for "green" energy. Even though most pathways based on non-biogenic feedstock are currently not available at industrial scale, in the mid-term they might replace substantially greater amounts of fossil kerosene than feedstock constrained fuel options (e.g., fuels based on lipid-biomass).

Also, for the alcohols considered the increasing importance of non-biogenic feedstock based conversion pathways is apparent. Increasing availability of "green" methanol and ethanol is more likely than for butanol, as "green" butanol production capacities are of lower importance compared to the others. In contrast to ethanol, the conversion efficiency for methanol

and butanol can potentially improve. A decrease in costs appears rather unlikely, as for methanol not only feedstock availability but also demand is likely to increase. For ethanol and butanol (mostly from biogenic feedstock) the feedstock availability is additionally limited.

Among the gaseous fuel options, the ranking of hydrogen can change drastically within the next decade. With increasing industry wide demand for hydrogen from renewable sources, the presently (very disadvantageous) criteria for logistics infrastructure can improve substantially. At airports, however, the effects of industry-wide interest are less pronounced and the need for infrastructure modification / development is substantially greater. Thus, a non drop-in fuel option will only become available, if broad industry consensus for its use is reached. Only if the weight toll to store liquid hydrogen is drastically reduced, its high gravimetric energy density would pay off. Increased availability of liquid hydrogen at airports and improved fuel storage in airports are prerequisites for a market introduction of an aircraft using liquid hydrogen directly. These prerequisites can be achieved within this decade, whereas a hydrogen fuelled aircraft would rather be available in the decade thereafter, if at all.

The wide-spread and large-scale use of renewable aviation fuels can potentially be expected in the mid-term (e.g., from 2030 onwards). Comparing the current and next decade status reveals that those options with an advantageous ranking for today's application (drop-in fuels in general, HEFA-SPK in particular) are not necessarily the most advantageous options in the long-term. For example, at the end of the next decade, FT-SPK and AtJ-SPK (for drop-in options) and hydrogen as non drop-in option could be seen far more advantageous as they are today.

Table 3.14 Overall assessment results (AtJ Alcohol-to-Jet; BtL Biomass-to-Liquid; CH Catalytic Hydrothermolysis; SK Synthesized Kerosene; FT Fischer-Tropsch; HEFA Hydroprocessed Esters and Fatty Acids; HFS-SIP Hydrofermented Sugars Synthesized Isoparaffins; SK Synthesized Kerosene; SPK Synthetic Paraffinic Kerosene; PtL Power-to-Liquid)

#	Fuel option	Feedstock and production			Logistics and airports		Fuel and aircraft		Economics and environment	
		Feedstock potential	Production capacities	Fuel conversion efficiency	Logistics infrastructure	Airport infrastructure	Fuel properties	Aircraft modifications	Lifecycle CO_2-eq	Fuel costs
1	Blended Synthetic Kerosene	2→ (HEFA-SPK, CH-SK)	3↑ (FT-SPK, AtJ-SPK)	2? (FT-SPK (BtL), HFS-SIP) 2↑ (AtJ-SPK, FT-SPK (PtL))	5→	5→	4→	5→	4→ (HEFA-SPK, biogenic AtJ-SPK, HFS-SIP) 4↑ (non-biogenic AtJ-SPK)	1↓ (HFS-SIP)
		3→ (HFS-SIP)	3→ (other)	3? (CH-SK)						2? (FT-SPK (PtL))
2	Neat Synthetic Kerosene	5↑ (FT-SPK, AtJ-SPK)		4→ (HEFA-SPK)	4↑	4↑	4→	4↑	5→ (CH-SK, FT-SPK (BtL)) 5↑ (FT-SPK (PtL))	4↓ (AtJ-SPK, HEFA-SPK, FT-SPK (BtL), CH-SK)
3	Methanol	5↑	3↑	3↑	3?	3→	1→	2→	4↑	4?
4	Ethanol	5↑	5→	2↓			1→	2→	4→	4↓
5	Butanol	3→	2→	1→			2↑	2→	2→	4↓
6	Ammonia	5↑	2?	3↑	4?	1→	1→	1→	4↑	4?
7	Methane	5↑	3?	3↑ (except Biomethane)	4↑		2↑	1→	4↑	4?
8	Hydrogen	5↑	3↑	5↑	1↑	1↑	2↑	1?	4↑	4?
Ranking:		1 "very disadvantageous"		2 "disadvantageous"	3 "neutral"		4 "advantageous"		5 "very advantageous"	
Trend:		↑ improvement		↓ deterioration	→ no change		? unclear		-	

3.2.6 Conclusion

Alternative fuels are considered as a key measure to reduce greenhouse gas emissions in the air transport system and thus lower its contribution to anthropogenic climate change. But, current usage-shares are below 1 %. Among seven conversion pathways certified by ASTM only one (HEFA-SPK) is produced by several companies at an industrial scale. Against this background, this paper investigates blended synthetic kerosene as drop-in aviation fuel and neat synthetic kerosene fuels, three alcohols (methanol, ethanol and butanol) and three gases (methane, ammonia and hydrogen) as non drop-in aviation fuel options. These fuel options are selected because they are discussed as alternative aviation fuels (e.g., synthetic kerosene), are already produced from renewable resources (e.g., ethanol), or considered to play a central role in the defossilation of the global energy system (e.g., hydrogen). Therefore, a set of nine technological and system-related assessment criteria is used to cover the central elements of the entire fuel value chain. A multi-criteria assessment based on a five-step ordinal scale is performed, taking into account the criteria feedstock potential and extra-sectoral demand, aviation fuel conversion efficiency, conversion technology readiness level (TRL), production capacities, logistics and airports, fuel properties, aircraft modifications, fuel costs and environment. The studies' main results can be summed up as follows.

- The availability of some biogenic feedstock is not sufficient to replace the present overall energy demand of aviation. Either the feedstock's limited physical availability (e.g., lipid wastes) or potential conflicts with the food and fodder sector are constraining factors. Additionally, lacking capacities for the provision of renewably sourced energy limit the availability of fuels of non-biogenic origin.
- Synthetic kerosene options are mainly constrained by a clear lack of production capacities. Nevertheless, the integration of these fuels into the existing air transport system seems easily feasible from a technological point of view. In contrast, the use of alcohols would at least require modifications of aircraft and engines. Additionally, using such fuels results in a loss of range due to their lower energy density. In contrast, significant capacities to produce renewably sourced methanol and ethanol exist. The use of gaseous fuels (e.g., hydrogen) would require the development of new aircraft, with resulting delays for the fuel's market introduction,

significant economic risks for aircraft manufacturers and operational constraints for airlines.

- All of the discussed fuel options have the potential to mitigate most of the life cycle greenhouse gas emissions of aviation fuels. A prerequisite for a highly efficient greenhouse gas reduction is a favorable combination of feedstock and renewably sourced energy provision. Large uncertainties exist with regard to the non-CO_2 related climate effects of non drop-in fuel options.
- Long-term price parity with fossil kerosene is highly unlikely for any of the fuel options studied. Cost of the renewable fuel options considered are mainly driven by feedstock and energy costs.

For the next decade the following conclusions can be drawn.

- The further development of fuel provision for aviation cannot be seen independently from the development within the ongoing developments within the overall energy system. If hydrogen develops as currently expected to become the main molecular energy carrier by the mid of this century, most likely hydrogen-based solutions will become market mature also for the aviation sector.
- Some fuel options appear more likely to reach significant market shares than others. On the one hand, these are synthetic kerosene options with (intermediate) products experiencing demand from other sectors (e.g., FT-SPK, AtJ-SPK). On the other, the broad interest in ramping up the production of hydrogen from renewable energy sources might induce a fast increase in its availability and decreasing costs. This might provide a mid- to long-term option for carbon-free aviation, assuming that a hydrogen fueled aircraft will be brought successfully to the market.
- Within the next decade it is most unlikely that gaseous fuels or non drop-in fuels will gain a significant market importance due to numerous reasons. Thus, if greenhouse gas emission reductions are politically enforced also within the aviation sector, the use of biomass-based drop-in fuels (HEFA-SPK) need to be promoted. Non-biogenic FT-SPK might gain importance in the early / mid thirties if the respective technological and market development is strongly supported. If this materializes, their outlook as commercial aviation fuel can improve clearly, as non-biogenic FT-

SPK fuels show large development potentials for several of the assessment criteria.

The most relevant uncertainties are the implications resulting from the potential introduction of a second fuel type next to kerosene in the air transport system for the years to come. Not only the aircraft itself would need to be modified / developed, but also a separate / additional infrastructure would need to be provided at airports and in case of hydrogen also on a global scale. Network interdependencies among airports would require broad consensus for one fuel-option, as economic operation of an aircraft between two (or few) airports seems unlikely. Taking also the high safety and resulting certification standards within commercial aviation into account, these implications are non-negligible and difficult to estimate a priori.

Most of the present climate change mitigation strategies in aviation focus on the reduction of greenhouse gas emissions. However, scientific understanding of the non-CO_2 related climate effects of aviation has improved significantly. A better understanding of these effects for non drop-in fuels would help to understand each of the fuel options' potential to mitigate the entire climate effects of aviation and not only CO_2 related climate effects.

3.3 Sustainable Aviation Fuels – Status and Prospects

Quante, Gunnar; Kaltschmitt, Martin (2025): Sustainable Aviation Fuels – Status and Prospects. In : Research Handbook on Air Transport Management. [S.l.]: EDWARD ELGAR, in Press.
Typesetting and formatting are slightly adjusted to ensure consistency within this thesis.

Abstract

Commercial air transport contributes approximately 4% to global anthropogenic climate forcing. The use of so-called "Sustainable Aviation Fuels", i.e., fuels from renewable energy sources instead of fossil fuel-based sources can help to mitigate a large fraction of aviation's climate forcing. Such "green" fuels reduce carbon dioxide (CO_2) emissions by using feedstock based on carbon dioxide (CO_2) bound from the atmosphere. Additionally, their use can lower non-CO_2 related climate impacts. Various feedstock and several provision pathways for such "green" fuels are available, but their market shares are still clearly below 1% on a global scale.

This chapter outlines the context of climate impact mitigation in aviation (section 3.3.1) and derives systemic requirements for renewably-sourced kerosene. On the consumption side, the air transport system requires a fuel characterized ideally by identical fuel properties as fossil fuel-based kerosene (section 3.3.2). On the provision side, a wide variety of feedstock and provision pathways for renewably-sourced kerosene is available (section 3.3.3). To bridge the gap between provision and consumption, selected pathways for the provision of renewably-sourced kerosene are described (section 3.3.4). Comparing these provision pathways indicates a trade-off between low conversion efforts and a high theoretical availability (section 3.3.5).

3.3.1 Motivation

Aviation contributes about 4 % towards net anthropogenic climate forcing [5]. This contribution is mainly caused by contrails, the emission of carbon dioxide (CO_2), as well as climate effects caused by NO_x emissions, water vapor emitted within the stratosphere, aerosol radiation and aerosol cloud interaction. In 2015, the so-called Paris Agreement was adopted by the international community of states stating to "hold the increase in the global average temperature to well below 2 °C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5 °C above pre-industrial levels" [2]. This goal is to be transmitted into policies / political measures via so-called nationally determined contributions. As of now, 194 states and the European Union (EU) have defined such commitments for climate change mitigation [272]. Thus, most measures contributing to the achievement of the Paris Agreement's goals are defined and implemented at national level. At the same time, the majority of aviation climate impacts are caused by international air travel and thus typically not covered by nationally determined contributions [5].

Against this background, the two international aviation organizations, the International Civil Aviation Organization (ICAO) and the International Air Transport Association (IATA), both defined a "Net-Zero Carbon Emissions" target by 2050 [3, 4]. These targets focus on the abatement of carbon dioxide emissions; other climate terms of aviation are not explicitly targeted so far. Already in the year 2016, ICAO started developing the so-called Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA) as a global market-based approach to reduce aviation emissions, either by extra-sectoral offsets or the intra-sectoral use of renewably-sourced kerosene[9] [40].

Additionally, regions with a high flight density, mainly the US and the EU have introduced policies to reduce the climate impacts of aviation, such as the "SAF Grand Challenge" targeting a production of around 9 Mt/a of renewably-sourced kerosene by 2030 within the US [273] or the ReFuelEU Aviation directive, which defines increasing mandatory blending quotas for renewably-sourced kerosene within the EU [205]. Several Asian states (e.g.,

[9] Such fuels are often referred to as "sustainable aviation fuel" or "SAF". However, this term is not used here, as the fuel's renewable origin does not guarantee the fulfilment of other sustainability aspects (e.g., biodiversity or social criteria).

Malaysia and India) also consider the introduction of a blending quota [274].

Individual airlines have also defined climate impact mitigation targets and strategies. For example, more than 25 airlines (e.g., Air France – KLM, United Airlines and Azul) joined the "Science Based Targets Initiative" (SBTI) and defined a near-term and potentially also a long-term emission reduction goal [275, 276]. Additionally, large airline customers, such as freight forwarders or companies with large business air travel volumes, incentivize voluntary demand for renewably-sourced kerosene.

The IATA estimates that in 2023 about 500 kt of renewably-sourced kerosene were used, corresponding to a market share of less than 1 % [79]. At the time of writing (spring 2024), eight different provision pathways for renewably-sourced kerosene and two options to co-process feedstock from renewable sources in conventional refineries are approved by the responsible authorities. Among those pathways, virtually all consumption realized so far is based on the Hydroprocessed Esters and Fatty Acids (HEFA) pathway. These approved options to provide "green" kerosene closely mirror the physical and chemical properties of conventional jet fuel. Additionally, some technological developments like, e.g., aircraft capable of directly using liquefied or compressed hydrogen(H_2), are planned to target the next generation of airplanes. E.g., Airbus announced that it is developing a hydrogen aircraft with a market entry, however, expected not before 2035 at the earliest [78]. Thus, the possible contribution of renewably-sourced kerosene towards achieving the climate targets for 2050 is inherently limited.

All over, the aviation sector consumed around 300 Mt of kerosene in the year 2018 (mainly crude oil based kerosene), resulting in carbon dioxide emissions of about 1 Gt (2018) [5, 6]. Despite being roughly reduced to 50 % in the year 2020 during the COVID-19 pandemic, kerosene demand and resulting carbon dioxide emissions in 2024 might even surpass 2019 levels [277]. Without mitigation measures, these emissions might increase to about 1.5 to 2.5 Gt in the year 2050 [157].

Carbon dioxide emissions from aviation are primarily caused by the combustion of kerosene derived from fossil crude oil. If kerosene is produced based on carbon which has recently been removed from the atmosphere (e.g., by photosynthesis or technical processes), balanced net carbon dioxide emissions could be realized (assuming no secondary fossil fuel based emissions, e.g., from conversion or transportation processes). In this

way, substituting the presently used fossil fuel based kerosene with a renewably-sourced kerosene could allow for large carbon dioxide emission reductions.

Additionally, due to their slightly different chemical composition, renewably-sourced kerosene can also contribute to the reduction of contrail-related climate impacts [10, 16, 17, 28, 131]. Other climate impact mitigation measures, e.g., technological measures such as engine efficiency improvements or more efficient air traffic management, can also help to reduce (but do not substitute) the use of fossil fuel based kerosene.

These facts are taken into account in most studies on pathways towards aviation's carbon dioxide neutrality by 2050. E.g., a recent study estimates that about 40 % of carbon dioxide emission reductions could result from renewably-sourced kerosene, and an additional 10 % could result from a demand reduction caused by higher airfares as a result of increased kerosene costs [157]. IATA reports that renewably-sourced kerosene would have to account for 65 % of the emission reductions required to achieve the stated net-zero carbon dioxide emissions goal by 2050.

In conclusion, a substitution of the presently fossil fuel based energy carrier by renewably-sourced ones is indispensable for the aviation industry to achieve its climate mitigation targets and thus to align it with the Paris Agreement.

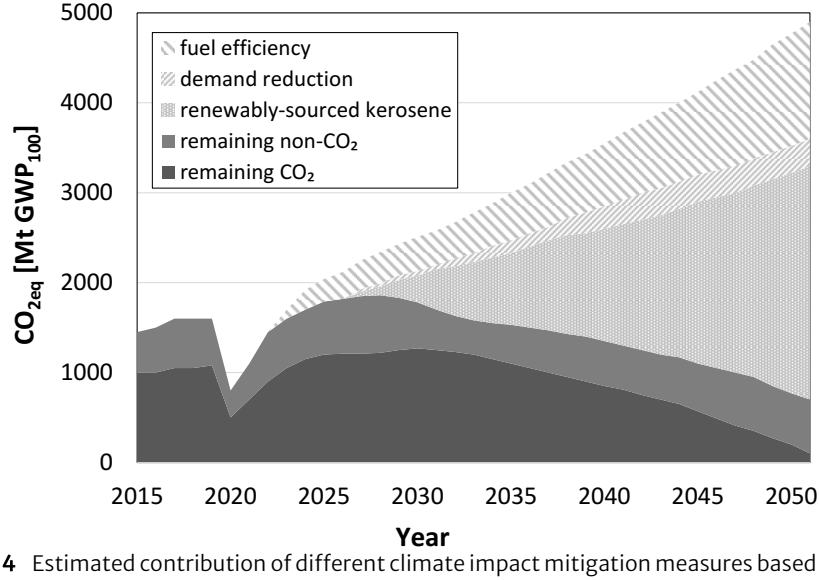


Figure 3.14 Estimated contribution of different climate impact mitigation measures based on [157]

Against this background, this chapter describes requirements and conversion pathways for renewably-sourced kerosene. Section 3.3.2 discusses kerosene consumption-related and section 3.3.3 kerosene provision-related requirements. Based on these, section 3.3.4 outlines several provision pathways for renewably-sourced kerosene.

3.3.2 Consumption-related Requirements and Resulting Kerosene Specifications

3.3.2.1 Requirements

Requirements related to a large-scale use of renewably-sourced kerosene can be clustered into three groups: supply chain, flight operations, and aircraft technology (Figure 3.15). In the following section, each of these groups and their requirements are described. In particular, requirements from flight operations and aircraft technology have shaped existing kerosene specifications, which will be addressed in the subsequent section.

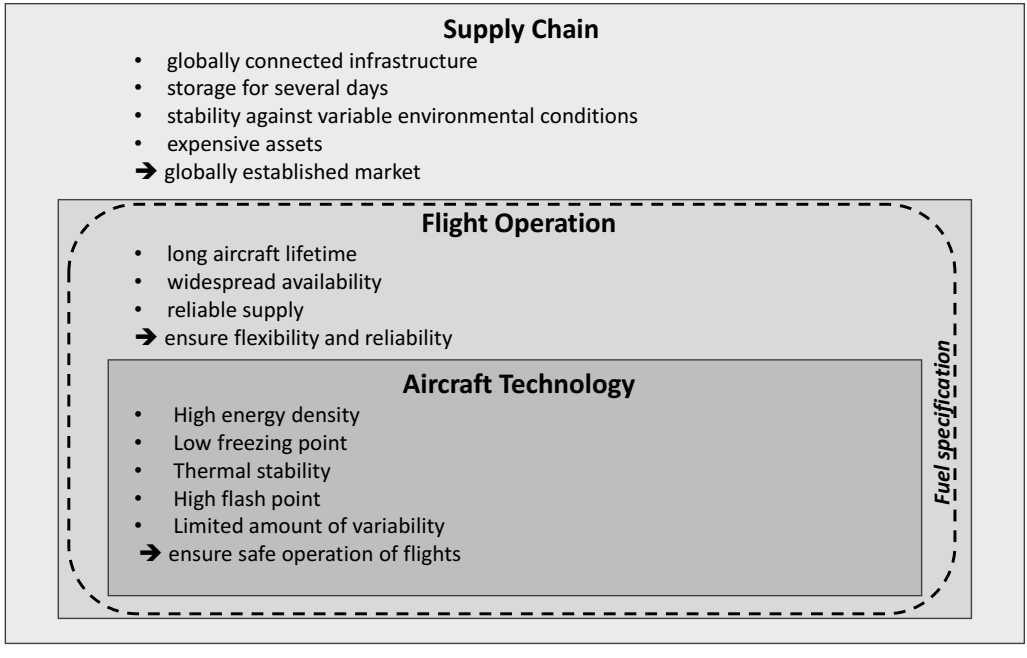


Figure 3.15 Categories within the kerosene consumption perspective and consumption-related requirements for aviation kerosene (own figure)

The supply chain for conventional fossil fuel based kerosene is part of the crude oil value chain. Such crude oil value chains have been developed and optimized in the past century to ensure the efficient delivery and availability of a broad range of hydrocarbon products for various markets. Especially at large, international airports, huge amounts of kerosene are being consumed – e.g., in San Francisco/USA around 7 200 t/d or Munich/Germany about 5 200 t/d [278]. Such high rates require a globally connected infrastructure to ensure reliable supply.

At airports, fuel suppliers are required to stock an amount of kerosene equaling the consumption of several days. Typically, this is performed by a common fuel storage facility, where deliveries of different fuel suppliers commingle [279]. The resulting requirement for fuel is that it can easily be stored for several days.

Such a common fuel storage at airports results in further requirements. At first, any fuel used within this system should be stable against variable environmental conditions to ensure its specification compliance even for storage over extended periods of time. Hence, its stability against changing environmental conditions is another requirement for aviation fuel.

Furthermore, the refinery technology for the conversion of crude oil to specification-compliant kerosene and the associated supply infrastructure are comparatively capital-intensive [178]. Not using this infrastructure would result in stranded investment and thus constitute an economic disadvantage by fuel producers / suppliers. As a result, this enforces fuel producer / supplier to maximize the utilization and extend the technical lifetime of their refineries and supply infrastructure as much as possible.

Overall, from a supply chain perspective, a widely (ideally globally) standardized fuel would be desirable. In this way, the globally established market for kerosene can be served efficiently. The introduction of a fuel which cannot be transported within the existing supply infrastructure (e.g., for physical, chemical and/or environmental reasons) would lose this advantage.

For **flight operations**, the typical technical lifetime of a commercial aircraft ranges between 20 to 30 years and partly even longer. Furthermore, the design and certification of new aircraft is very time-consuming and capital-intensive; this is even true for rather incremental adjustments [144, 232]. Assuming that present-day aircraft will be used for similar technical lifetimes, it is required that present-day kerosene types are also available in

the future (i.e., the decades to come). Notably, this primarily refers to existing kerosene standards but not necessarily to its origin (fossil / renewable, cf. section 3.3.2.2).

In order to match offered air travel / freight capacity and demand as closely as possible, airlines (a) require flexibility to start or close specific routes in the mid-term and (b) require the ability to switch the aircraft type on a specific route in the short-term. Both demands can be supported by offering the same fuel at most (ideally all) airports globally and by certifying most (ideally all) aircraft for the same fuel type.

In addition to fuel flexibility, airlines require a reliable fuel supply. With typical turnaround times below 45 min [232], airlines usually mitigate the risk of a supply failure by establishing supply agreements with at least two fuel supplier per airport [279].

Again, those characteristics of airline flight operations, i.e., long aircraft lifetimes, widespread availability, and reliable supply, result in the requirement for comprehensive fuel standardization.

In terms of **technology**, also aircraft and engine technology put certain requirements on aviation fuels. First of all, a high energy density is required for aviation fuels, due to the trade-off between fuel's energy density and maximum achievable payload (i.e., weight of passengers and cargo). Typical air temperatures at aircraft cruise altitudes are below -40 °C, sometimes considerably lower. In order to avoid fuel freezing during prolonged flights, the aviation fuel in use should exhibit a low freezing point. For the same reason, large temperature changes exist between cruise flight and on ground. Accordingly, aviation fuel should also exhibit sufficient thermal stability within this wide temperature window. Additionally, to avoid unintended fuel ignition (e.g., during refueling) the fuel's flash point should be sufficiently high. Current fuel specifications encompass a range of several further properties to ensure the technological functionality of the fuel together with aircraft and engine [181].

Ultimately, all these requirements serve to ensure a flight's safe operation. Any combination of fuel, engine, and aircraft design, regardless of whether they correspond to "conventional" or "innovative" designs, must fulfill these requirements.

In particular, the flight operation- and technology-related requirements emphasize the need for a standardized and widely available fuel. Since conventional fossil fuel based kerosene has taken this role for more than 70

years, these requirements pose a high barrier against the introduction of innovative technologies and "new" fuels, such as hydrogen (H_2) or electricity for battery-electric flights. For these reasons, for many actors within the commercial aviation industry renewably-sourced kerosene options with similar properties as conventional kerosene are the preferred option.

3.3.2.2 Kerosene Specification

Technological conditions and flight operation requirements are a strong driver in developing a virtually global standard for kerosene. The American Society for Testing Materials (ASTM) specification ASTM D1655 [181] has taken this role as a basically globally applied fuel specification for kerosene. In some regions (e.g., in China and Russia), a few, slightly different specification standards exist, but their requirements are very similar to those defined by the respective ASTM standard [200]. ASTM D1655 defines ranges and in some cases maximum or minimum permissible values for a broad range of kerosene properties [254]. Notably, while the design of aircraft and engines has undergone substantial incremental improvements within recent decades to increase their overall efficiency, specification standards for the used fuel largely remained unchanged [138]. Nevertheless, in 2018 and 2020, two options for the common processing ("Co-Processing") of renewable feedstock and fossil crude oil have been added to ASTM D1655 [181].

An additional standard, ASTM D7566, exists for renewably-sourced kerosene. It lays out a range of requirements for neat renewably-sourced kerosene derived from currently eight different conversion pathways. Table 3.15 summarizes these conversion pathways defined by ASTM D7566 and the Co-Processing options of ASTM D1655.

Nevertheless, ASTM D7566 still requires blending of renewably-sourced kerosene with conventional kerosene by up to 50 %, depending on the respective conversion pathway. The resulting blend must also fulfill the requirements laid out by ASTM D1655. As a result, a specification-compliant blend can be considered Jet A-1 by definition and thus used in the existing infrastructure and aircraft without any further modifications. For this reason, such kerosene is often called "drop-in" kerosene.

A blend ratio of 50 % renewably-sourced kerosene is clearly insufficient to achieve the industry goals of net-zero carbon dioxide emissions. Therefore, ASTM is developing a specification for neat renewably-sourced kero-

sene [142]. This should be a drop-in kerosene, meaning it would still be usable in any legacy aircraft certified for the use of conventional Jet A-1 kerosene. Beyond this, in order to improve local air quality and also to mitigate contrail climate impacts, an aromatic-free / fully paraffinic renewably-sourced kerosene would be desirable. As of now, however, this seems to require the development of a new kerosene specification and leaves open questions as to its compatibility with some older, legacy aircraft [142, 281].

Table 3.15 Approved production pathways for synthetic kerosene (own table based on [181, 280])

ASTM	Annex	Year of approval[a]	Process	Blending-limit[b]
D7566	1	2009	FT-SPK	50 vol.-%
	2	2011	HEFA-SPK	50 vol.-%
	3	2014	HFS-SIP	10 vol.-%
	4	2015	FT-SPK/A	50 vol.-%
	5	2016	AtJ-SPK	50 vol.-%
	6	2020	CH-SK	50 vol.-%
	7	2020	HC-HEFA-SPK	10 vol.-%
	8	2023	AtJ-SKA	50 vol.-%
D1655	-	2018	Co-Processing of vegetable oils	5 vol.-% [c]
	-	2020	Co-Processing of FT-crude	5 vol.-%

Note: at the time of writing; **A** aromatics; **AtJ** Alcohol-to-Jet; **CH** Catalytic Hydrothermolysis; **FT** Fischer-Tropsch; **HC** Hydrocarbons; **HEFA** Hydroprocessed Esters and Fatty Acids; **HFS** Hydroprocessed Fermented Sugars; **SIP** Synthetic Isoparaffins; **SK** Synthetic Kerosene; **SKA** Synthetic Kerosene with Aromatics; **SPK** Synthetic Paraffinic Kerosene)
[a] This refers to the initial approval. After the initial approval, approved processes were partially adapted, for example by increasing the maximum blending limit or by expanding the raw materials that can be used. [b] Precautionary maximum blending limit of the synthetic kerosene component. [c] An increase of the blend ratio to 30 vol.-% is currently prepared for approval as ASTM. This increase will require that the co-processing includes a hydrocracking step.

3.3.3 Provision-related Requirements

In contrast to the primary feedstock of conventional kerosene, crude oil, a mature supply chain for renewable feedstock to produce kerosene has not yet been developed. In principle a large variety of renewable feedstock options exists, however, with largely differing characteristics. The following section classifies these options and then describes their main characteristics.

Renewable feedstock can broadly be distinguished according to their energy input into biogenic and power-based options[10].

- Biogenic options. Depending on their primary components, biogenic feedstock can be classified as lipid-, starch-, sugar- and lignocellulose-containing feedstock.
- Power-based options. In terms of power-based feedstock, typically water, carbon dioxide (CO_2) and as energy source renewably-sourced electricity are distinguished.

Table 3.16 summarizes the different feedstock types, based on typical sources, their feedstock potential and demand for this feedstock from other sectors.

Table 3.16 Qualitative discussion of feedstock options for renewably-sourced kerosene (own table)

	Biogenic feedstock			**Non-biogenic feedstock**		
	Lipid-containing	Starch- / Sugar-containing	Ligno-cellulose-containing	Water (H_2O)	Carbon dioxide (CO_2)	Renewably-sourced electricity
Typical sources	used cooking oil animal fats	crops food / feed waste	plantation wood, stalks agricultural and forestry waste and residues	almost any source of water, including seawater	point sources (cement plant, biogas plant) direct-air-capture	wind and photovoltaic power plants
Feedstock potential	limited	limited, mostly due to regulatory constraints	very high	very high	limited	theoretically very high
Demand from other sectors	moderate	very high	moderate	moderate, in some cases very high	currently low, but most likely increasing in the future	very high

3.3.3.1.1 Feedstock for Biomass-based Pathways

3.3.3.1.1.1 Lipid-containing Feedstock

Typical sources for lipid-containing feedstock currently in use are wastes and residues, such as used cooking oil or animal fats from meat production.

[10] A combination of both feedstock options might be advantageous from a process engineering perspective. For greater clarity, such combinations are not discussed here. More information can be found in the literature. [282].

Certain crop species also contain relatively high amounts of lipids (e.g., rapeseed, oil palms, or *Jatropha Curcas*). However, such crops are currently only used for the production of renewably-sourced kerosene to a certain extend. This is mainly due to regulatory constraints intended to preserve the used agricultural land with priority for food and feed production [32, 154]

The **feedstock potential** for lipid-containing wastes and residues is inherently limited, while the potential for dedicated crops is rather constrained by regulatory and sustainability aspects e.g., due to land-use change aspects and a potential competition with the food and feed production [32, 125, 167, 237].

Simultaneously, lipid-containing feedstock experiences a strong **demand from other sectors**, mainly due to its high energy content. Edible feedstock (e.g., rapeseed or palm oil) is demanded for food and feed production, but typically not approved for the production of renewably-sourced kerosene. Like any feedstock suitable for the production of renewably sourced kerosene, it can also serve as feedstock for other fuels, e.g., road transportation fuels. Additionally, this biomass feedstock is also demanded by the chemical industry as well as other industry branches.

3.3.3.1.1.2 Sugar- / Starch-containing Feedstock

Typical sources of sugar- / starch-containing feedstock are almost all food and feed crops. Examples are sugar beet, potatoes, wheat, or corn. Their use within the food and feed industry also creates substantial amounts of food waste [283].

The **feedstock potential** of sugar- / starch-containing feedstock is in principle very high. However, it needs to be weighted with the **demand from other sectors**, particularly the need for food and especially feed. A common concern is that the use of this feedstock type as an energy crop results in a reduced availability / in higher prices of food and feed in average. Political approaches to mitigate this risk and to deal with the resulting challenges differ largely by region, partly affected by the respective population density and the local / regional availability of arable land. E.g., in Brazil, ethanol based on sugar is widely used within road transportation. In the US mainly corn is used as an energy crop for bioethanol production. Compared to that, within the EU a clear political intention is visible towards an ongoing shift to lignocellulose-based feedstock [284–286].

3.3.3.1.1.3 Lignocellulose-containing Feedstock

Typical sources for lignocellulose-containing feedstock could either be plantation wood, such as poplar, meadow, or eucalyptus wood, or stalks, such as straw or reed [154]. Also, e.g., agricultural or forestry wastes and residues can provide a large source of lignocellulose-rich feedstock [285, 287].

The **feedstock potential** of such lignocellulose-based material is very high, even though it is associated with a large uncertainty range [32, 237]. As a potential alternative to sugar- / starch based feedstock, technological development for the use of lignocellulose as feedstock is ongoing, but has not yet reached full commercial scale [285].

There is a substantial **demand from other sectors** related to lignocellulosic material. This is true for the use as an energy carrier as well as for a material use. However, the widespread availability alleviates the competitive situation. Additionally, since lignocellulose is – in contrast to sugar or starch – indigestible, a competition with the food market can largely be ruled out.

3.3.3.1.2 Feedstock for Power-based Pathways

3.3.3.1.2.1 Water

Typical sources show a broad range from underground water as well as surface water e.g., from rivers. But also the use of seawater is possible. The subsequent electrolysis step requires a pre-cleaning and deionization of the water input in most cases. Thus, seawater can be made available via desalination at comparatively low efforts [102].

As a result, the **feedstock potential** is generally very high, however, for some local regions, e.g., deserts with typically high potentials of solar radiation, it may be necessary to enable a water supply via a pipeline or other means of transport.

As many sectors, not only households but also industrial production, require large amounts of water. Thus, a **competition with other sectors** can be expected. In general, the high feedstock potential and the comparatively low supply effort dampens the competitive situation. However, additional stress on sweet water resources might arise.

3.3.3.1.2.2 Carbon Dioxide

Either point sources or direct-air-capture processes are **typically discussed sources** for the provision of carbon dioxide for fuel production. Point sources can be fossil-fueled power plants, cement plants, or e.g., biogas or bioethanol plants. In this case, the origin of the carbon plays an important role. In case of a biogas or a bioethanol plant, the carbon contained within the CO_2 molecule originates from the biomass (renewable resource), while e.g., at a cement plant or a lignite fired power plant, the carbon dioxide would be clearly of fossil origin. Direct-air-capture technology allows for the capture of carbon dioxide directly from ambient air. However, the currently available technology shows high energy, material, and area requirements and thus high cost, while the potential of scale effects in the future is uncertain [102, 288].

The **feedstock potential** of point sources providing carbon dioxide of renewable origin is limited [289]. Carbon dioxide from the ambient air is theoretically abundantly available, however, at a very low concentration of about 419.5 ppm (as of 2023). Hence, the feedstock potential of carbon dioxide is indirectly limited by energy, material, and area requirements for direct-air-capture plants.

Demand from other sectors is currently rather low, but assuming increasing efforts to defossilize the overall economic system, demand from other sectors will most likely increase. In addition to fuel production, also the chemical industry will require large amounts of renewably-sourced carbon.

3.3.3.1.2.3 Renewably-sourced Electricity

A wide variety of **typical sources** for renewably-sourced electricity exists, from which the most important ones, in terms of potential and costs, are wind and photovoltaic power [290]. Since they directly depend on the availability of wind and solar irradiation, certain regions around the globe show substantially higher potential than others [198].

In principle, the **feedstock potential** of renewably-sourced electricity, in particular for wind and photovoltaic power, is abundantly high [290]. As of now, however, only a small fraction of this potential is utilized since the ramp up of these technologies has begun only about two decades ago [239]. Due to their strong increase in installed capacity throughout the globe, it

can be expected that the wind and solar potential will be more widely exploited in the years to come.

Demand from other sectors for renewably-sourced electricity is very high, especially due to global efforts to lower the dependency on (imported) fossil-based fuels and to mitigate greenhouse gas emissions. Most likely, this demand will further stipulate the ramp up of renewable energy sources, but the competitive situation is likely to remain high in the next decades.

3.3.4 Provision Pathways

As outlined in section 3.3.2, kerosene-type renewably-sourced aviation fuels are favorable from a fuel consumption perspective. Simultaneously, a broad range of feedstock options for such fuels exists (section 3.3.3). Thus, below pathways to convert such feedstock into specification compliant kerosene are outlined. Due to its impending approval [218], the Methanol-to-Jet conversion pathway is also discussed. The provision of intermediates is covered first, followed by upgrading steps toward specification-compliant kerosene. Figure 3.16 depicts the various conversion pathways available.

3.3.4.1 Provision of Intermediate Products

3.3.4.1.1 Alcohols

Alcohols are a group of organic compounds that contain a hydroxyl group attached to a saturated carbon atom (chain). Currently, only selected alcohols such as ethanol and iso-butanol are approved, but ASTM D7566 explicitly mentions the objective to approve all C_2 to C_5 alcohols [280]. Depending on feedstock and alcohol, a wide variety of pathways are available for the provision of alcohols [223]. Therefore, this section focuses on two well-established processes, namely methanol synthesis, and fermentation.

Methanol synthesis is a heterogeneously catalyzed, thermochemical conversion of a gas mixture consisting of carbon monoxide (CO) and hydrogen (H_2)[11]. Today, over 100 Mt/a of methanol are produced from such a CO and H_2 containing synthesis gas; however, the feedstock for the provision of

[11] Note that this gas mixture is also often referred to as synthesis gas, similar to the gas mixture of carbon monoxide (CO), carbon dioxide (CO_2) and hydrogen (H_2) used for Fischer–Tropsch Synthesis. To improve clarity, the term synthesis gas is used here only for a gas mixture of carbon monoxide (CO) and hydrogen (H_2).

this synthesis gas are almost exclusively fossil fuels (i.e., natural gas, coal) [32, 291]. This type of catalyst-steered synthesis is also known as conventional methanol synthesis. Since such catalysts used within a methanol synthesis also show a certain activity for CO_2, methanol can also be produced from a CO_2- and H_2-rich gas in the so-called direct methanol synthesis. Both synthesis pathways are exothermic and take place at elevated pressures (~75 bar) and temperatures (~250 °C) under the presence of typically Copper-Zinc based catalysts [291, 292]. The required feedstock for a power-based ("green") production, H_2 and CO_2, can be provided via electrolysis (section 3.3.4.1.2) from water and either from point sources such as bioethanol plants or direct-air-capture processes. Sustainable synthesis gas for conventional synthesis can be produced by gasification or reforming and conditioning of lignocellulosic biomass (section 3.3.4.1.2).

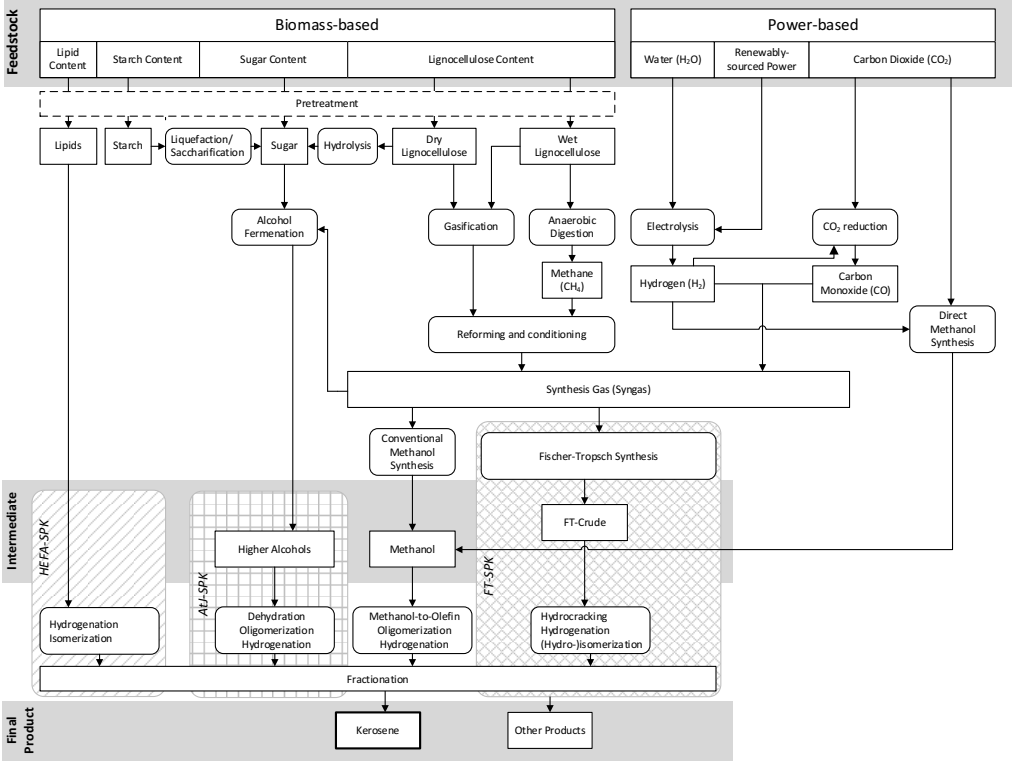


Figure 3.16 Possible main conversion pathways for the provision of renewably-sourced kerosene, based on [94, 106, 291]; AtJ Alcohol-to-Jet; FT Fischer-Tropsch; HEFA Hydroprocessed Esters and Fatty Acids; SPK Synthesized Paraffinic Kerosene

Fermentation refers to the biochemical conversion of sugars by microbes into ethanol or higher alcohols (e.g., iso-butanol) [293]. When appropriate

process steps are applied (e.g., liquefaction or saccharification of starch or hydrolysis of lignocelluloses), starch or, in principle, also lignocelluloses can be used as fermentation feedstock [285, 293]. The most prominent and oldest fermentation process is the "classical" ethanol fermentation, where yeast is used to produce ethanol and carbon dioxide (CO_2) as a side product from sugar molecules. This biochemical process is widely implemented on a global scale, e.g., for the production of beer and yeast dough.

ABE-fermentation in turn, which uses *Clostridium acetobutylicum* bacteria, yields acetone, butanol, and ethanol. It has been used at large scale until the second half of the 20th century, until it has been replaced by cheaper production processes [293]. Today this process option is basically irrelevant due to much more promising competing, fossil-based processes.

Synthesis-gas fermentation is also based on a biochemical conversion of synthesis gas (CO and H_2) using acetogenic bacteria [223]. In contrast to the "classical" ethanol fermentation, synthesis gas fermentation is less dependent on sugar as feedstock and could theoretically also be operated using lignocellulose or even non-biogenic feedstock. The scale-up of this process is currently under development [294].

In all of these cases, subsequent separation of the alcohols from the fermentation or synthesis by-products is required. This can be achieved e.g., by means of distillation and/or fractionation.

3.3.4.1.2 Fischer–Tropsch (FT) crude

Fischer-Tropsch (FT) crude is the product of Fischer-Tropsch (FT) synthesis. This process is a catalyst-supported thermochemical conversion of synthesis gas (CO and H_2). During the respective synthesis, hydrocarbons of various types and chain lengths (C_1 to beyond C_{20}) are formed under the presence of an iron- and/or cobalt-based catalyst [74]. Process conditions are pressures in the range of 20 to 40 bar and temperatures either between 320 to 350 °C ("high temperature FT-Synthesis") or 220 to 250 °C ("low temperature FT-Synthesis"). The hydrocarbon distribution in the product ("syncrude") varies depending on the synthesis gas composition, the reactor technology, the operation mode and the utilized catalyst [74].

A wide variety of processes based on biogenic and non-biogenic feedstock is available for the provision of synthesis gas. For biogenic feedstock, the central process steps are gasification, anaerobic digestion with subsequent reforming and conditioning. For non-biogenic feedstock, synthesis

gas is primarily provided based on electrolysis and carbon dioxide reduction.

Gasification of biomass entails the thermal deconstruction of the lignocellulosic feedstock into a product gas through partial oxidation. Either air, oxygen, steam or mixtures thereof can be used as gasification agents [295]. In addition to the synthesis gas components (CO and H_2), the main components of the product gas are CO_2 and light hydrocarbons. Despite several attempts to commercialize this technology, no plant has been built at commercial scale so far [32].

Anaerobic digestion entails the biochemical conversion of biogenic feedstock, typically wastes and residues, by bacteria in an oxygen-free environment. The bacteria release a gas mixture of mainly methane (CH_4) and carbon dioxide (CO_2). This process step is particularly suitable for biogenic feedstock with a comparatively high water content. In some global regions, e.g., Germany, anaerobic digestion is widely applied for combined heat and power generation and biomethane production.

Reforming and conditioning enable synthesis gas production from product gas and biogas. Reformation of light hydrocarbons is usually catalyst-supported and operated at high temperatures with H_2O (steam reforming), O_2 (partial oxidation), or CO_2 (dry reforming) as oxidizing agent. While product gas from biomass gasification usually contains a lower proportion of hydrocarbons and reforming is therefore not necessarily required, extensive reforming is essential for converting biogas or biomethane into synthesis gas.

Conditioning is usually needed to adjust the synthesis gas ratio according to the synthesis requirements. The H_2 deficit that usually prevails can be compensated for by a water-gas shift with subsequent CO_2 separation or by adding power-based H_2. Reforming and conditioning is globally applied in many synthesis plants and refineries, however, mainly converting natural gas or product gas from coal gasification [39].

Electrolysis is the electrochemical splitting of water (H_2O) into hydrogen (H_2) and oxygen (O_2). Different technologies are available for this process, namely the alkaline water electrolysis, proton-exchange membrane electrolysis and solid oxide electrolysis. Among these, only the alkaline water electrolysis has reached commercial stage [154].

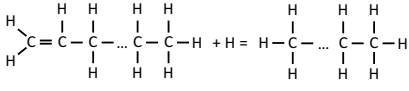
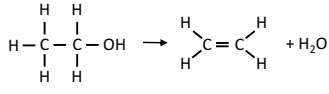
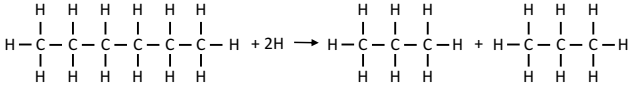
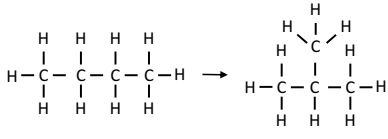
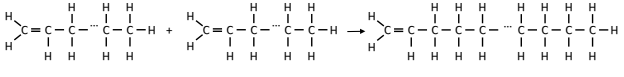
Carbon dioxide (CO_2) reduction via the so-called reverse water-gas shift (RWGS) reaction is required since low-temperature FT-Synthesis,

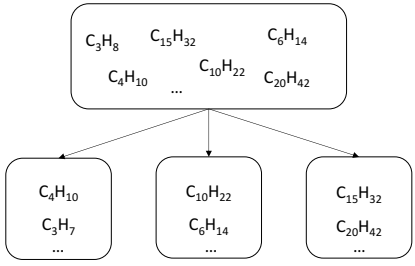
mainly used for producing long-chain paraffinic fuels, does not allow for a direct CO_2 conversion. Within this RWGS reaction, hydrogen (H_2) and carbon dioxide (CO_2) react at high temperatures (700 to 1000 °C) catalyst-controlled to water (H_2O) and carbon monoxide (CO) as the mainly desired product [296, 297]. In contrast to the other process steps, the RWGS reaction has not been realized large-scale at a commercial scale yet [298].

3.3.4.2 Conversion and Upgrading of Intermediate Products

The upgrading of the abovementioned intermediate products to specification-compliant kerosene is based on different combinations of process steps being widely used since decades primarily within the petrochemical industry [74]. Table 3.17 lists the names and provides a short description and a visualization of each of these individual process steps. The respective combinations of process steps for the upgrading of each of the intermediate products are described thereafter.

Table 3.17 Petrochemical process blocks, note that the carbon chain lengths of the molecules depicted may vary (own table)

Name	Visualization	Description
Hydrogenation		Addition of hydrogen (H_2) for saturation, e.g., of alkenes into alkanes
Dehydration		Removal of oxygen and hydrogen as water
(Hydro-) cracking		Cracking of longer-chain hydrocarbons into shorter ones
(Hydro-) isomerization		Branching of hydrocarbons to isomers
Oligomerization		Combination of short-chain alkenes to longer ones

Fractionation		Separation of hydrocarbons based on their chain lengths

3.3.4.2.1 Upgrading of Lipids

Upgrading of lipids to specification-compliant kerosene requires typically at least a hydrogenation, an isomerization, and a final fractionation step [280]. Most lipids consist mainly of triglycerides, i.e., molecules consisting of an ester and three attached fatty acids. Compared to that, di- or monoglycerides contain only two or one fatty acid group, respectively. Hydrogenating the triglycerides replaces the oxygen contained within such a molecule with hydrogen by forming water; additionally, any potentially existing double bonds within the fatty acid groups are saturated. Thus, the main product of such a treatment are n-alkanes with a chain length corresponding to the length of the former fatty acids. As this length does not necessarily correspond to the desired kerosene fraction, cracking combined with a subsequent hydrogenation may be necessary to increase the product yield. As n-alkanes show a higher freezing point compared to iso-alkanes, isomerization may additionally be required to meet the fuel specification requirements [154, 299, 300].

3.3.4.2.2 Upgrading of Alcohols

Upgrading of alcohols to specification-compliant kerosene requires at least a dehydration, an oligomerization, a hydrogenation, and a final fractionation step [280]. By definition, any alcohol contains a hydroxy (OH) group. ASTM D7566 requires the removal of any oxygen from the kerosene; hence dehydration is applied to remove this group as water. The remaining, short alkene group corresponds to the chain length of the former alcohol (e.g., C_2H_4 for ethanol). An exception to this is the dehydration of methanol, where carbon bonds are formed between the individual molecules in parallel with the water separation, and a mixture of light alkenes is produced (methanol-to-olefin; MtO). In order to achieve a carbon chain length within

the kerosene range, an oligomerization step is required to combine several short-chain alkenes into longer-chain molecules. To saturate the alkenes, hydrogen (H_2) is added during hydrogenation and fractionation is applied to divide the hydrocarbon mixture into different product fractions [154, 285].

3.3.4.2.3 Upgrading of Syncrude

Syncrude has a comparatively similar chemical composition as fossil-based crude oil. Still, (hydro-) cracking, hydrogenation, (hydro-)isomerization, and fractionation are necessary to achieve specification-compliant kerosene from syncrude [280]. Compared to fossil crude oil, syncrude usually contains a substantially larger fraction of waxes, i.e., hydrocarbons with a greater chain lengths compared to kerosene [74]. Therefore, these molecules have to be cracked to increase the amount of hydrocarbons being within the kerosene range. Subsequently, remaining alkenes are saturated to alkanes by hydrogenation. Again, to ensure a sufficiently low freezing point, additionally (hydro-)isomerization is typically required. During fractionation, the last step, the products are separated based on their carbon chain length [74, 154, 291].

3.3.5 Final Considerations

Air transport contributes approximately with 4 % to global anthropogenic climate forcing. Both the International Civil Aviation Organization (ICAO) and the International Air Transport Association (IATA) aim to achieve net-zero carbon dioxide emissions by 2050, primarily by replacing fossil fuel based kerosene with renewably-sourced kerosene. Their feedstock contains carbon recently bound from the atmosphere. As a result, the carbon dioxide emissions released by using such renewably-sourced kerosene are circulated within a closed loop and do not contribute to an increase of the carbon dioxide inventory within the atmosphere. However, renewably-sourced kerosene has a market share of currently clearly less than 1 %.

In light of these aspects, this chapter provides an overview of requirements from kerosene consumption and provision as well as currently discussed provision pathways for renewably-sourced kerosene. Its main conclusions can be summarized as follows:

- Requirements from the view point of the kerosene consumption can be clustered into requirements from the supply chain, the flight operations and the given / available technology. The latter two play an influential role on the development of almost globally applied kerosene specifications. Additionally, the use of a kerosene-type fuel is enforced, while different fuels, e.g., hydrogen (H_2), face substantial barriers in this regard.
- Requirements from kerosene provision emerge from the properties and availability of the individual feedstock options. Feedstock for renewably-sourced kerosene can be classified as biomass-based and power-based feedstock. Among the biomass-based feedstock, lipids have the highest energy content but also the most strictly constrained availability. Among power-based feedstock, especially energy, material and area requirements for the provision of carbon dioxide constitute so far a substantial barrier, while power-based hydrogen production remains the main energy consumer within all power-based pathways.
- A broad range of provision pathways for renewably-sourced kerosene is available. The main routes concern the conversion of lipid-containing feedstock (Hydroprocessed Esters and Fatty Acids, HEFA), the conversion of alcohols (Alcohol-to-Jet, AtJ), and the provision and conversion of Fischer-Tropsch Crude (FT) crude. To ensure specification compliance, further upgrading of the intermediates to specification-compliant kerosene is necessary.

By connecting these results, a trade-off between efforts for conversion and theoretical availability becomes apparent (Figure 3.17). The conversion of lipids is comparatively easy in terms of processing steps and energy requirements. Moving along the feedstock options towards power-based feedstock, energy requirements, processing steps and also the process complexity increase. On the other hand, the theoretical availability describes the physical availability, e.g., the amount of solar irradiation which would be physically available, neglecting the still required ramp up of wind turbines and photovoltaic modules. Here, the theoretical availability of lipids is lowest and increases via lignocellulose-containing biomass towards power-based feedstock. Each conversion pathway for renewably-sourced kerosene can be allocated somewhere along this spectrum, indicating that there is not a “one size fits all” solution for renewably-sourced kerosene.

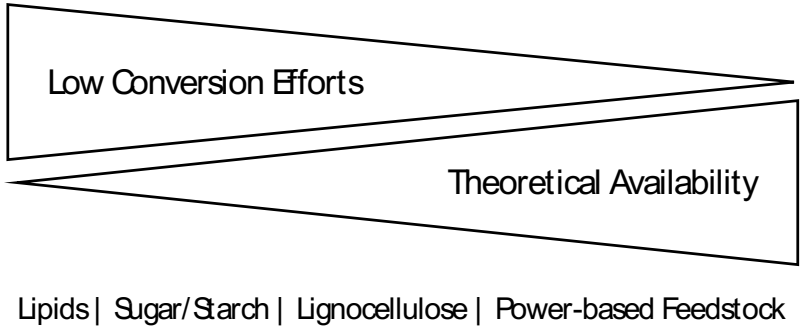


Figure 3.17 Trade-off between low conversion efforts and theoretical availability (own figure)

In the years to come, the development of air travel demand, the (potential) approval of new conversion pathways and the development of the overall energy transition will be highly influential to the market development of renewably-sourced kerosene.

Air travel demand determines the energy demand of the aviation sector and thus, also the demand for renewably-sourced kerosene. A slower air travel demand growth would also require lower volumes of renewably-sourced kerosene for achieving the industries climate targets. The approval of new conversion pathways might allow for the use of a broader feedstock range and potentially also higher conversion efficiencies. A range of interdependencies arises from the evolvement of the overall energy transition. If, e.g., the electrification of the road transport sector occurs quickly, also demand from road transportation for fuels based on lipid-containing feedstock would decrease, in turn increasing their availability for renewably-sourced kerosene. Hence, the future development of the air transport sectors energy transition cannot be estimated individually, but should rather be seen as part of the global energy transition.

3.4 Synthesis – Fuel Provision

The previous sections cover the technological provision of alternative fuels, either by hydroprocessing of conventional kerosene or by providing aviation fuels from renewable sources of energy. These sections are summarized now and discussed against other, technological climate forcing mitigation measures. Accordingly, provision pathways for alternative fuels are outlined and discussed first (*Research Question 1,* section 3.4.1) and then main influential factors on their carbon dioxide- (*Research Question* 2*,* section 3.4.2) and contrail-related climate forcing (*Research Question 3,* section 3.4.3) are summarized and analyzed. This section closes by discussing potential trade-offs and interdependencies among these mitigation measures in the overall synthesis (section 3.4.4).

3.4.1 Provision Pathways

In the following, first the different provision pathways for alternative aviation fuels are introduced and their key characteristics are summarized (section 3.4.1.1). Thereafter, the other, technological climate forcing mitigation measures are described (section 3.4.1.2).

3.4.1.1 Synthesis

Alternative aviation fuels can be provided either by altering the properties of conventional kerosene or by replacing it. For example, by removing soot precursors (i.e., mainly aromatic components) from conventional kerosene, the optical thickness and lifetime of potentially formed contrails can be reduced and thus also the absolute value of their climate forcing (section 3.1.1). Replacing the current fossil fuel-based feedstock of kerosene by feedstock from renewable sources of energy would in turn mitigate a substantial fraction of aviation's carbon dioxide-related climate forcing. Since most renewably sourced kerosene options contain hardly any aromatic components (cf. section 3.2.4 [18, 138]), their use would additionally lower contrail-related climate forcing, in particular when they are used at high blend ratios with conventional kerosene.

One option to lower the content of aromatic components in conventional kerosene is an additional hydroprocessing step to transform / hydrogenate the kerosene's aromatic components to cycloalkanes or even crack

them into alkanes. Hydroprocessing is a well-established process in present-day crude oil refineries [39, 74, 178, 301]. While this process is typically not used for the treatment of conventional kerosene, it is required for other processes (for example the treatment of vacuum gas oil [39], cf. section 3.1.2.1). Hydroprocessing is also used for the desulfurization of fuels to be sold for the road transport market to fulfill the legal sulfur limits, e.g., for conventional Diesel fuel (section 3.1.1 [301]). Thus, hydroprocessing could be implemented in the short-term on a large scale.

Mild and harsh hydroprocessing can be distinguished, where in the first case it is assumed that the kerosene content of aromatic components remains at or above 8 %, while in the latter case, the content of aromatic components is reduced to near zero (section 3.1.2.1). Reducing the content of aromatic components below 8 m-% could, however, be contradictory to the presently valid fuel specifications (cf. section 3.1.3.2.2 [181, 280]). Thus, harshly hydroprocessed kerosene would rather be available in the medium-term, since the adoption of these specifications will presumably be completed at the earliest in the medium-term (cf. section 3.1.3.3).

Renewably sourced aviation fuels can be sub-divided in the categories: kerosene-like fuels, alcohol-based fuels, and gaseous fuels. For kerosene-like fuels, currently (November 2024) eight pathways are certified by ASTM [280].[12] Three of these pathways are of central relevance, while the remaining five options are either company-specific or so far less relevant processes (section 3.3.2.2).

- Hydroprocessed Esters and Fatty Acids Synthesized Paraffinic Kerosene (HEFA-SPK) is the pathway currently providing most of the renewably sourced kerosene for commercial use (section 3.2.2.2 [87, 240]). It uses lipids as a feedstock and is thus technologically and economically advantageous because of the associated low conversion efforts (section 3.3.4.2.1) by making maximum use of the synthesis efforts already realized by nature. But lipid-based feedstock is a priori limited on a global scale and thus most likely not enough feedstock will be available also on the longer term to cover the overall energy demand of the global civil air transport system especially when considering other demands for lipids (e.g., human nutrition) (section 3.3.3.1.1.1 [158, 237, 240]).

[12] When the corresponding research article (section 3.2) was published in October 2022, one pathway (AtJ-SKA) was not yet included in the specification. For this reason, the article only lists seven options.

- Besides lipid-based feedstock, kerosene can also be provided based on different alcohols via the Alcohol-to-Jet Synthesized Paraffinic Kerosene (AtJ-SPK) pathway (section 3.2.4.1 [119, 216, 223, 285]). The alcohol typically used as feedstock for such conversion processes are either iso-butanol or ethanol [280]. But also methanol as the simplest alcohol can be used as feedstock from a technological perspective; the certification of a pathway for methanol is currently ongoing [302]. If such alcohols are to be provided from biogenic feedstock, a trade-off exists between sugar- or starch-based as well as lignocellulose-based feedstock. The first two options require less intense processing, but their feedstock availability is a priori limited and might compete with the food and feed as well as industrial markets (section 3.3.3.1.1.2 [216, 223]). In contrast, lignocellulose-based feedstock is available at greater amounts, less competitive with food and feed provision, but in turn requires clearly more intense processing (section 3.3.3.1.1.3 [216, 223]) and is for the time being not state of technology.
- The third of the main provision pathways is Fischer-Tropsch Synthesized Paraffinic Kerosene (FT-SPK). This kerosene can be provided either from biogenic or from non-biogenic feedstock (section 3.2.4.1 [291]). Various parts of this process have been realized at an industrial scale, but their combination for the feedstock considered here has not been demonstrated on a large scale (i.e., at industrial scale) [216]. In terms of feedstock, the heterogeneity of biogenic feedstock (section 3.3.3.1.1.3) or – in case of non-biogenic feedstock – the provision of carbon from renewable sources of energy (section 3.3.3.1.2.2 [102, 216, 291]) currently constitute main barriers for the application of this process at industrial scale.
- The other certified conversion pathways are either company-specific (e.g., Alcohol to Jet Synthesized Kerosene with Aromatics (AtJ-SKA) [303]) and / or have been abandoned since they were economically unviable (e.g., Hydroprocessed Fermented Sugars Synthesized Isoparaffins (HFS-SIP)) (section 3.2.4.1). For this reason, these processes are not discussed here.

For these kerosene-based options, a trade-off exists between the technical efforts for conversion and the market availability of the respective feedstock (section 3.3.5). Lipid-based pathways, such as HEFA-SPK, show rather low technical efforts for the conversion of the feedstock into specification-

compliant kerosene, while their market availability is limited on a global scale (e.g., in comparison to non-biogenic feedstock). For basically unlimited available feedstock, however, the efforts for a conversion to specification-compliant kerosene are substantially higher. As a result, to replace the majority of aviation's kerosene demand, the scale-up of processes with higher conversion efforts and thus higher associated fuel provision cost (e.g., FT-SPK) will be indispensable to achieve aviation's climate mitigation targets.

Most certified pathways for kerosene provision do not yield noteworthy amounts of aromatic compounds (section 3.3.2.2). Currently valid ASTM fuel specifications, however, define a minimum content of aromatic components [280]. For this reason, renewably sourced kerosene is presently only certified as a blend of up to 50 % with conventional kerosene. Such a specification-compliant kerosene is often referred to as drop-in kerosene, because it can be treated like conventional kerosene and supplied via the same infrastructure (section 3.3.2). For this reason, it can be considered as usable in the short-term. Simultaneously, the use of neat renewably sourced kerosene would allow for substantially larger lifecycle carbon dioxide emission reductions and kerosene without aromatic compounds would be beneficial in terms of contrail-related mitigation potentials (section 3.2.4.4). Thus, from a climate protection perspective, using neat renewably sourced aromatic component-free kerosene would be most desirable. However, such fuel would not be compliant with the currently valid fuel specifications and thus be a non drop-in kerosene. For these reasons, neat renewably sourced kerosene might be available in the medium-term at the earliest.

For the direct use of alcohols as renewably sourced aviation fuel, methanol, ethanol and butanol have been investigated (section 3.2.2.2). In principle, all of them can already be provided from renewable sources of energy. But these options show disadvantageous properties compared to conventional kerosene (e.g., a lower energy density compared to conventional kerosene) (section 3.2.4.3). Another barrier for their use is the provision infrastructure and the aircraft modifications required for their use (sections 0 and 3.2.4.3). Thus, renewably sourced alcohols used directly as an aviation fuel constitute a long-term option, if at all.

The situation is similar for the gases investigated, namely ammonia, methane, and hydrogen (section 3.2.2.2). In principle, all of these gases can al-

ready be provided from renewable sources of energy, but with highly disadvantageous properties compared to conventional kerosene (e.g., the low freezing point of hydrogen or the comparatively low energy density of ammonia and methane) (section 3.2.4.1). Again, due to the required modifications of the existing infrastructure and / or the aircraft's fuel system, these options seem to be usable in the (very) long-term only, if at all.

3.4.1.2 Discussion

Technological mitigation measures other than fuel-related measures can be distinguished as modifications of engines or airframes [304]. The following sections discuss exemplary measures from both fields as listed in Table 3.18. Some of these measures might also affect other than contrail- or carbon dioxide-related climate forcing (e.g., climate forcing from nitrogen oxide emissions), which will not be discussed in-depth here.

Table 3.18 Exemplary technological mitigation measures and their description

Category	Measure	Description
Engine	Geared-turbofan	Additional gearbox to differentiate the rotational speeds of the fan and the low-pressure compressor / turbine
	Lean-burn combustion chamber	Favor conditions for lean combustion to lower nitrogen oxide and other emissions
	Counter-rotating open rotor	New engine design to improve the fan's aerodynamic efficiency
Airframe	Advanced wing design	Modified wing profile and shape to improve its aerodynamic efficiency
	Structures with reduced specific weight	Reduce weight to lower energy required for flight
	Blended-wing body design	Adjust the shape of the fuselage to improve aerodynamic efficiency

- In terms of engine technology, the mitigation measures selected are incremental measures such as a geared-turbofan and a lean-burn combustion chamber and a more radical change by a counter-rotating open rotor engine. A geared-turbofan utilizes a gearbox to differentiate the rotational speeds of the fan and the low-pressure compressor / turbine. In this way, higher and thus more efficient rotational speeds of the low-pressure compressor / turbine can be achieved, since the fan's rotational speed is limited by transsonic flow velocities at its outer tips [31]. A lean

burn combustion chamber is another engine design option. Here, the fuel is burned with excess air mainly reducing the formation of nitrogen oxide and soot, while fuel consumption is not substantially affected (section 1.2.3 [31, 49]). The third option, a counter-rotating open rotor engine design would encompass two fan blade rows rotating in opposite direction, which are located outside of the engine's cover similar to propeller engines [305]. This would allow for efficiency improvements by a further increase in the engine's bypass ratio and a reduction of the fan's airflow residual swirl by the second fan row [305].

- In terms of airframe technology, most options either aim at reducing aerodynamic drag or at reducing weight. Typical examples for incremental drag reduction options are adjustments in wingtip design to lower induced drag with an estimated fuel consumption (and thus carbon dioxide climate forcing) [306]. Reducing weight incrementally (e.g., by an increased use of composite materials or reducing cabin weight) can reduce the required energy for a flight, since less lift is required, which would induce aerodynamic drag [306]. A more radical option constitutes the "blended-wing-body" design, where the aircraft's fuselage is shaped similar to the wing in order to also contribute towards the aerodynamic lift force [307].

3.4.2 Carbon Dioxide–related Mitigation Potentials

In this section, the carbon dioxide-related mitigation potentials of the different provision pathways for alternative aviation fuels are discussed (section 3.4.2.1) and these fuel-related mitigation potentials are compared against the mitigation potentials of the other, technological climate forcing mitigation measures (section 3.4.2.2).

3.4.2.1 Synthesis

Altering the properties of conventional kerosene mainly aims at contrail-related mitigation potentials and can theoretically also result in an increase in carbon dioxide emissions, caused by the additional hydroprocessing step of the crude-oil based feedstock (cf. section 3.1.2.1.2). Compared to this, renewably sourced aviation fuels reduce carbon dioxide-related climate forc-

ing by either not containing carbon (e.g., liquid hydrogen, ammonia) or using feedstock which has been synthesized by using carbon dioxide from the atmosphere and thus constitutes a closed carbon cycle.

Altering the properties of conventional kerosene by hydroprocessing requires large amounts of hydrogen being presently typically provided from fossil fuel energy (section 3.1.2.1 [37, 38, 118]). In this case, a climate penalty has to be expected in terms of carbon dioxide-related climate forcing. This climate penalty needs to be carefully weighed against the contrail-related mitigation potentials. Assumed that production capacities for renewably sourced hydrogen increase in the future, the provided hydrogen can be used for hydroprocessing helping to minimize the carbon dioxide-related climate penalty of additional hydroprocessing (section 3.1.3.1.2 [266]). This is due to the fact that the main influential factor for carbon dioxide emissions for hydroprocessing conventional (i.e., crude oil-based) kerosene are the indirect emissions incurred by the provision of hydrogen (section 3.1.2.1 [39]).

Hypothetically, kerosene-like aviation fuel options from renewable sources of energy allow for reducing the entire lifecycle carbon dioxide-related climate forcing of their use, since their feedstock is entirely provided using carbon recently bound from the atmosphere (section 3.3.1). As a result, the carbon dioxide emissions released by using such renewably sourced kerosene are circulated within a closed loop and do not contribute to an increase of the carbon dioxide inventory within the atmosphere on average (section 3.3.1). However, the processing of feedstock might incur a climate penalty, e.g., due to the use of fertilizer which is produced with fossil fuel-based energy or energy demands for transportation covered by fossil fuels [94, 102]. Such climate penalties can be substantial, resulting in a broad range of net lifecycle emission values for renewably sourced aviation fuels (Figure 3.12). The values range from negative values (>100 % reduction compared the same amount of crude oil-based kerosene, where the carbon captured is partially removed into waste streams) to values higher than for conventional kerosene (about 30 % increase compared to the same amount of crude oil-based kerosene). Such cases with (very) high emission values are usually related either to (indirect) land use change effects for feedstock provision and / or indirect emissions caused by the provision of renewably sourced energy (e.g., manufacturing of the conversion plant

with, e.g., steel and cement) (section 3.2.4.4 [94, 123]). Concluding, influential factors on carbon dioxide-related climate forcing of renewably sourced aviation fuels are, e.g., greenhouse gas emissions caused by the used biogenic feedstock as well as emissions related to the energy provision for feedstock processing. The latter might decrease with an increasing defossilation of our global society [102, 291] and the former might be reduced due to a better understanding of the various controlling factors in the time to come (cf. section 3.2.4.4 [94, 123]).

3.4.2.2 Discussion

The carbon dioxide-related mitigation potentials of such other technological mitigation measures are summarized in Table 3.19 and subsequently their main influencing factors on carbon dioxide-related climate forcing are discussed and compared against the main influencing factors of alternative fuels.

In the field of engine technologies, the geared-turbofan has been introduced commercially with the PW1000G engine option for the Airbus A320neo aircraft in 2016 and is estimated to lower fuel consumption by about 12 % to 14 % compared to its predecessor [31]. A lean burn combustion chamber mainly reduces the formation of nitrogen oxide and soot, while fuel consumption is not substantially affected [31, 49]. A counter-rotating open rotor engine is estimated to reduce carbon dioxide-related climate forcing by 20 % to 40 % compared to a conventional A320 aircraft engine (CFM56-5) [306, 307].

Table 3.19 Exemplary technological mitigation measures and their carbon dioxide-related climate forcing mitigation potential (based on the provision that the respective measure is fully adopted); ? – unknown mitigation potential, low – less than 10 %, medium – up to 50 %, high – up to 100 %

Category	Measure	Carbon dioxide-related mitigation potential
Technology *engine*	Geared-turbofan	**Medium**
	Lean-burn combustion chamber	**Low**
	Counter-rotating open rotor	**Medium**
Technology *airframe*	Advanced wing design	**Low**
	Structures with reduced specific weight	**Low**
	Blended-wing body design	**Medium**

In the field of airframe modifications, options to reduce aerodynamic drag are estimated to lower fuel consumption (and thus carbon dioxide climate forcing) by about 3 % compared to present designs [306]. Reducing weight is expected to lower fuel consumption by about 2 % against conventional materials [306]. A blended-wing-body is assumed to lower fuel consumption by around 30 % compared to a conventional design [307].

Clearly, most of these technology-related measures only allow for low carbon dioxide-related mitigation potentials (i.e., less than 10 %). A geared-turbofan, a counter-rotating open rotor and a blended wing body design are expected to yield higher mitigation potentials but also require by far greater modifications within the respective components as well as within the overall aircraft system. Bearing the historic and projected future growth rates of the air transport system in mind, it seems unlikely that these measures can substantially reduce aviation's carbon dioxide emissions in absolute terms.

Such technology-related measures reduce the specific energy consumption being the energy required for a certain "air transport service" (e.g., carrying a certain amount of payload over a specified distance). However, regardless of the extent to which any technology reaches towards its thermodynamic optimum, a certain amount of energy will always be required to provide the respective air transport service. If this is to be achieved in line with the global climate mitigation targets, alternatives to the current use of fossil fuel-based energy carrier should be adopted as quickly as possible.

None of the technology-related options provides an alternative towards the current use of fossil fuel-based energy carrier. Alternative aviation fuels from renewably sourced energy constitute such an alternative and thus also allow for far larger carbon dioxide-related climate forcing mitigation potentials of up to 100 %. For this reason, they appear indispensable for the mitigation of aviation's carbon dioxide-related climate forcing. Reducing the (specific) energy requirements of the air transport system can facilitate the replacement of conventional kerosene by renewably sourced kerosene since it also reduces their required amount.

3.4.3 Contrail-related Mitigation Potentials

Besides the carbon dioxide-related mitigation potential discussed above, now the contrail-related mitigation potentials of the different provision pathways for alternative aviation fuels are discussed (section 3.4.3.1).

These fuel-related mitigation potentials are compared against the mitigation potentials of the other, technological climate forcing mitigation measures (section 3.4.3.2).

3.4.3.1 Synthesis

Altering the properties of conventional kerosene, namely reducing its content of aromatic components, results in substantial contrail-related climate benefits. Using mildly hydroprocessed kerosene (reducing the content of aromatic components to about 8 %) is found to lower the contrail energy forcing by about 18 %, with a carbon dioxide-related climate penalty of a few %-points (Figure 3.2). Such a kerosene treated with hydrogen could still be compliant with the currently valid fuel specifications (section 3.1.3.2.2). Harsh hydroprocessing conditions, i.e., transforming almost all aromatic compounds into alkanes, could reduce about 38 % of the contrail energy forcing at a carbon dioxide-related climate penalty of about 5 %-points (Figure 3.2). Using hydrogen from renewable sources of energy with hardly any lifecycle carbon dioxide emissions could mitigate the carbon dioxide climate penalty and thus slightly increase the mitigation potential of such a hydroprocessed kerosene [266]. Overall, the main influential factor on contrail-related climate forcing in this case is the hydroprocessing intensity (i.e., to which extent the content of aromatic components is reduced / the hydrogen content is increased compared to the use of conventional kerosene, cf. section 3.1.3.3).

Renewably sourced kerosene can also lower contrail-related climate forcing. Since it typically contains less aromatic components compared to conventional kerosene, fewer soot precursors are formed during combustion subsequently resulting in a reduced contrail optical thickness and lifetime, which both reduce the magnitude of a contrail's climate forcing. For drop-in kerosene (i.e., blends of up to 50 % neat paraffinic kerosene and conventional kerosene) this potential is limited by the minimum content of aromatic components required by the currently valid fuel specifications (chapter 3.2.4.4 [280]). Assuming a hydrogen content of 14.4 m-% for the blend, the contrail energy forcing could be reduced by about 20 %, based on the assumptions outlined in section 3.1. If neat, renewably sourced kerosene could be used, the mitigation potential would further increase to more than 40 % (section 3.1.3.1). In this case, the blend ratio of renewably

sourced and conventional kerosene is the main influential factor for the reduction of contrail-related climate forcing.

For the alcohols and gases studied, hardly any data are available on the relationship between soot formation and contrail evolution from jet engine exhausts. First flight measurement campaigns for a hydrogen jet engine are currently ongoing [133]. Hence, the impact of using the alcohols or gases studied here directly in a jet engine are highly uncertain. Beyond this, the introduction of these technologies will rather take place in the long-term (if at all) and thus not significantly affect aviation's climate forcing until 2050.

3.4.3.2 Discussion

The contrail-related mitigation potentials of the technological climate forcing mitigation measures are summarized in Table 3.20 and subsequently their main influencing factors on contrail-related climate forcing are described compared against the main influencing factors of alternative fuels.

Table 3.20 Exemplary technological mitigation measures and their contrail-related climate forcing mitigation potential (based on the assumption that the respective measure is fully adopted); ?: unknown mitigation potential, low – less than 10 %, medium – 50 %, high – 100 %

Category	Measure	Contrail-related mitigation potential
Technology *engine*	Geared-turbofan	**Low**
	Lean-burn combustion chamber	**?**
	Counter-rotating open rotor	**?**
Technology *airframe*	Advanced wing design	**Low**
	Structures with reduced specific weight	**Low**
	Blended-wing body design	**?**
Operations and Infrastructure	Flight route modifications for contrail avoidance	**High**
	More efficient flight operations (continuous descent, direct routing, single-engine taxi)	**Low**
	Airspace harmonization	**Low**

A geared-turbofan mainly reduces specific fuel consumption by increasing its overall efficiency [31]. Since a higher propulsive efficiency of an aircraft increases contrail formation probability [11, 12, 308], it appears unlikely that this technology yields any noteworthy reductions in contrail-related

climate forcing. Engines equipped with lean burn combustion chambers lower nitrogen oxide emissions and they also reduce soot particle emission numbers by several orders of magnitude compared to the current "Rich-Quench-Lean" combustor types [10, 172, 191]. However, the ice nucleation behavior for contrail formation of engines with lean-burn combustors is not yet well understood [8, 21] and thus the resulting contrail-related climate forcing is highly uncertain. For counter-rotating open rotor engine designs, no data are available for contrail-related climate impacts. Possibly, similar to the geared-turbofan, their higher efficiency increases contrail formation probability [11, 12, 130, 308].

In terms of airframe technology and weight reductions, all options discussed here achieve their emission reductions by improving an aircraft's propulsive efficiency. As a result, an increased contrail formation probability appears likely [11, 12, 130, 308]. To which extent this affects the overall contrail-related climate forcing has not yet been investigated in detail [130].

Among the options discussed above, the technological measures increasing the propulsive efficiency of an aircraft are likely to increase contrail-formation probability and thus could potentially even cause an increase in contrail-related climate forcing. The impact of lean-burn combustors on contrail-related climate forcing is not yet scientifically well understood. Both, a lean-burn combustor and the use of paraffinic kerosene significantly affect soot particle emissions. An in-depth understanding of the associated ice nucleation behavior and the related contrail climate forcing of a lean-burn combustor might potentially indicate further technological options for engine modifications to lower contrail-related climate forcing.

3.4.4 Overall Synthesis

Figure 3.18 shows a comparison of the different measures in terms of carbon dioxide- and contrail-related climate forcing. Replacing conventional, i.e., fossil fuel-based, kerosene by fuels from renewable sources of energy can mitigate the entire carbon dioxide-related climate forcing of aviation. Renewably sourced drop-in (i.e., kerosene-like) aviation fuels appear particularly promising among aviation fuels from renewable sources of energy, since they can be used without infrastructure / aircraft modifications.

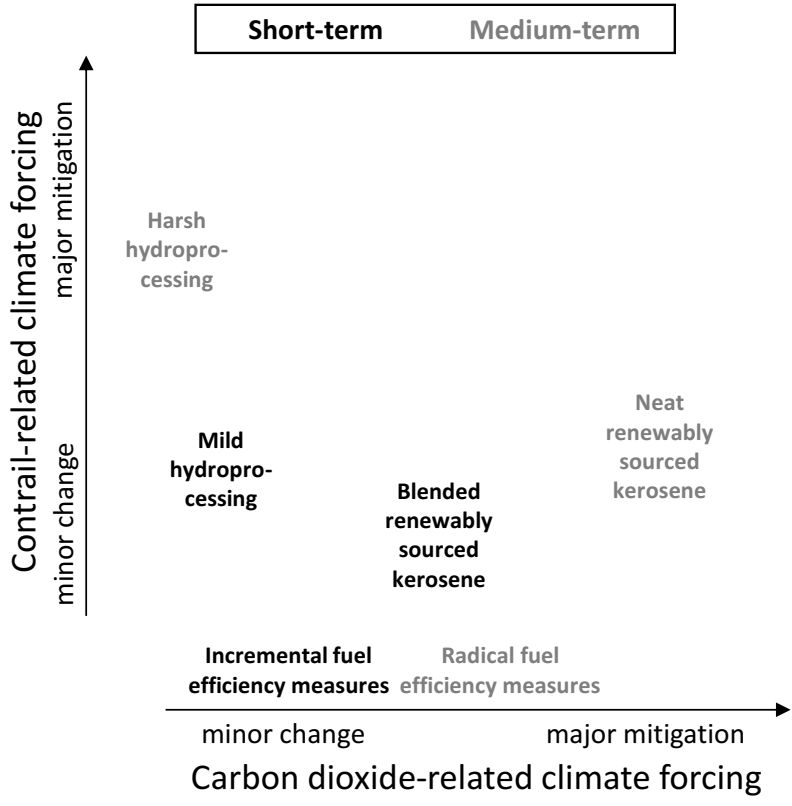


Figure 3.18 Carbon dioxide- and contrail-related mitigation potentials of the fuel-related and other mitigation measures discussed in this section; incremental fuel efficiency measures: geared-turbofan, lean-burn combustor, advanced wing design, reduced structural weight; radical fuel efficiency measures: counter-rotating open rotor, blended wing-body

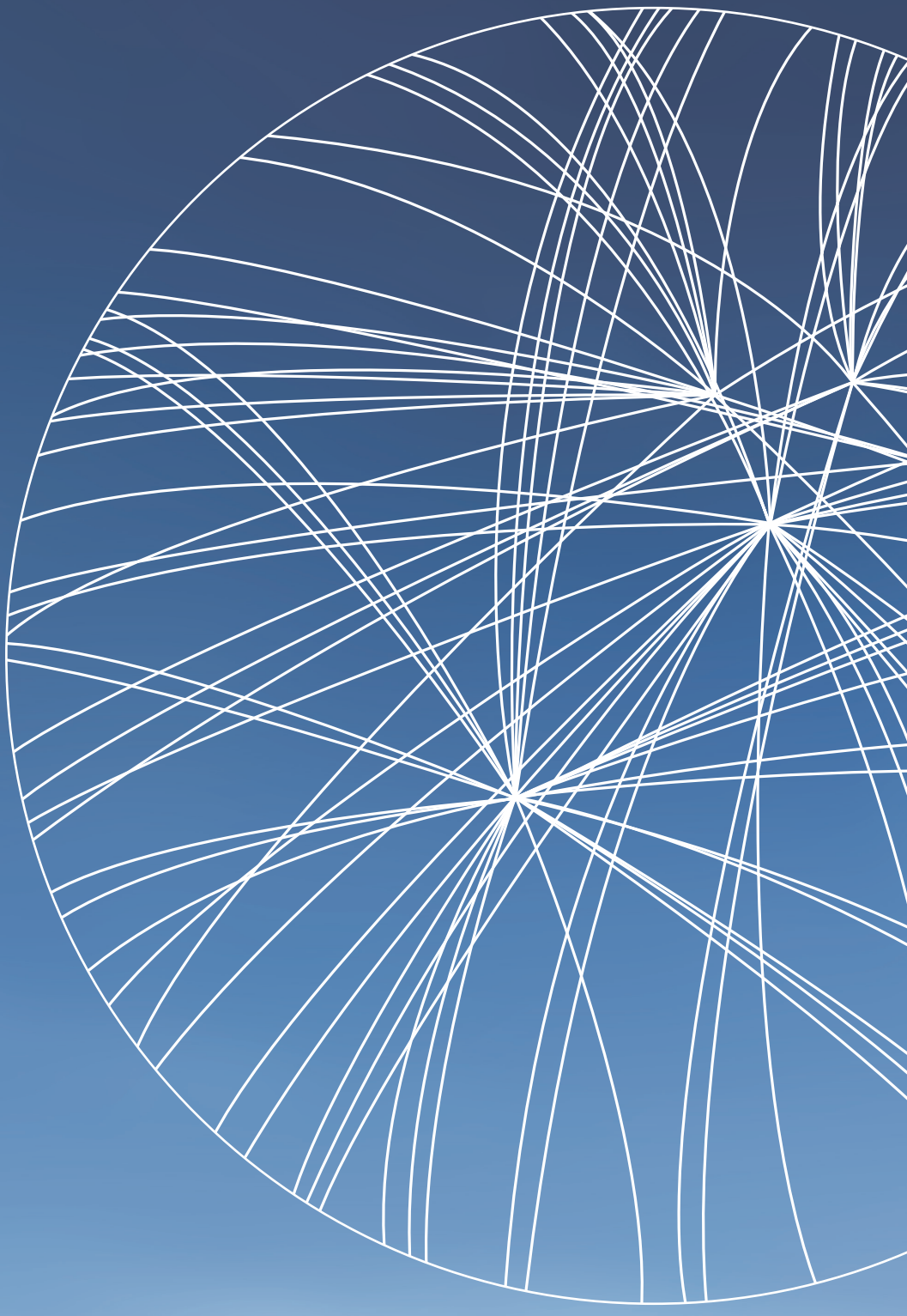
In the short-term, such a renewably sourced kerosene will most likely be used as a blend component within conventional kerosene, while in the medium-term their neat use could be approved in order to allow for a complete replacement of the currently used conventional kerosene. Incremental fuel efficiency measures are available in the short-term and more radical fuel efficiency measures are rather available in the medium-term. As long as the global commercial air transport system continues to grow, its growth rates extenuate such emission reductions.

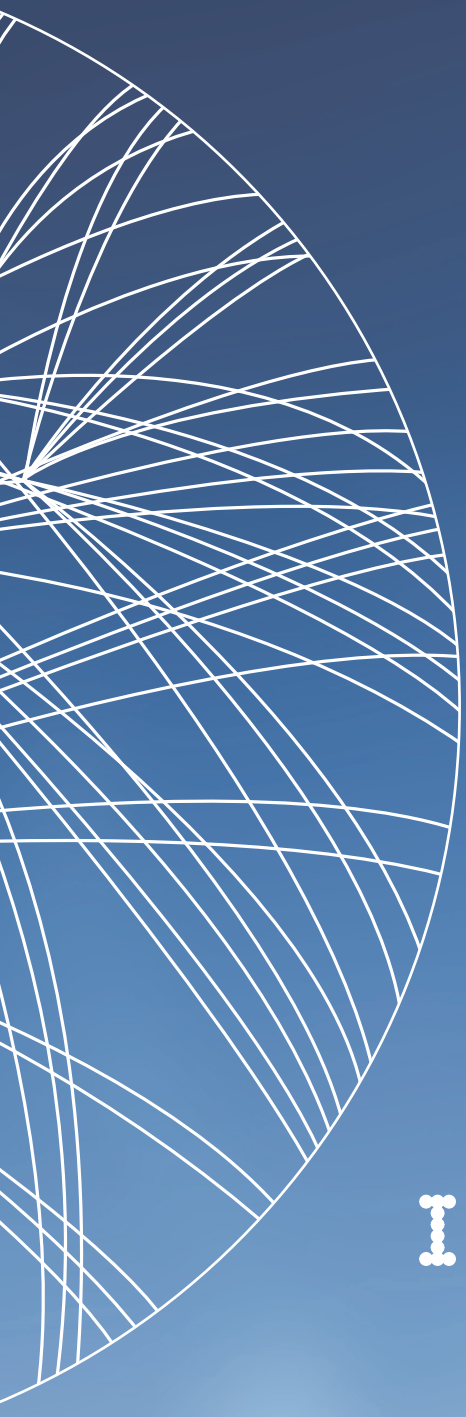
In terms of contrail-related climate forcing, mild hydroprocessing appears as viable option in the short-term, while harsh hydroprocessing would rather be available in the medium-term. None of the technological measures discussed here yields significant potentials to mitigate contrail-related climate forcing.

Most fuel efficiency measures (e.g., counter-rotating open rotor engine, blended wing body design) improve the overall propulsive efficiency and thus potentially increase the probability of contrail formation and presumably also the associated climate forcing [11, 12, 130, 308]. However, the contrail-related climate forcing of such radical design changes and also of engines equipped with a lean-burn combustor, are not yet thoroughly investigated and thus only understood to a certain extend [130].

Especially for the lean-burn combustor it cannot be ruled out that different environmental objectives are subject to trade-offs. For example, such a measure might reduce climate forcing from nitrogen oxide emissions, but simultaneously increase contrail-related climate forcing [309].

The use of paraffinic kerosene appears promising to mitigate contrail-related climate forcing. It can be provided from additional hydroprocessing of conventional kerosene (section 3.1) or by using kerosene from renewable energy sources (section 3.2 and section 3.3). Hydroprocessing of conventional kerosene could allow for the provision of larger shares of paraffinic kerosene in the short-term, while the market shares of renewably sourced kerosene are still low.





4

SYSTEM INTEGRATION

4 System Integration

The system integration of the aforementioned fuel provision options is examined based on a simulation study (section 4.1) and the demonstration of a segregated supply of low-contrail kerosene (section 4.2). Implications for blending powerfuels are discussed (section 4.3) and the dynamics of the air transport system are studied (section 4.4). Again, this chapter closes by summarizing implications for climate forcing and system integration of the different system integration strategies (section 4.5).

4.1 Targeted Use of Paraffinic Kerosene: Potentials and Implications

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Typesetting and formatting are slightly adjusted to ensure consistency within this thesis.

Abstract

Aviation contributes to anthropogenic climate change mainly by contrails, CO_2 and NO_x emissions, whereof contrails are considered the largest single contributor to the radiative forcing from aviation. Powering aircraft with kerosene containing fewer or no-aromatics, i.e., "Sustainable Aviation Fuels" (SAF) or hydroprocessed, fossil-based kerosene, can significantly reduce contrail climate forcing. However, such kerosene is currently scarcely available. Moreover, less than 10 % of the flights worldwide cause more than 80 % of the contrail climate forcing. Hence, this study investigates a targeted allocation of paraffinic i.e., aromatics-free kerosene to flights and flight segments with the highest contrail climate forcing, by calculating the resulting contrail energy forcing (in J) on 844 364 flight trajectories worldwide departing from five large European airports in 2019. The contrail radiative forcing integrated over contrail evolution (i.e., contrail energy forcing [J]) is simulated for a reference fleet powered with conventional kerosene of 14.1 m - % hydrogen content. 5 % of overall kerosene demand assumed to be paraffinic kerosene with 15.3 m - % hydrogen content is allocated via a uniform, a flight-specific and a segment-specific approach. The uniform allocation assumes that all flights receive the same blend of 5 % paraffinic kerosene. The other cases target 100 % paraffinic kerosene either to flights or segments with highest contrail energy forcing. Compared to the reference, the results indicate a reduction on contrail energy forcing by 4 %, 36 % and 55 %, respectively. For market shares of paraffinic kerosene up to 30 %, a segment-specific allocation appears advantageous compared to a flight-specific allocation. However, they might require airport and aircraft modifications. Uncertainties in contrail climate benefits can be reduced by providing additional information on kerosene properties and accurate meteorological data. Overall, this study highlights robust potentials of paraffinic kerosene to significantly reduce the climate forcing from aviation.

4.1.1 Introduction

The air transport sector contributes with 3.5 to 4 % to global anthropogenic climate forcing [5]. The release of greenhouse gases (GHG), mainly CO_2, and several other emission effects ("non-CO_2" effects) are the primary causes of air transport's climate impact. While CO_2 presently accounts for roughly one third of aviation's effective radiative forcing (ERF) [5, 159], the other two thirds are comprised of contrail effects, indirect effects of NO_x emissions, and direct and indirect aerosol effects (in decreasing order of magnitude) [5]. The effective radiative forcing (ERF) of contrails has been estimated as 58 mW per m^2 (variation: 17 to 98 mW per m^2) corresponding to about 57 % of the overall aviation-related ERF until 2018 [5, 159].

Historic air traffic volume growth rates have been around 3 to 4 % per year. After a disruption by the COVID-19 pandemic [129, 310], growth rates currently return to pre-pandemic levels [311, 312]. Simultaneously, passenger / freight-specific fuel consumption has been reduced by about 1.3 % per year due to numerous technical and organisational measures [156]. Thus, as long as growth rates remain higher than fuel efficiency improvements, aviation kerosene consumption on a global scale and as a result also the climate impact of air transport will increase. Based on these assumptions, it is expected that the global air transport system's CO_2 emissions might more than double within the next 20 years to values clearly above 2 Gt of CO_2 in the year 2050 [156]. Since non-CO_2 effects are an indirect result of fuel combustion, it is also most likely that they also increase in the future; however, it is expected that they increase slightly slower due to the different lifetimes of both effects [156]. Accordingly, an effective reduction of both, CO_2 and non-CO_2 effects, is required to swiftly reduce the overall climate impact of the global air transport sector.

The use of kerosene with a reduced aromatics content may provide an option to lower the climate impacts of contrail formation [10, 17, 20, 28, 86]. However, such fuels are currently available at small volumes [32]. Bearing in mind that a few (2 to 10 %) of all flights account for the majority of the contrail energy forcing [9, 29, 177, 186, 313, 314], it seems promising to allocate currently small amounts of such kerosene to the flights or segments producing those contrails. Thus, this study aims to analyze the targeted use of paraffinic kerosene. Paraffins are saturated, acyclic hydrocarbons [315]

and therefore paraffinic kerosene refers to kerosene free of aromatics and cycloalkanes.

Four different allocation cases are investigated; i.e., the contrail climate forcing of allocating a given market share of paraffinic kerosene uniformly, for individual flights and for segments of flights is compared to a base case where only conventional kerosene is used. Flight trajectories of departing flights from the years 2017 to 2019 of the five largest European airports (by passenger number) are considered.

Contrails form when water vapor emitted by fuel combustion condensates on aerosol particles and subsequently freezes into ice crystals due to the low temperatures at typical flight levels. Depending on temperature and humidity of the surrounding atmosphere, contrails can be short lived, but in ice supersaturated air they can also persist for several hours [24, 25]. Persistent contrails can spread over large areas, potentially lose their linear shape and develop into so-called contrail cirrus [25, 26]. Finally, the ice crystals of the contrail (cirrus) sublimate, e.g., caused by sedimentation into warmer and dryer air masses / atmospheric layers.

Aerosol particles originate from the combustion of kerosene and from the surrounding air [8, 10, 131]. Aircraft engines with differing combustor designs, e.g., shifting from presently used "Rich-Quench-Lean" (RQL) combustion chambers to "Twin Annular Premixing Swirler" (TAPS) lean burn combustors can reduce soot particle emission numbers by several orders of magnitude [10, 172, 191]. The majority of engines presently used in commercial aviation typically operate in the so-called soot-rich regime (10^{14} to 10^{16} particles per kg_{fuel}), while a few new engines equipped with lean-burn combustors emit substantially fewer particles ("soot-poor" regime, $<10^{13}$ particles per kg_{fuel}). In the soot-rich regime, ice nucleation on soot particles from fuel combustion is the dominant process, while for the soot-poor regime, ice nucleation on volatile particles emitted by the engine or on aerosols of the ambient air become the dominant cause for ice nucleation [8].

The use of aviation kerosene with a reduced sooting tendency could also reduce particle emission numbers. The use of neat renewably-sourced kerosene has been found to reduce soot particle emission numbers by up to 60 % compared against neat conventional kerosene [18, 131]. Soot forming aviation kerosene components are poly- and mono-cyclic aromatics, cyclo-,

iso- and n-alkanes (by decreasing order of magnitude) [15, 18]. The hydrogen content of these components decreases in the same order. Therefore, the average hydrogen content of a kerosene is often used as proxy for its sooting tendency [10, 18, 131, 281]. Additionally, the fuel sulfur content is another cause for soot particle activation [17, 131, 194–197]. Fuel lubricant oil is considered a further source of contrail-ice nucleation [316]. For modern jet turbines with soot emissions in the low-soot regime, these effects might gain importance for contrail formation [131]. In addition to using neat renewably-sourced kerosene as paraffinic kerosene, hydroprocessing of crude oil-based kerosene allows to (partially) transform aromatic components to alkanes. This provides a technical option to adjust the composition of kerosene to reduce the sooting tendency of fossil-based kerosene.

Reducing soot emission numbers leads to the formation of fewer but larger initial ice crystals [17]. Due to the reduced particle number, the optical thickness and thus the resulting contrail climate forcing is reduced [10, 23, 28, 164]. Due to the increased ice crystal weight, ice crystals sediment faster into warmer and / or drier air layers [8]. This results in faster sublimation, a shorter contrail lifetime, and hence also a reduced climate forcing [10, 23, 28, 164].

The climate impact of contrails is distributed strongly heterogeneously among flights; about 3 % of all flights globally within a year (or 11 % of the contrail-forming flights) accounted for 80 % of the global contrail energy forcing in 2019 [9]. While the net climate impact of contrails is positive (i.e., warming), the climate impact of individual contrails varies by several orders of magnitude. During the night contrails have a warming climate impact, but during the day contrails can also have a cooling impact due to the reflection of solar radiation and less solar energy input at the surface. [9, 26, 317]

More than 99 % of the global kerosene supply is presently produced from fossil fuel sources (i.e., crude oil). Roughly 310 Mt per year of such conventional kerosene are consumed. Compared to that, the production volumes of renewably sourced kerosene[13] are estimated at around 200 kt per year, i.e. more than three orders of magnitude smaller compared to conventional kerosene [167, 168]. Most studies indicate significant market shares

[13] Colloquially, such fuels are often referred to as "Sustainable Aviation Fuel" (SAF). However, this term is not used here, because renewable origin does not guarantee compliance with other sustainability aspects (e.g., biodiversity or social criteria).

of renewably sourced kerosene (>10 %) not before 2030 [125, 144, 169]. Simultaneously, hydroprocessing of conventional kerosene to increase the content of acyclic alkanes (i.e. paraffins) is technically possible but not realized on a large scale. In this study, 5 % of overall kerosene demand are assumed to be available as paraffinic kerosene at all airports considered.

This work adds to the previous analysis by Teoh et al. by additionally evaluating a segment-specific allocation [10]. The study by Woeldgen et al. focusses on allocation strategies which avoid large infrastructure modifications, e.g., by allocating kerosene based on season or time of the day [134]. The allocation cases in this study would require infrastructure and in the case of the segment-specific allocation even aircraft modifications. Thus, both studies complement each other indicating a broad range of options for the targeted use of paraffinic kerosene.

The remainder of this study is structured as follows: Section 4.1.2 details methods and data used for both fuel options, their allocation cases and the contrail cirrus prediction (CoCiP) model to estimate the different climate impacts. In section 4.1.3, the climate impact reduction potential is analyzed and discussed for increasing market shares of paraffinic kerosene, changes in the weather data used for fuel allocation and influential factors for a flight's contrail climate forcing. Finally, the results are summarized and discussed.

4.1.2 Methods and Data

This study evaluates the targeted use of paraffinic kerosene via different allocation strategies (Figure 4.1). The main criterion for the assessment is the relative change in contrail energy forcing compared to the exclusive use of conventional kerosene ("base case"). The contrail energy forcing is chosen as a metric to assess the climate impacts of each allocation case [10, 177]. It is defined as the amount of energy added to the earth-atmosphere system, calculated as the instantaneous radiative forcing of contrails integrated over their individual lifetime (section 4.1.2.1.2). The different cases are simulated using the Contrail Cirrus Prediction model (CoCiP) [185].

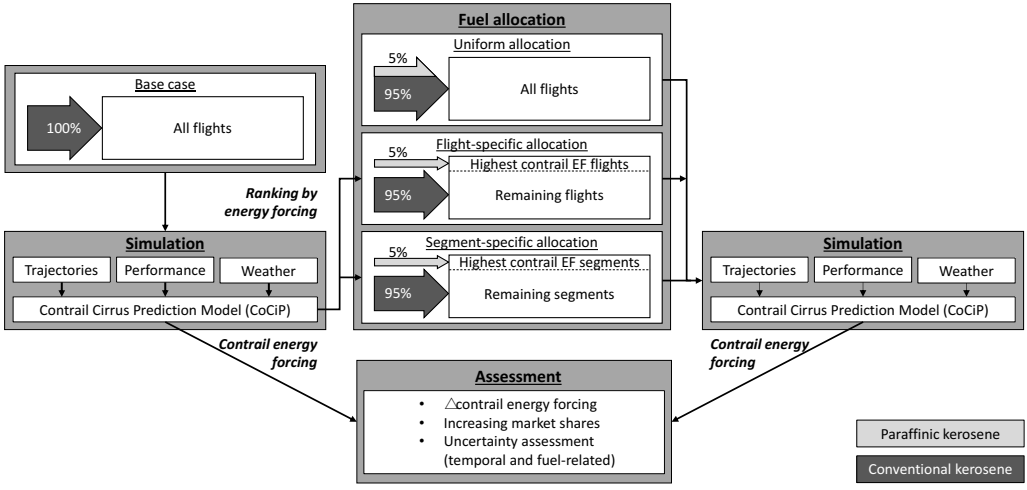


Figure 4.1 Methodological approach: For each of the allocation cases (uniform allocation, flight-specific allocation, segment-specific allocation) the contrail energy forcing is calculated and its relative change compared to the base case is used for the assessments (EF energy forcing)

4.1.2.1 Methods

4.1.2.1.1 Allocation Cases

Paraffinic kerosene is allocated in three different ways being

- a uniform,
- a flight-specific and
- a segment-specific

allocation case. Fuel allocation is based on the results of a base case simulation, assuming the exclusive use of conventional kerosene. The amount of paraffinic kerosene available equals the fuel consumption of the flights in the dataset multiplied by an assumed market share of 5 %, corresponding to about 200 kt for the entire year 2019 and the flights selected (cf. 4.1.2.2.1).

The **base case** constitutes of an initial simulation where only conventional kerosene is used. The resulting contrail energy forcing is used as reference for the mitigation potentials of each allocation cases. The results from this simulation are used to derive the ranking of flights and segments for the flight and segment-specific allocation cases.

The **uniform allocation** case distributes the paraffinic kerosene uniformly among all flights considered. It corresponds to a situation, where

each flight receives a conventional / paraffinic kerosene blend with a blend share of 5 %.

The **flight-specific allocation** distributes the paraffinic kerosene available on a flight by flight basis. Individual flights are prioritized on a daily basis by their overall contrail energy forcing; the flight with the highest overall contrail energy forcing receives paraffinic kerosene first until the remaining paraffinic kerosene is insufficient to cover the fuel consumption of the next flight. The remaining paraffinic kerosene is discarded from the analysis. In reality, this remainder would rather be blended with conventional kerosene to fuel the remaining flight(s) or added to the next day's paraffinic kerosene volume. However, discarded amount is small (on average < 1.7 % of all paraffinic kerosene) and thus the error induced by omitting these options is negligibly small compared to other uncertainties (cf. 4.1.3.1.3.).

Currently, large international airports typically supply fuel from their fuel storage towards individual aircraft via a pressurized hydrant system. Special vehicles provide a tube connection between the underground hydrant system at the aircraft's parking position and the aircraft tank inlets. Typically, the system's main pipeline constitutes a closed loop around the terminal, allowing to circulate the fuel within the system to prevent fuel degradation due to aging [278]. Such a circular system impedes the targeted supply of various fuel types to specific aircraft. Accordingly, targeting a certain share of flights with paraffinic kerosene would require additional infrastructure to store and supply two different fuel types.

For the **segment-specific** allocation, flight trajectories are split into segments of three categories, namely segments causing warming contrails, segments without contrail formation and segments causing cooling contrails. Segments are prioritized based on their contrail energy forcing. Since typically only a fraction of each flight causes a contrail, for the segment-specific allocation less paraffinic kerosene is required to provide fuel for all warming contrails than in the flight-specific allocation.

In this case, a real-world application would not only require additional infrastructure at airports, but also aircraft modifications. These could be the addition of a monitoring system for contrail formation and a control system for in-flight fuel switching, among others. Despite the fact that most commercial aircraft have several fuel tanks and a switching between different tanks during a flight has been demonstrated in flight experiments [17, 131],

it is not yet clear to which extent this can be realized during regular airline operations [169].

4.1.2.1.2 Contrail Cirrus Prediction (CoCiP) Model

The contrail climate forcing of all flights and segments in the dataset is estimated using the contrail cirrus prediction model (CoCiP) [185, 318]. The life cycle of contrail segments formed along individual flight trajectories is simulated and used to estimate the resulting contrail radiative and energy forcing [164]. Since CoCiP is well documented [9, 10, 164, 177, 185, 186], only the basic principles and the particularities of this study are outlined below.

When consecutive waypoints meet conditions for contrail formation, i.e., the Schmidt-Appleman criterion [11, 164, 308], contrail formation is assumed in CoCiP. The soot emissions number of the respective engine-airplane combination determines the initial number of formed ice crystals within the contrail. However, a lower limit of 10^{13} particles per kg_{fuel} is introduced to consider ambient aerosols and organic particles as ice nuclei [8]. Additionally, the ambient temperature affects the initial number of ice crystals, as well as the soot activation rate [16] and the fraction of ice particles which survive the wake vortex phase [164]. The simulations do not account for changes in fuel sulfur content. However, a decreasing fuel sulfur content could potentially lower the ice nucleation efficiency of soot particles [17, 131, 194–197].

Contrail segments enduring the wake vortex phase are simulated in the model using time steps of 30 min until they reach their end-of-life conditions; i.e., the contrail ice crystal number decreases below the background ice nuclei concentration ($<10^3$ m^{-3}), the contrail's optical depth $\tau_{contrail}$ is less than 10^{-6}, or the lifetime surpasses a maximum of 24 h [164]. The CoCiP model calculates the local instantaneous contrail radiative forcing (RF′) for each waypoint representing the change in radiative flux over the contrail area [10]. The contrail energy forcing is calculated as the product of the contrail segment RF′, length, and width integrated over the contrail segment's lifetime [14, 177, 186]. The default settings of the CoCiP model are applied with two exceptions. On the one hand, the humidity data of the ECMWF reanalysis 5 (ERA5) data scaling to in-situ measurements [317] is performed using the "exponential boost with latitude scaling" method [9] (cf. Appendix C). On the other, radiative heating effects, i.e., the influence of radiative

heating on the contrail plume and thus contrail lifetime are taken into account [9]. A comparison of this CoCiP configuration with previous studies can be found in the Supporting Info of Quante et al. (2024) [281].

4.1.2.1.3 Assessment

First, the contrail energy forcing for each allocation case is compared to the base case, where no paraffinic kerosene is used. Then, increasing market shares of paraffinic kerosene are studied and the temporal and fuel-related sensitivity is assessed.

The European Union (EU) recently introduced a blending mandate for renewably sourced kerosene [205], requiring kerosene suppliers to supply e.g., 6 % renewably sourced kerosene in the year 2030, 20 % in the year 2035 and 34 % in the year 2040. Hence, increasing market shares are investigated in the first sensitivity study. For the uniform allocation, a paraffinic kerosene market share of 5 % is assumed, which roughly matches the European Union's (EU) blending quota of 6 % by the year 2030 [319]. To study the effects of increasing market shares of paraffinic kerosene, assumed market shares are gradually increased between 1 and 100 %. To reduce computation time, the simulations are performed for each third day in 2019, starting January 1st.

Second, the temporal variability of the base case's contrail energy forcing is studied. In addition to the year 2019, simulations are also performed for the years 2017 and 2018. The results are used to compare the day-to-day variability of the contrail energy forcing and also the variability of the annual mean energy forcing for different years. Additionally, the mitigation potentials for each allocation case and year are discussed.

Uncertainties by fuel composition are assessed in another sensitivity study. Because only few data on the hydrogen content of conventional kerosene are publicly available, the fuel properties assumed in the main study may be different from the fuel being used at the airports studied. Thus, three different hydrogen contents corresponding to the mean and the single standard deviation of publicly available datasets (13.9 m-%, 14.1 m-% and 14.3 m-%) [135, 179, 180] are used for the simulations. Again, each third day in the year 2019 is considered to reduce computation time, starting January 1st.

4.1.2.2 Data

4.1.2.2.1 Fuel

The composition of **conventional kerosene** might vary depending on the crude oil's respective reservoir and refinery operations. The components typically contained in conventional kerosene, e.g., paraffins or aromatics differ by hydrogen content. Thus, the hydrogen content of conventional and paraffinic kerosene are used as proxies for the detailed fuel composition. The potential impact of fuel sulfur on emissions and contrails is not considered due to the lack of data [10, 131]. For conventional kerosene, the hydrogen content is distributed around a mean hydrogen content of 14.1 m-% with a standard deviation σ = 0.2 m-%-points and based on a sample size of n = 57 [135, 179, 180]. Most of the analyzed samples originate from Europe and North America, where a large fraction of aviation kerosene is consumed [179]. Against the large volumes of conventional kerosene in use, this sample size is rather small. However, as of now no larger fuel sample is publicly available.

The properties of **renewably sourced kerosene** are derived from the US Federal Aviation Administration's (FAA) National Alternative Jet Fuels Test Database [138, 320] including about 400 alternative fuels / fuel blends from which 21 samples of neat, renewably sourced kerosene options were selected. Only samples for which the hydrogen content was determined by ASTM D7171 or inferred from GC × GC measurements were selected here; other testing methods were excluded due to the expected measurement uncertainty [86].

The selected samples have a mean of about 15.3 m-% (σ = 0.1 m-%-points, n = 21) and the distribution is shown in Figure 4.2. Other fuel properties, e.g., heating value and water emissions, are adopted using a linear relationship with increasing aviation kerosene hydrogen content [10].

Typical soot precursors (e.g., aromatics) can also be reduced / removed from conventional kerosene, e.g., by hydroprocessing or extractive distillation [83]. So far, it is uncertain how much technological efforts are needed to provide a purely paraffinic kerosene with a similar hydrogen content as renewably sourced kerosene. For this study, the hydrogen content of neat renewably sourced kerosene (15.3 m-%) is assumed for the paraffinic kerosene. Note that this implies the use of unblended, almost aromatics free

kerosene which is not compliant with current kerosene specifications [280]. Thus, it rather indicates the theoretical maximum potential of a targeted use concept.

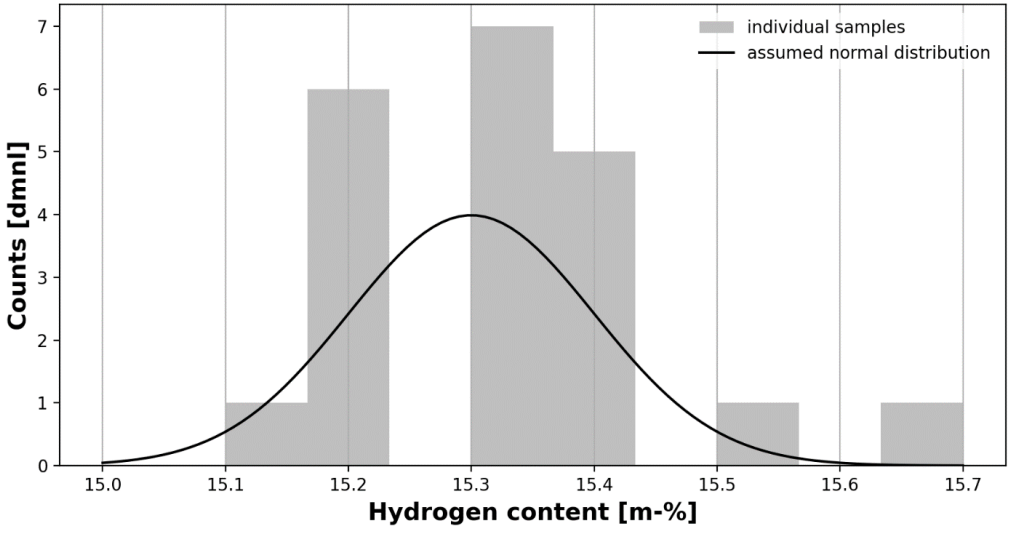


Figure 4.2 Frequency distribution (grey bars) and assumed density function (black line) for the hydrogen content of neat, renewably sourced kerosene (data source [138, 320]), the abscissa shows the frequency and the ordinate the associated hydrogen content

4.1.2.2.2 Flight Trajectories

The simulations cover 844 364 departing flights from the five largest European airports by passenger numbers [187] (i.e., London-Heathrow, Paris Charles-de-Gaulle, Amsterdam Schiphol, Frankfurt International, Madrid-Barajas) during the year 2019. In the base case, their fuel burn is estimated at about 3 908 t (about 1.4 % of the global fuel burn [9]) and their contrail energy forcing amounts to about 1.47×10^{19} J (about 1.5 % of the global contrail energy forcing [9]). To study the interannual variability of meteorological conditions and traffic volume fluctuations, the years 2017 and 2018 are compared against the results for 2019. Flight trajectories are provided from the OpenSky Automatic Dependent Surveillance Broadcast (ADS-B) database [188] (cf. Figure 4.3, Appendix C).

As shown by Figure 4.3, the focus on European airports results in a higher flight density above Europe and the North Atlantic compared to other regions, e.g., Southeast Asia. Therefore, the meteorological conditions above Europe and the North Atlantic play an important role for the overall results. Due to the strong temporary effect of the COVID-19 pandemic [129],

the years after 2019 are not considered. The use of ex-post data reduces influences of potential future developments, such as the use of less soot emitting engines or different air traffic growth scenarios.

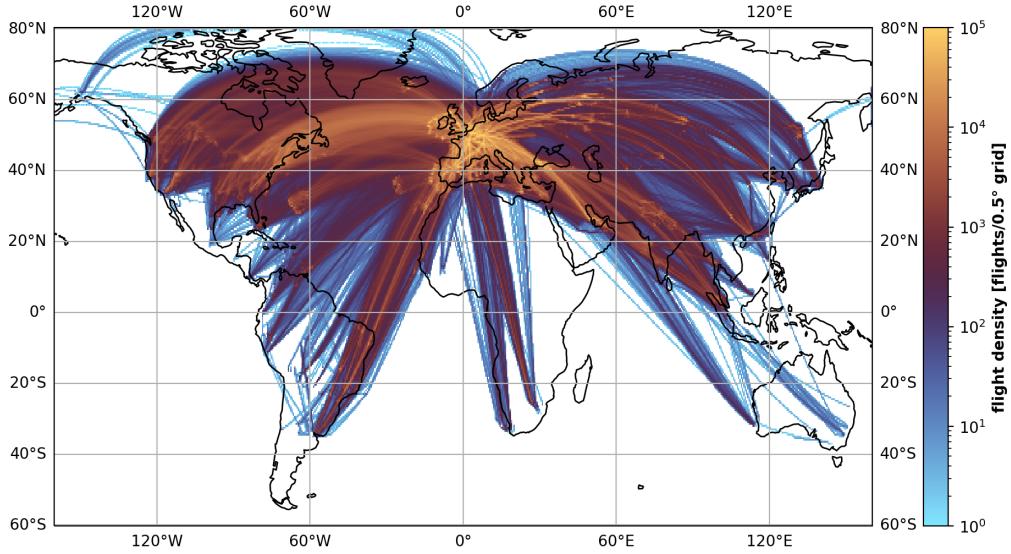


Figure 4.3 Number of flights per 0.5° × 0.5° latitude / longitude grid cell for the year 2019, note the logarithmic scaling of the colorbar. Basemap plotted using Cartopy 0.21.1 © Natural Earth; license: public domain.

4.1.2.2.3 Performance

The performance data used to simulate aviation kerosene consumption and emissions of each flight is calculated using the Eurocontrol Base of Aircraft Data (BADA) version 3.15 [190]. This data base covers 1409 aircraft types, of which 250 aircraft types are directly supported and the remaining aircraft types are matched with a directly supported aircraft type considered to be equivalent [190]. The assignment of engine types to specific aircraft is also based on BADA, which assumes a "typical" engine model for a specific aircraft. In reality, however, most aircraft can be equipped with different engine models (e.g., the CFM56-5 or the IAE V2500 engine for the A320 aircraft). In case the emissions of both engine models differ significantly, the use of a "typical" engine model by BADA incurs a bias for e.g., soot or NO_x emissions. A recent study on global contrail climate effects finds an increase of 18 % in contrail radiative forcing for a BADA-based aircraft-engine assignment compared with an assignment on the individual aircraft level from

commercially available data [9]. For this study, the bias would primarily affect the absolute values of the contrail energy forcing estimates, but to a lower degree the relative mitigation potentials where identical aircraft fleet are compared against each other.

4.1.2.2.4 Weather Data

Weather data are used from the European Centre for Medium-Range Weather Forecast fifth generation high-resolution reanalysis (ECWMF ERA5) [192] (0.25° × 0.25° horizontal resolution for 37 pressure levels and at a temporal resolution of 1 h). Meteorological conditions for flights between those pressure levels are interpolated from the two nearest pressure levels [317]. The ERA5 humidity fields are adjusted to in-situ observations using the so-called method of exponential scaling with latitude correction [9] (cf. Appendix C). This dataset is an ex-post analysis and as such it would not be available for flight planning purposes.

4.1.3 Results and Discussion

4.1.3.1 Results

4.1.3.1.1 Allocation Cases

Figure 4.4 shows the change in median contrail energy forcing for all allocation cases and the years 2017, 2018 and 2019 compared the base case, which assumes conventional kerosene only.

A uniform allocation reduces median contrail energy forcing by less than 5 %, while a flight- and segment-specific allocation would reduce median contrail energy forcing by about 36 % and 55 % respectively. The variation among the three years evaluated is clearly smaller compared to the differences among the allocation cases.

Figure 4.5 shows the simulation results in the year 2019 on a daily basis for the base case and each of the allocation strategies. Each data point (●) represents the contrail energy forcing for one day. The data mean is indicated as blue data point and the median as orange data point. The grey shaded areas indicate the frequency distribution of the data points. With increasing allocation precision (from a uniform allocation to a segment-specific approach), arithmetic mean and median of the data points move to

smaller values, even though this is barely visible due to the large spread of the data points. the value range decreases and the distribution becomes more narrow and moves closer to lower energy forcing values. In all cases, the values range from high positive values (2.7×10^{17} J, base case) to small negative values (e.g., -0.78×10^{16} J, base case). The large majority (almost 98 % for the base case) of the data points is positive, indicating a warming climate impact for most of the days in 2019. Additionally, the flight- and segment-specific allocation strategies yield some days with substantially lower energy forcing values ($- 2.2 \times 10^{16}$ J, segment-specific allocation).

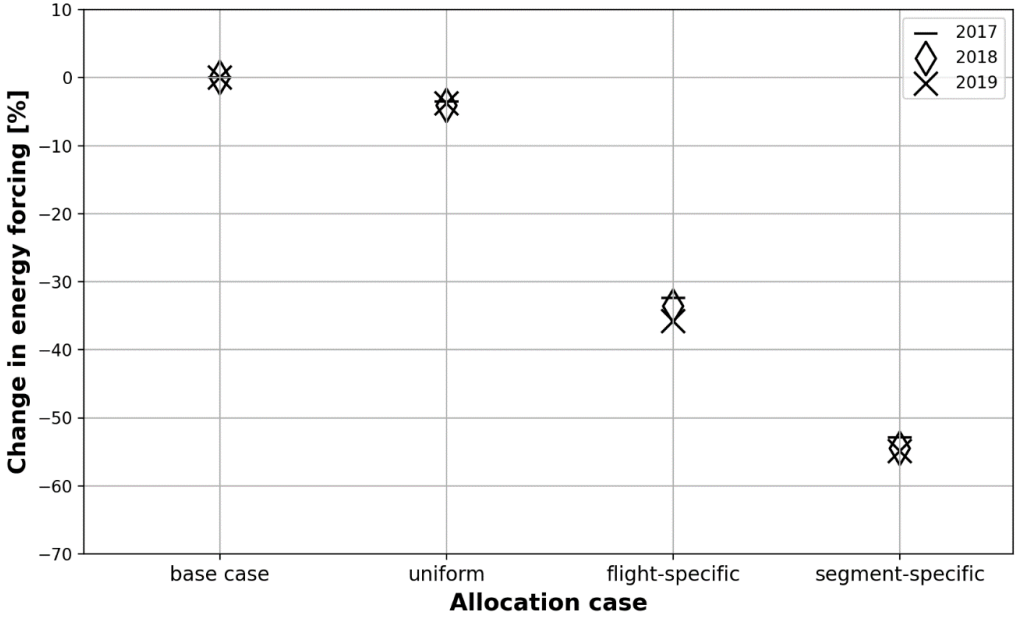


Figure 4.4 Relative change of the median contrail energy forcing [%] for all allocation cases and the years 2017, 2018 and 2019

As indicated by the decreasing mean and median, the more precisely the paraffinic kerosene is allocated, the lower the resulting contrail energy forcing. The large variability can be explained by the influence of the strong daily variation of meteorological conditions (cf. Figure 4.8).

Most of the days in the dataset indicate a net warming contrail energy forcing. The more precisely the paraffinic kerosene is allocated, the more contrails originate from paraffinic kerosene. The associated reduction in contrail lifetime and optical thickness yields a decrease in contrail energy forcing. Days with a net cooling energy forcing become more cooling, since the few warming contrails during these days receive paraffinic kerosene.

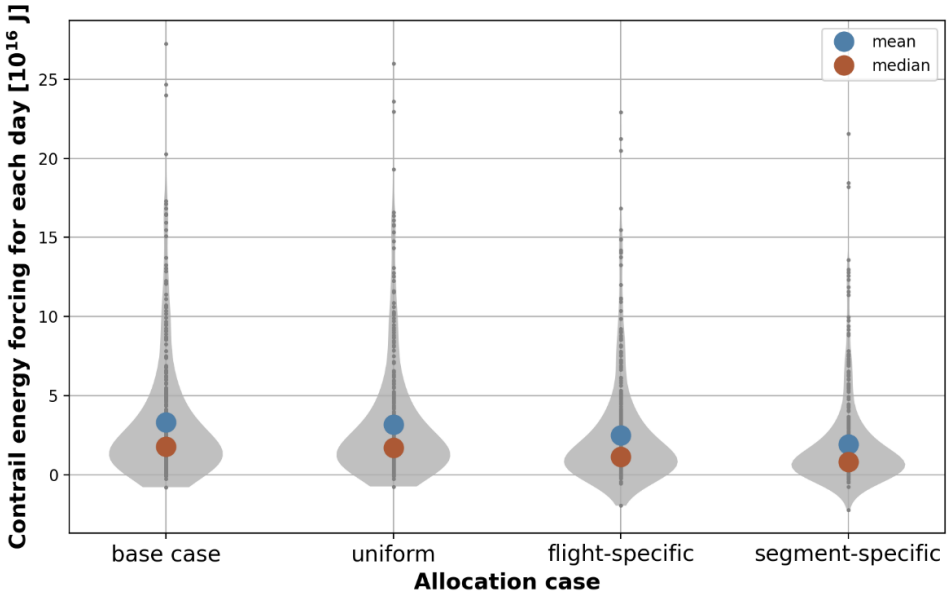


Figure 4.5 Contrail energy forcing (ordinate) for each day (•) and frequency distribution of the data points (grey shaded areas) for the base case and each allocation case (abscissa)

Figure 4.6 provides more details concerning the daily energy forcing for values between -1 × 10^{16} J and +5 × 10^{16} J. This includes about 80.3 % of all data points for the year 2019. The reduction potential of each option becomes more visible in Figure 4.6: While the median contrail energy forcing of the base case is at 1.8 × 10^{16} J, it decreases by about 4 % for a uniform allocation, by about 36 % for the flight-specific allocation and by 55 % for the segment-specific allocation. As already indicated by Figure 4.5, the frequency distributions of the data points shift towards lower contrail energy forcing values, while some data points show a stronger cooling climate impact.

If the paraffinic kerosene is allocated uniformly, the used kerosene's hydrogen content increases by about 0.4 % from 14.10 m- % to 14.16 m-%. As a result, the reduction in contrail energy forcing is clearly limited. A flight-specific allocation strategy uses the limited amount of paraffinic kerosene more effectively, since only flights which form warming contrails (about 25 % of all flights considered) are assumed to receive neat paraffinic kerosene (15.3 m-% hydrogen content) and accordingly, the median contrail energy forcing decreases by about 36 %. For low paraffinic kerosene market shares (including the 5 % market share studied here), some flights with a lower, but still warming contrail energy forcing will not receive paraffinic kerosene. In contrast, a segment-specific allocation strategy targets a

greater fraction of flights, since the paraffinic kerosene is assumed to be used only on those segments of flights where a warming contrail is formed. Thus, this allocation strategy lowers the median contrail energy forcing even by 55 % for the same amount of paraffinic kerosene.

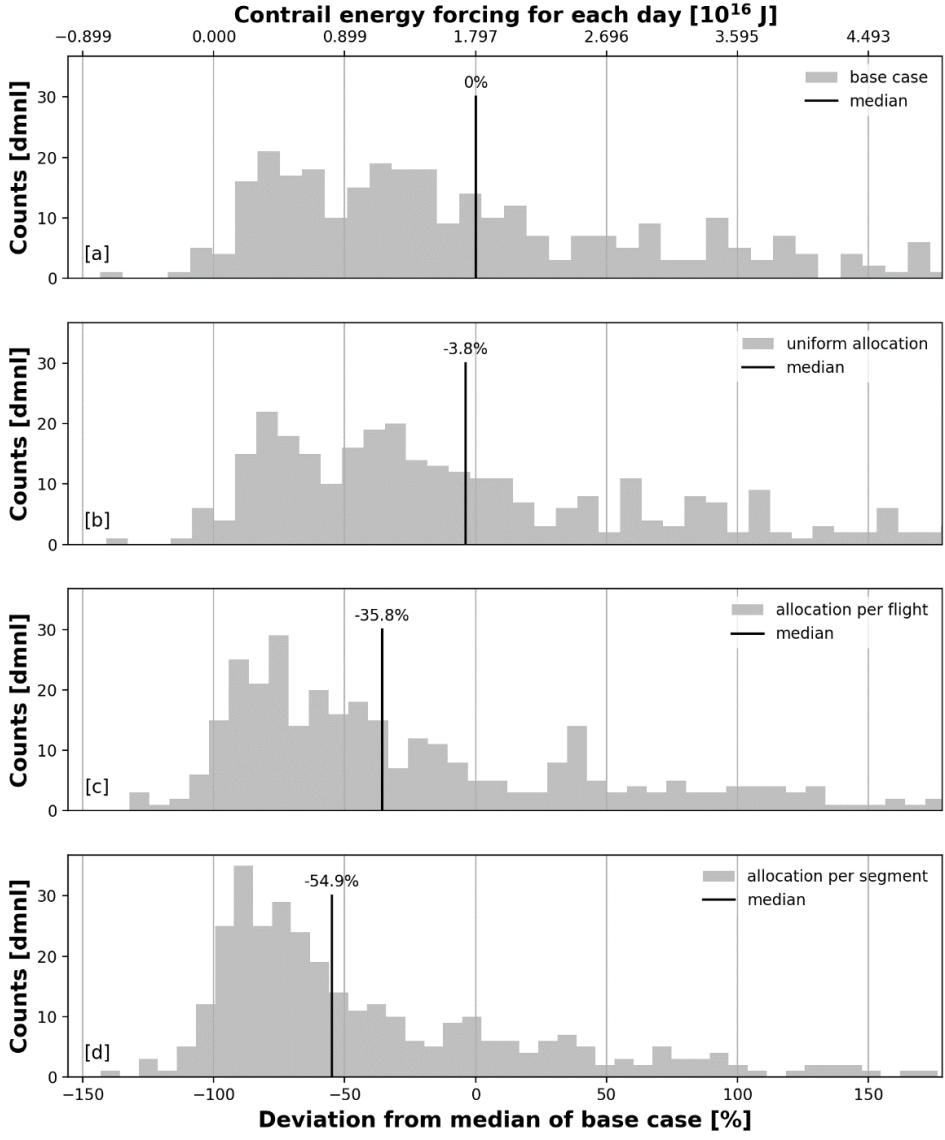


Figure 4.6 Histograms for the daily energy forcing for 2019 conditions for the base case [a], a uniform allocation [b], a flight-specific allocation [c] and a segment-specific allocation strategy [d] (dmnl dimensionless), the ordinate shows the frequency of the data points, the top abscissa the absolute energy forcing and the bottom abscissa the relative change compared to the median of the base case

4.1.3.1.2 Increasing Market Shares

Figure 4.7 shows the relative mitigation potentials for each allocation case by increasing paraffinic kerosene market shares. Data points represent the results for each third day related to the year 2019 and lines correspond to resulting arithmetic means for each allocation case. While the mean mitigation potential for the uniform allocation (solid line) decreases slowly monotonically with increasing market shares, the average mitigation potential of the flight-specific allocation (dashed line) declines steeply and reaches a reduction of > 60 % for a paraffinic kerosene market share of about 25 % and remains constant up to market shares of around 75 %. This effect is even more pronounced for the segment-specific allocation strategy (dash-dotted line), reaching a mitigation potential of > 60 % at a market share of about 10 %. Again, at very high market shares, the reduction in contrail energy forcing decreases until all allocation strategies converge at a mitigation potential of about 40 % for a market share of 100 %.

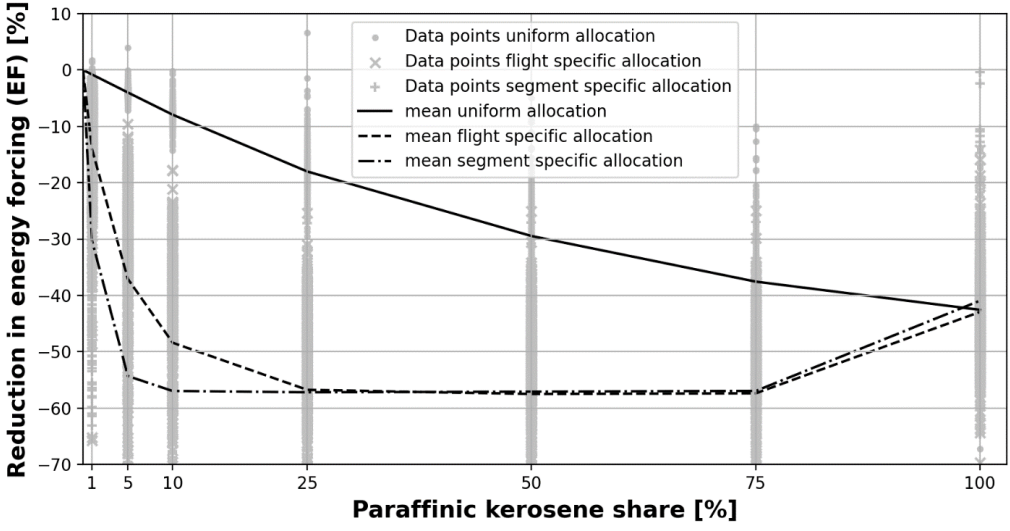


Figure 4.7 Change in contrail energy forcing (ordinate) for increasing paraffinic kerosene shares (abscissa) for each third day in the year 2019. Grey data points show individual days, and the black lines connect the mean for each market share and allocation strategy.

For a uniform allocation, energy forcing decreases almost linearly by increasing paraffinic kerosene market shares. For market shares > 50 % the curve flattens slightly. This can be explained by the assumed non-linear relationship between kerosene hydrogen content and soot emission number (nvPM EI_n) [10], which comes into effect at an increase in hydrogen content

> 0.5 m.p.p. (corresponding to a hydrogen content of 14.6 m - % or a uniformly allocated market share of about 42 %).

In terms of the flight-specific allocation strategy, the steep reduction in energy forcing at market shares up to 25 % is the result of targeting the flights with the highest contrail energy forcing first. As market shares for paraffinic kerosene increase (e.g., from 5 to 10 %), an increasing share of flights with warming contrail energy forcing receive paraffinic kerosene. At a market share of around 25 %, all flights causing warming contrails receive paraffinic kerosene. Thus, the maximum reduction in energy forcing (about 60 %) is achieved. For market shares between 25 and 75 %, flights with a warming contrail climate forcing and an increasing amount of flights without contrail formation receive the paraffinic kerosene, while flights with a cooling contrail climate forcing still receive the conventional kerosene.

The segment-specific allocation strategy targets only segments of flights with a warming contrail energy forcing and accordingly, lower market shares of paraffinic kerosene achieve larger mitigation potentials compared with the other strategies. In this case, the maximum reduction of about 60 % is already achieved at a market share of about 10 %. Again, if market shares increase further, also segments without contrail formation receive paraffinic kerosene.

For both strategies, flight- and segment-specific allocation, the mitigation potential decreases once also flights / segments with a cooling energy forcing receive paraffinic kerosene (market shares > 75 %). The reason behind this counter-intuitive result is the contrail lifetime reduction. If the lifetime of a cooling contrail is reduced, the absolute value of its energy forcing is reduced, but its sign remains negative (i.e., cooling). Thus, the cooling effect of such contrails decreases, and in relative terms the mitigation potential of the respective allocation strategy decreases. As a result, all curves converge for a paraffinic kerosene market share of 100 % at a reduction in contrail energy forcing of about 40 %.

4.1.3.1.3 Uncertainty Assessment

4.1.3.1.3.1 Temporal Variability

Due to different weather patterns, daily and seasonal variations in energy forcing from contrails can be large [186], and only a few studies investigate interannual variations in contrail forcing [9, 10, 186]. A larger effect has

been observed during the COVID-19 pandemic, when contrail occurrence was significantly reduced due to restrictions in air traffic [193, 310, 321, 322]. Therefore, the temporal variability of the contrail energy forcing for different days and years is investigated by comparing the resulting contrail energy forcing from respective flight trajectories and weather data of the years 2017, 2018 and 2019 (Figure 4.8).

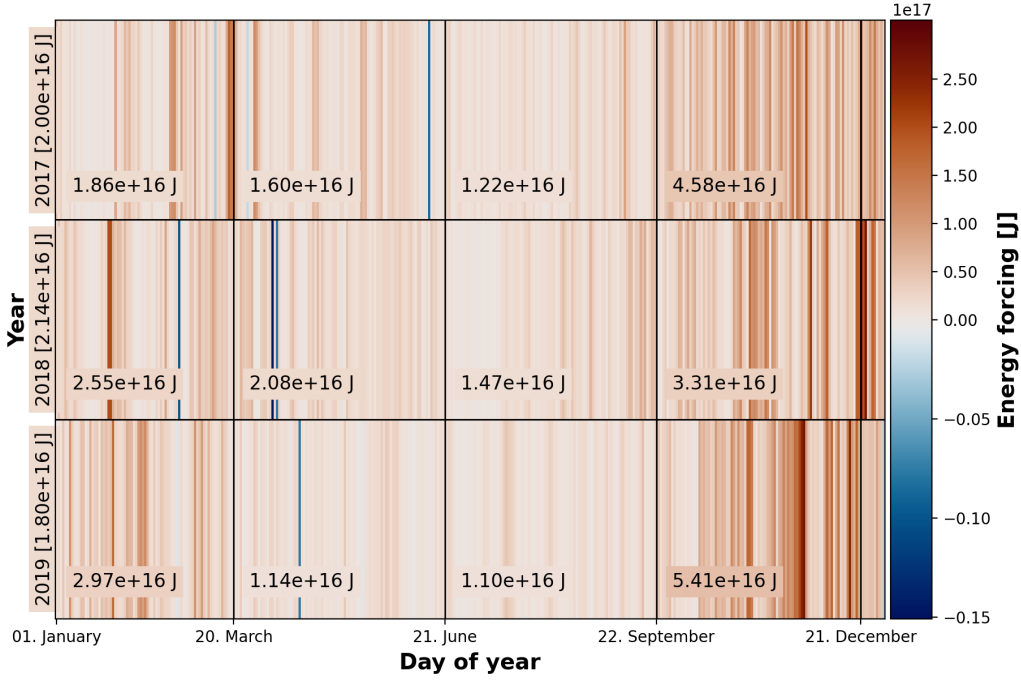


Figure 4.8 Contrail energy forcing by day of year (abscissa) for 2017, 2018 and 2019 (ordinate) (figures in each box show the median for the corresponding timeframe; medians of each year are shown in brackets on the ordinate; to increase the visibility of changes for negative (cooling) energy forcing values, a non-linear scaling is applied)

The color of each bar corresponds to the energy forcing of the entire dataset for each day. The large majority of the days has a warming energy forcing with most of the days ranging between 0 and 10^{17} J. Even as sum for all departing flights at the five airports chosen, a few days exhibit a net cooling climate impact, but with a substantially smaller magnitude (about 10^{16} J) compared to the strongly warming days (about 2×10^{17} J). Figure 4.8 also shows a seasonal pattern. From autumn equinox to winter solstice the median contrail energy forcing is highest (between 3.3×10^{16} J and 5.4×10^{16} J), while from summer solstice to autumn equinox days show a small to moderate contrail energy forcing (median < 1.5×10^{16} J). The median contrail energy forcing for 2017, 2018 and 2019 amounts to 2.00×10^{16} J, $2.09 \times$

10^{16} J and 1.80 × 10^{16} J, respectively. For the three years evaluated here, the inter-annual variation is small (about 10 %) when compared to the seasonal variation (up to five-fold) and even more the daily variation (-10^{16} J up to 3 × 10^{17} J), indicating a strong influence of daily and seasonal changes.

Two effects are probable causes for this temporal variability, namely variations in meteorological conditions and the traffic volume. The vast daily variation can most likely be explained by short-term changes of meteorological conditions such as the movement of ice-supersaturated regions in the atmosphere. Also, the solar cycle during day and night plays an important role for contrail energy forcing. The seasonal variation can be explained by longer nights in the winter months of the Northern hemisphere resulting in a higher probability of contrails with a warming climate impact. For the dataset used here, more flights (on average +11 %) travel greater distances per flight (on average +5 %) during autumn and winter (cf. Appendix C) than during the other seasons, which also increases the probability for contrail formation.

Table 4.1 shows the relative change in median energy forcing compared to the base case where no paraffinic kerosene is used for the entire years 2019, 2018 and 2017 and for each season. The annual values for 2017 and 2018 are in line with the results for 2019 discussed above. In general, the mitigation potentials appear highest in spring and lowest in winter. The variation among seasons is substantially larger than the variation among different years, e.g., about 14 %-points between spring 2019 and winter 2019, but only up to 6 %-points among winter months in 2017, 2018 and 2019.

Table 4.1 Change in median energy forcing relative to the base case by year and season

Timeframe	Uniform [%]	Flight-specific [%]	Segment-specific [%]
2019 [2017; 2018]	-3.8 [-3.5; -4.1]	-35.8 [-32.4; -33.6]	-54.9 [-52.9; -54.5]
Spring[a]	-5.5 [-1.2; -3.3]	-44.1 [-44.4; -42.7]	-62.9 [-61.3; -64.7]
Summer[a]	-4.0 [-3.4; -4.2]	-36.7 [-32.4; -38.3]	-59.6 [-52.0; -56.3]
Autumn[a]	-3.6 [-4.0; -4.6]	-26.7 [-24.4; -30.1]	-43.2 [-44.5; -48.6]
Winter[a]	-4.1 [-3.7; -4.3]	-27.8 [-32.6; -29.9]	-48.4 [-55.0; -52.6]

[a] based on astronomic seasons (i.e., Spring – March 21st to June 21st; Summer – June 22nd to September 22nd; Autumn – September 23rd to December 22nd; Winter – December 23rd to March 20th)

4.1.3.1.3.2 Kerosene Composition

The effect of the kerosene composition for conventional aviation kerosene is shown in Figure 4.9. It shows the distribution of the contrail energy forcing for each third day in 2019 for the base case (top), a uniform allocation (second from top), a flight-specific (second from bottom) and a segment-specific allocation strategy (bottom). Based on the hydrogen content distribution of the World Fuel Survey [179], the hydrogen content is varied between 13.9 m-%, 14.1 m-%, and 14.3 m-%. These values correspond to the mean (14.1 m-%) and a single standard deviation of the distribution of kerosene samples described in the World Fuel Survey [179].

Since the base case does not use any paraffinic kerosene, it allows for an estimate of the uncertainty in contrail energy forcing due to kerosene composition changes. Assuming a comparatively low hydrogen content (13.9 m-%), the median contrail energy forcing is about 12 % higher than for the medium hydrogen content (14.1 m-%). For a high hydrogen content (14.3 m-%), the contrail energy forcing decreases by about 16 %. This corresponds to a sensitivity of a 6 to 8 % change in contrail energy forcing per 0.1 m-% change in kerosene hydrogen content. This roughly corresponds to the inter-annual variability estimated in 4.1.3.1.3.1. Due to the non-linear relationship between kerosene hydrogen content and resulting contrail energy forcing (cf. Figure 4.7, [281]) this approximation is only valid for the hydrogen content of conventional kerosene.

A uniform allocation of paraffinic kerosene yields a small increase of the hydrogen content of all used kerosene for the market share of 5 % assumed here (14.1 m-% to 14.16 m-%). In essence, this results in a slight reduction of the absolute contrail energy forcing (- 4 %), but the variability due to kerosene changes (- 16/+ 12 %) is barely affected.

For a flight-specific allocation, the conventional aviation kerosene with a high hydrogen content reaches the greatest reduction (- 37 % compared to the base case and a hydrogen content of 14.1 m-%), while the smallest reduction is achieved by the conventional aviation kerosene with a low hydrogen content (- 30 %). The variability due to the changing kerosene hydrogen content is lower than in the base case (- 4/+ 3 % compared to - 16/+ 12 %). A similar variability can be observed for the segment-specific allocation strategy (- 3/+ 3 %). Additionally, for a segment-specific allocation, conventional aviation kerosene with a low hydrogen content results in

the largest contrail energy forcing reduction (- 56 %) and a high hydrogen content (- 50 %).

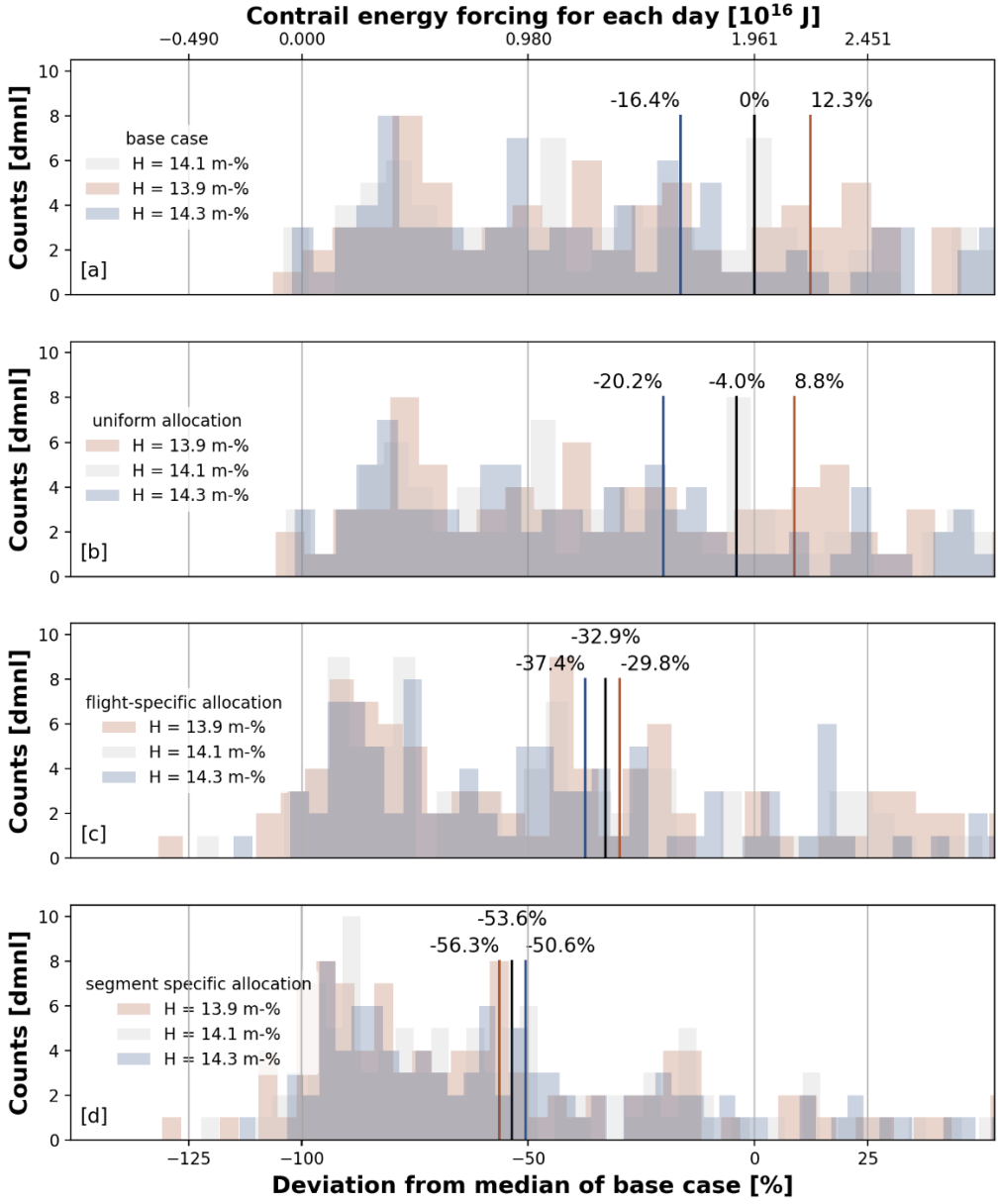


Figure 4.9 Distribution of contrail energy forcing for each third day in the year 2019 and the respective medians for a conventional kerosene hydrogen content of 13.9 m-%, 14.1 m-% and 14.3 m-% for the base case [a], a uniform allocation [b], a flight-specific allocation [c] and a segment-specific allocation strategy [d], the ordinate shows the frequency of the data points, the top abscissa the absolute energy forcing and the bottom abscissa the relative change compared to the median of the base case

For both targeted allocation cases (flight and segment-specific) the variability is reduced because the influence of the conventional aviation kerosene on contrail energy forcing decreases. This is due to the effect that the specific allocation strategies allocate paraffinic kerosene to flights / segments with a warming energy forcing first. As the hydrogen content of this kerosene is not varied, the climate impact of such flights segments is not affected by changes in the conventional aviation kerosene's hydrogen content. For the market share assumed here (5 %), the most impactful flights and almost all segments are fueled with paraffinic kerosene. Thus, changes in conventional aviation kerosene hydrogen content primarily alter the energy forcing of cooling flights / segments. For the large majority of the days and flight trajectories evaluated, the energy forcing of warming flights / segments outweighs the energy forcing of cooling flights / segments (Figure 4.8) and thus variations in paraffinic kerosene properties outweigh variations in conventional kerosene hydrogen content. Since paraffinic kerosene properties are not varied, the overall variability decreases.

A similar behavior explains that a flight-specific allocation for a conventional aviation kerosene with a *high* hydrogen content achieves the largest mitigation potential while for a segment-specific allocation a conventional aviation kerosene with a *low* hydrogen content achieves the largest mitigation potential. If the kerosene is allocated on a per flight basis, a paraffinic kerosene market share of 5 % is not sufficient to fuel all flights with a warming contrail energy forcing, only about 10 % of the net warming flights receive paraffinic kerosene. The energy forcing of these flights decreases for high hydrogen contents of the conventional kerosene and thus also the net energy forcing of all flights decreases. Since the segment-specific allocation is more specific, about 62 % of the net warming flights receive paraffinic kerosene. Thus, variations of the conventional kerosene's hydrogen content mostly affect the energy forcing of cooling segments. Here is the effect opposite: An increasing hydrogen content results in a shorter contrail lifetime and thus a reduced (cooling) energy forcing. As a result, a higher conventional kerosene hydrogen content results in less cooling segments and thus a higher overall energy forcing. If higher paraffinic kerosene market shares (e.g., 25 %) were assumed, also for a flight-specific allocation all warming flights would receive paraffinic kerosene and the same effect could be observed.

In general, the variability due to kerosene composition changes has an important effect on the resulting contrail energy forcing. For the overall contrail energy forcing of a representative fleet, such variations average each other out and the use of average values seems appropriate. But for the contrail energy forcing of individual flights the hydrogen content or ideally the composition (i.e., cycloalkanes, aromatics and naphthalene content) needs to be known more precisely.

4.1.3.2 Discussion

The results presented allow for distinct conclusions about (1) mitigation potentials of allocating 5 % of overall kerosene demand as paraffinic kerosene in a uniform, flight- or segment specific manner and (2) the temporal development of those potentials assuming increasing market shares of paraffinic kerosene. These conclusions are discussed in the following.

(1) For any of the allocation strategies investigated, paraffinic kerosene reduces the contrail energy forcing. Even without a targeted use, low or paraffinic kerosene can reduce contrail climate forcing considerably. The relative reduction in contrail energy forcing ranges from 4 % for a uniform allocation, about 36 % for a flight-specific allocation (10 % of net warming flights would receive paraffinic kerosene) and around 55 % for a segment-specific allocation, (62 % of net warming flights would receive paraffinic kerosene). For the flight and segment-specific allocation strategies, these reductions are significant and appear robust against most uncertainties studied.

(2) Assuming an increase in renewably sourced (and thus paraffinic) kerosene market shares also affects the mitigation potential of the different allocation cases. A segment-specific allocation shows higher mitigation potentials than a flight-specific allocation up to market shares of about 25 % (cf. Figure 4.7). Provided that the market shares foreseen by the EU's blending mandate materialize in time (20 % in the year 2035 and 34 % in the year 2040), a segment-specific allocation strategy would be beneficial for a bit more than a decade. It appears questionable to which extent this timeframe is sufficient to develop and roll-out the required airport and aircraft modifications. Another option might be the implementation of a flight-specific allocation strategy at scale and the use of a segment-specific allocation only on newly produced aircraft.

The absolute energy forcing values are largely affected by meteorological conditions (by orders of magnitude) and to a smaller extent seasonal effects, such as the day-night duration (up to five-fold), while the inter-annual variability is < 10 %. The conventional kerosene properties play another important role for the absolute contrail energy forcing (6 to 8 % change per 0.1 m-% change in conventional kerosene hydrogen content). Thus, to determine the contrail energy forcing of individual flights, more detailed information about each flight's kerosene composition would be required.

A segment-specific allocation strategy would require substantial infrastructure and aircraft modifications, which would result in substantial cost and delays for the implementation of this strategy. A flight-specific allocation strategy would require a segregated infrastructure to supply paraffinic kerosene in a targeted manner to flights with a high contrail energy forcing. Both allocation strategies strongly depend on how reliable the expected contrail climate forcing of individual flights can be estimated. All these factors, limitations from meteorological data, the magnitude of necessary infrastructure changes and aircraft modifications are beyond the scope of this investigation. Such efforts (cost- and time-wise) should be evaluated carefully to ensure that effective allocation strategies can be implemented.

Instead of all flights globally, this study uses departing flights from the five large European airports. This most likely induces two systematic errors, i.e., an increased relevance of weather conditions in Europe and the North Atlantic region and a high share of long-range flights. Thus, the results rather indicate the general mitigation potential of a targeted use concept, but exact airport-specific values may vary depending on its region and size. In particular, for airports located in other climate zones, such as the tropics, the mitigation potentials may vary.

Previous studies to mitigate the climate impact of contrails typically focus on route modifications to avoid ice-supersaturated regions [29, 30, 177], while the targeted use of paraffinic kerosene has been studied less often [10, 134]. In 2022, Teoh et al. reported a 10 % reduction in contrail energy forcing for a paraffinic kerosene market share of 1 % for a flight-specific allocation strategy. This value is slightly lower than the result for 1 % market share shown here in Figure 4.7, because Teoh et al. (2022) assume a 50 % blend of renewably sourced and conventional kerosene, while this study assumes neat paraffinic kerosene on the flights targeted. Woeldgen et al. recently published results for supplying flights with renewably sourced

kerosene using strategies which avoid large infrastructure modifications [134]. The paraffinic kerosene is allocated either during contrail-sensitive seasons (October to February), between 16:00 and 03:00 UTC and with a combination of days and aircraft-engine combinations for the highest warming contrail formation. They assume an overall paraffinic kerosene market share of 2 % and estimate a reduction in annual contrail energy forcing between 1.4 % and 2.6 % [134]. Their allocation strategies are not based on meteorological data but rather fixed external factors and thus their mitigation potential estimate is far lower than the values of Teoh et al., (2022) [10] and this study. Finding an allocation strategy which optimizes the trade-off between required infrastructure modifications and contrail climate mitigation potential could be an interesting area for further research.

Current kerosene specifications require a minimum aromatics content of 8 m-% for renewably sourced kerosene [280], while specifications for conventional kerosene do not include a minimum aromatics content [181]. This study assumes the use of neat, i.e., aromatics-free kerosene on a fraction of all flights (< 2 % for the flight-specific allocation). Further investigations are necessary to ensure compatibility with current aircraft systems, such as the sealing of fuel systems and fuel quantity measurements. Further research could be conducted about the mitigation potential of the targeted use of specification compliant kerosene (i.e., with a minimum aromatics content of 8 %).

The effectiveness of any targeted use strategy depends on the reliability of estimating an individual flight's contrail climate forcing, most significantly for the segment-specific allocation. This study uses an ex-post meteorological dataset (ERA5) which would not be available at the flight planning stage. Different data options are considered for the fuel allocation, e.g., ex-ante datasets (forecasts) and also observation based strategies, such as satellite remote sensing or on-board tracking of contrail formation and evolution conditions [10, 25, 313, 314]. Further research could be conducted to assess their potential and implications for flight operations.

Both, flight and segment-specific allocation achieve their highest mitigation potentials up to paraffinic kerosene market shares of about 75 %. For higher market shares, also the remaining contrails with a cooling climate forcing would be affected. The extent to which the cooling impact of such

flights could be maintained once market shares of renewably sourced kerosene increase beyond 75 % is another area for further research. One option might be the admixture of specific molecules, such as renewably sourced aromatics or cycloalkanes. However, further investigations are required to reduce uncertainties and potentially prevent adverse outcomes.

Concluding, this study quantifies the climate benefits of different paraffinic kerosene allocation strategies. For paraffinic kerosene market shares up to 25 %, a segment-specific kerosene allocation would be more effective than a flight-specific kerosene allocation. However, potential infrastructure and aircraft modification efforts need to be carefully considered. Meteorological and kerosene-related uncertainties as well as economic implications of these strategies remain areas for further research. Further investigations could allow for a derivation of specific marginal abatement cost and thus the comparison of this mitigation option with other strategies to reduce the climate impacts of aviation.

4.2 Segregated Supply of Sustainable Aviation Fuel to reduce Contrail Energy Forcing – Demonstration and Potentials

G. Quante, B. Enderle, P. Laybourn, P. W. Holm, L. W. Andersen, C. Voigt, and M. Kaltschmitt, "Segregated Supply of Sustainable Aviation Fuel to reduce Contrail Energy Forcing – Demonstration and Potentials" Journal of the Air Transport Research Society, p. 100049, 2024, doi: 10.1016/j.jatrs.2024.100049.
Typesetting and formatting are slightly adjusted to ensure consistency within this thesis.

Abstract

Aviation contributes about 4 % to net anthropogenic climate forcing, with contrails being the largest individual contributor to radiative forcing from aviation. One option to mitigate contrail-related climate impacts is using kerosene containing fewer or no aromatic components and thus showing a higher hydrogen content compared to conventional kerosene (i.e., fossil fuel-based). Such "low contrail" kerosene can be provided as a blend of conventional (crude oil-based) and synthetic kerosene or from hydroprocessing conventional kerosene.

Low contrail kerosene reduces contrail lifetime and optical thickness and thus the magnitude of contrail climate forcing. However, market shares of such kerosene are presently very low. Simultaneously, a small fraction (< 10 %) of all flights globally accounts for the majority (> 80 %) of global warming contrail climate forcing. Hence, the targeted use of low contrail kerosene on those flights appears promising. But such an approach would

require additional operational efforts, such as a duplication of supply lines and storage tanks.

This study evaluates the feasibility and operational efforts of a segregated supply of a 35 m-% SAF-blend (14.34 m-% hydrogen content) to 84 winter time demonstration flights to reduce contrail climate forcing. Between 17th January 2023 and 2nd February 2023, low contrail kerosene was supplied to commercial A320 type aircraft flights on the route between Stockholm and Copenhagen in northern Europe. The operational feasibility and related efforts to target flights with the highest contrail energy forcing as well as a large-scale application are described. The evolution of contrails is tracked using data from the Meteosat Second Generation (MSG) satellite. The contrail energy forcing is calculated for the corresponding flight trajectories assuming another, well-validated engine model (CFM56-5B4 for the simulations instead of LEAP1A-26 for the demonstration flights) using the Contrail Cirrus Prediction (CoCiP) model with meteorological input fields from European Reanalysis data (ERA5).

For the first time, the experiment demonstrates the operational feasibility for a segregated supply of low contrail kerosene to medium range aircraft at Stockholm airport. The segregated supply of low contrail kerosene can be realized for short to medium range flights, which can be fueled by a refueller truck. Targeting individual flights via single line hydrant fueling systems seems impractical as of now. Operational efforts to target single flights with highest contrail energy forcing are almost identical to the efforts in this demonstration experiment.

Simulations estimate that the segregated supply of the medium blend kerosene (14.34 m-% hydrogen content) can reduce contrail energy forcing by about 11 % assuming the use of a “Rich-Quench-Lean” (RQL) engine (CFM56-5B4). The contrail climate benefit increases to >20 % for a 50 % blend ratio (14.7 m-% hydrogen content). Also, the location and evolution of the demonstration flights’ 28 contrails calculated with CoCiP was tracked with satellite data.

The uncertainty of absolute contrail climate forcing estimates is mainly limited due to meteorological data input and also by lacking information on fuel composition in terms of cycloalkane, mono- and polycyclic aromatics content. Contrarily, the uncertainty of relative changes in contrail climate forcing is subject to low uncertainty, since it compares the use of different fuels for an identical fleet and identical weather conditions.

4.2.1 Introduction

Aviation contributes about 4 % towards net anthropogenic climate forcing [5]. Its climate impact can be attributed to contrails, carbon dioxide (CO_2) emissions, effects caused by NO_x emissions, and several other effects. In terms of radiative forcing, contrails are the largest individual contributor to the total radiative forcing from aviation, being even larger than the radiative forcing from historically accumulated aviation carbon dioxide (CO2) emissions [5, 9]. Hence, the mitigation of aviation's climate impact is considered a key challenge in air transportation research [323, 324].

One option to mitigate contrail climate impacts is the use of kerosene[14] with a reduced content of aromatic compounds compared to conventional kerosene ("low contrail kerosene"). Such kerosene lowers contrail climate forcing by reducing average contrail lifetime and optical thickness [10, 17, 28, 68, 86, 134, 281, 325]. The content of aromatic components within conventional kerosene can be reduced technically by hydroprocessing of the fossil fuel-based kerosene [17, 18, 131, 135] or by blending conventional (untreated) kerosene with synthetic kerosene [131, 309, 326] This synthetic kerosene is derived from non-crude oil based sources such as biomass or coal [280] and typically does not contain any aromatic compounds. Synthetic kerosene from renewable sources is colloquially referred to as "Sustainable Aviation Fuel" (SAF). Since the renewable origin does not necessarily guarantee compliance with other sustainability aspects (e.g., biodiversity, no child labour), the term renewably sourced kerosene is used here instead of the term "Sustainable Aviation Fuel" (SAF).

The use of low contrail kerosene has further environmental impacts than contrail-related climate forcing. The reduced aromatics content of such fuel reduces soot particle emissions and can thus improve the local air quality around airports [18, 324, 326]. Kerosene from renewable energy sources can also reduce aviation's carbon dioxide-related climate impact, depending on feedstock and provision pathway being used [32, 324, 327]. The choice of any renewably sourced feedstock type needs careful consideration, since it might affect land use or could stipulate competition with food and feed markets [221, 286, 328].

[14] Typically, kerosene denotes a certain fraction of hydrocarbon molecules containing about eight to 16 carbon atoms. Thus it is not per se compliant with aviation turbine fuel specifications. Note that the term kerosene refers to specification compliant jet fuel here.

Low contrail kerosene is currently scarcely available on the global fuel markets; neither large scale production units are under operation nor the economic environment supports the use of such fuel and additionally the valid fuel standards do not address the use of such fuels. Simultaneously, about 3 % of all flights in 2019 (or 11 % of the contrail-forming flights) are estimated to account for 80 % of the global contrail energy forcing [9]. For this reason, the targeted use of low contrail kerosene on flights with a substantial probability to cause high contrail climate forcing seems to be a promising way to reduce aviation's climate forcing impact. However, such a concept would imply additional operational efforts, e.g., due to the provision of segregated supply lines, additional storage tanks and specific equipment for a segregated aircraft refueling.

Against this background, this study reports about the operational efforts required for a segregated kerosene supply to 84 demonstration flights between Stockholm airport and Copenhagen airport. These efforts are weighed against the contrail climate benefits of using low contrail kerosene. To reduce uncertainties in the contrail climate forcing for lean burn engine (turbine) technologies, a predecessor of the demonstration flights' aircraft with a rich-quench-lean engine was assumed within this assessment. Additionally, implications for supplying flights based on their climate forcing ("targeted use") are derived and their general applicability at large-scale is discussed.

Initially, contrails are formed when the mixture of ambient air and aircraft engine exhaust cools down and reaches supersaturation against water. The required threshold air temperature and pressure can be determined by the Schmidt-Appleman criterion [11, 12, 308]. The combustion of kerosene in a jet engine produces water (among others) formed from the hydrogen chemically bound within the aviation fuel and oxygen from the ambient air. This water mainly condenses on soot particles (from incomplete combustion) emitted in parallel from the aircraft engines. The majority of present-day engines (turbines) emit in the so-called "soot-rich" emission regime (10^{14} to 10^{15} particles/kg_{fuel}). If the temperatures of the ambient air masses are sufficiently low, the formed water droplets subsequently freeze into ice crystals. When the humidity of the surrounding air is below ice saturation, the ice crystals will sublime after a short while. Contrarily, in ice-super-saturated regions, the initial ice crystals will trigger the formation of additional ice crystals from the humidity of the ambient air and thus cause a persistent

contrail, which can persist for several hours and – depending on vertical wind shear – can spread over large areas [25, 329, 330]. Typically, such persistent contrails exhibit a large climate impact. Finally, the contrail cirrus dissolves because its ice crystals sublimate [161], e.g., by sedimentation into warmer and / or dryer air masses.

At night, contrails trap outgoing terrestrial radiation in the atmosphere, while during day they also reflect incoming solar radiation [164]. Hence, the climate impact of individual contrails is largely dependent on the solar zenith angle during its life time. Most contrails at night have a warming climate impact, while contrails during the day can also exhibit a cooling climate impact. On the long-term average, the global net climate impact of contrails is clearly warming [9].

The sooting tendency of kerosene decreases roughly from poly- to mono-cyclic aromatics via cyclo-, iso- and n-alkanes [15, 18]. The reduced soot particle emissions number causes a marginally higher amount of water to condense onto substantially fewer soot particles. As a result, those soot particles covered by more water tend to be heavier and sediment earlier compared to the current situation. The reduced ice particle number also results in a decreased contrail optical thickness. Both, reduced optical thickness and faster sedimentation lower the absolute value of a contrail's climate impact; i.e., it shows either less warming or less cooling effects [28, 131, 164, 177, 318, 331].

The aromatics content of aviation kerosene can be reduced either by using kerosene produced based on renewable sources (which typically does not contain any aromatics) or based on an additional processing step of crude oil based kerosene [281]. The targeted supply of such low contrail kerosene to flights with a high contrail climate impact has been studied theoretically in several simulation studies [10, 134, 325]. The majority of these studies focus on the climate forcing mitigation potential [10] or on approaches avoiding infrastructure modifications [134]. This investigation adds a weighting of operational efforts and contrail climate benefits to the existing literature, based on a practical application of a segregated low contrail kerosene supply.

From 17th January to 3rd February 2023, 84 demonstration flights between Stockholm airport and Copenhagen airport have been conducted with low contrail kerosene. A blend of 35 % synthetic and 65 % conven-

tional (crude oil based) kerosene was supplied specifically to the demonstration flights segregated from the usual kerosene supply chain. The synthetic blend component was provided based on renewable sources via the Hydroprocessed Esters and Fatty Acids Synthesized Paraffinic Kerosene (HEFA-SPK) pathway [94, 124, 332]. These demonstration flights have been conducted as part of the ALIGHT project [333]. Data from the respective measurement campaign are used in this ex-post analysis to study the operational efforts and potential climate benefits of a segregated low contrail kerosene use. First-hand experiences from planning and conducting the demonstration flights are the basis to describe the corresponding operational efforts. The resulting demonstration flight's contrail climate forcing is estimated with a well-validated engine model (CFM56-5B4) for different conventional, crude oil based and low contrail kerosene options using the Contrail-Cirrus Prediction Model (CoCiP).

The remainder of this study is structured as follows: Section 4.2.2.1 details methods and section 4.2.2.2 data used to derive the operational efforts and to estimate the contrail climate forcing. Additionally, uncertainties of the contrail modeling and the Contrail Cirrus Prediction Model (CoCiP) are discussed qualitatively in section 4.2.2.3. Based on the experiences during these demonstration flights, operational efforts for targeting flights based on their contrail energy forcing and for a large-scale application are discussed (section 4.2.3.1). The satellite detection of individual contrails (section 4.2.3.2) and contrail climate benefits are described (section 4.2.3.3). As such, this study can be seen as an initial experimental demonstration of a segregated low contrail kerosene supply.

4.2.2 Methods, Data and Model Uncertainties

The weighting of operational efforts and contrail climate benefits of a segregated and targeted use is based on a discussion of the operational efforts and a contrail climate benefit estimation based on simulations. Drawing from the experiences made by conducting the demonstration flights, operational efforts for targeting flights with the highest contrail energy forcing are derived for a short-term perspective and their general applicability at large scale for multiple airports are discussed. The Contrail Cirrus Prediction model (CoCiP) is used to estimate the contrail climate benefits of using low contrail kerosene during the demonstration flights, assuming a prede-

cessor of the aircraft used for the demonstration flights to reduce model uncertainties. The evolution of individual contrails is studied to assess the model's uncertainties and their energy forcing is subsequently used as a metric for the weighting of operational efforts and contrail climate benefits.

4.2.2.1 Methods

This section covers the segregated supply of low contrail kerosene as it was realized for the demonstration flights first (section 4.2.2.1.1). Then, the methods to estimate the change in contrail climate forcing are discussed (section 4.2.2.1.2).

4.2.2.1.1 Segregated Supply of Low-contrail Kerosene

The demonstration flights were carried out with the primary objective to measure the local air quality impacts of using a kerosene with a low content of aromatic compounds. To supply this specific kerosene blend to the demonstration aircraft, a segregated supply infrastructure was required. Kerosene handling standards advocate that only kerosene in compliance with the respective applicable kerosene standards (e.g., ASTM D1655, Def Stan 91-091 [181, 334]) is delivered to an airport [335]. Since the applicable fuel specification (here: ASTM D7566) presently limits the use of synthetic kerosene to blends with at least 50 % conventional (crude oil based) kerosene [280], this regulation implies that blending takes place before the blend is supplied to an airport. Up to the point of blending, the supply of neat synthetic kerosene is segregated in any case, since an upstream blending of different synthetic kerosene components is not permitted by the respective standards. Therefore, the current (non-segregated) and the investigated (segregated) supply chains differ only from the point where all kerosene supplies for a particular airport merge and usually commingle. For the demonstration flights, this point is Gävle fuel terminal, located in Sweden north of Stockholm airport (Figure 4.10).

Overall, 84 demonstration flights with a low contrail kerosene consisting of about 35 m-% HEFA-SPK and 65 m-% conventional (crude oil based) kerosene were conducted between 17th January to 2nd February 2023. The aircraft, a commonly used single-aisle commercial airliner equipped with LEAP1A-26 engines, carried out scheduled passenger services between Stockholm airport and Copenhagen airport. For logistical reasons, fueling

took place at Stockholm airport only, where this aircraft was fuelled for both flight legs, to and from Copenhagen airport.

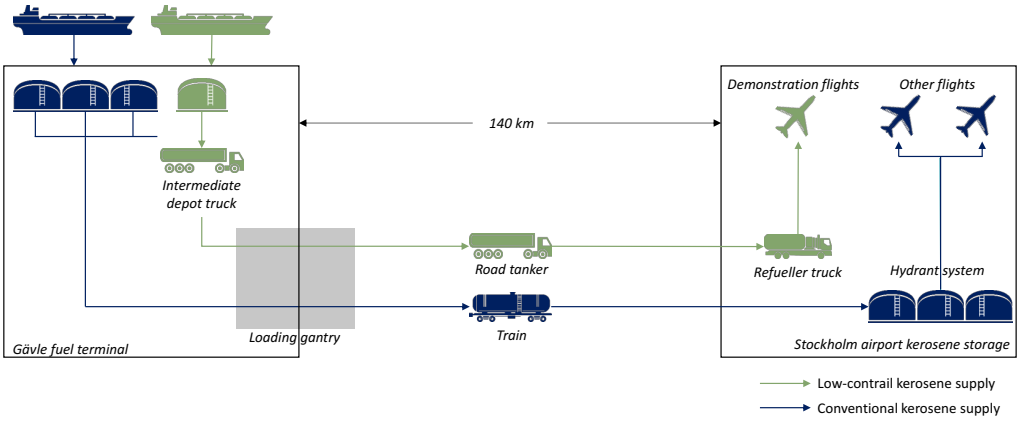


Figure 4.10 Schematic overview of the kerosene supply to Stockholm airport

Kerosene supply to Stockholm airport is realized from Gävle fuel terminal, where kerosene is supplied from a global range of refineries. From Gävle, the kerosene is transferred by train over a distance of about 140 km to a station nearby Stockholm and then supplied by a pipeline to the airport's fuel depot.

The low contrail kerosene was initially stored at Gävle's fuel depot in an individual tank. Usually, kerosene supplies from different tanks commingle in the supply lines for fueling the various train wagons. To avoid this, another outlet directly connected to the respective tank was used for filling a road tanker. This tanker served also as an intermediate storage, carrying the low contrail kerosene to the loading gantry, where it was transferred to another road tanker. Aviation kerosene handling standards require using filter / water separators to be installed at road / rail tank cars, marine vessels or entries into delivery pipelines which directly supply airport service tanks [335]. With a filter capacity of more than 800 L, residual kerosene in a filter/water separator can substantially alter the properties of the kerosene transported. Hence, the road tankers were drained and cleaned prior to fueling them with low contrail kerosene. Upon arrival at Stockholm airport's fuel depot, the low contrail kerosene was transferred to a segregated refueller truck of Stockholm airport.

Fueling at Stockholm airport is usually performed by the airport's hydrant system. In principle, such systems constitute a closed-loop with hy-

drants at most aircraft parking positions. Fueling is performed here by dispenser trucks basically connecting the hydrant system with the aircraft's fueling coupling. In a hydrant system, kerosene is continuously circulated to prevent fuel degradation [278]. This inhibits the segregated supply of a particular kerosene blend volume to a specific aircraft. Accordingly, for the measurement campaign, refueling was performed by a refueller truck, equipped with a pump, couplings and filters suitable for an aircraft refueling fulfilling the given legal requirements. Prior to its use, the refueller truck was drained and cleaned to prevent commingling of the low contrail kerosene with former conventional (crude oil based) volumes.

With an approximate capacity of 8,000 L, one trip of the refueller truck to the aircraft's position was usually sufficient to supply both flights (i.e., from Stockholm airport to Copenhagen airport and vice versa). Due to their tank volume, refueller trucks require more space than fuel dispensers. As a result, the aircraft was boarded at a remote stand instead of a contact stand during the demonstration flights. Remote stands are distant from the airport terminal and require the transportation of passengers by bus to and from the aircraft. Contact stands are in close proximity to the airport terminal, allowing passengers to board either via a boarding bridge or simply by walking. Additionally, the flights of the demonstration aircraft were scheduled with at least 40 min turnaround time to ensure sufficient time for fueling and boarding. To prevent commingling with residual kerosene in its tanks, the aircraft was defueled the night before the start of the measurement campaign and exclusively fuelled by low contrail kerosene for the entire duration of the measurement campaign.

4.2.2.1.2 Contrail Climate Forcing Estimation

The contrail energy forcing of the demonstration flights is estimated using the contrail cirrus prediction model (CoCiP) [185, 318]. This model simulates the life cycle of contrail segments formed along individual flight trajectories and derives the resulting contrail radiative and energy forcing [164] based on an ex-post weather dataset (section 4.2.2.2). In the following, the basic principles of CoCiP are highlighted [9, 10, 132, 164, 177, 185, 186].

When consecutive waypoints meet conditions for contrail formation (i.e., the Schmidt-Appleman criterion [11, 164, 308]) CoCiP assumes that contrails are formed. The soot emissions number being a main criterion for

the contrail formation potential is derived from the ICAO's engine emissions database [191] for a particular combination of a specific aircraft and its corresponding engine. The soot emissions are subsequently adjusted to the assumed average hydrogen content of the respective kerosene blend and the thrust setting (which is directly correlated with the fuel flow) estimated from aerodynamic data [185]. The higher a fuel's average hydrogen content, the lower it's sooting tendency ceteris paribus. The hydrogen content within the kerosene is mainly influenced by the composition of the kerosene because various component groups are characterized by different average shares of hydrogen; e.g., aromatic compounds show a hydrogen content of typically < 10 m-%, while alkane compounds have a hydrogen content > 15 m-%.

The amount of soot particles (non volatile organic particles) emitted by the airplane's engine due to incomplete combustion serve as condensation nuclei for the formation of ice crystals. A lower limit for the soot emissions number is introduced at 10^{13} particles/kg_{fuel} since also ambient aerosols and volatile organic particles emitted by the airplane's engine can serve as ice nuclei [8]. The ambient temperature at flight attitude, the soot activation rate [16] and the fraction of ice particles surviving the wake vortex phase [164] affect the initial number of ice crystals. A potentially enhanced activation of ultrafine aqueous particles at temperatures well below the formation threshold temperature [8] is not taken into account.

Contrail segments surviving the wake vortex phase are simulated with time steps of 30 min until they reach their end-of-life conditions defined as follows:

- The contrail ice crystal number decreases below the background ice nuclei concentration ($<10^3$ m^{-3});
- The contrail's optical depth $\tau_{contrail}$ is less than 10^{-6}, or
- The lifetime surpasses a maximum of 24 h [164].

Based on the contrail evolution, the local instantaneous contrail radiative forcing (RF′) for each waypoint is calculated based on the change in radiative flux over the contrail area [10]. This change is affected by the outgoing longwave radiation at the top of the atmosphere and the effective albedo from the atmospheric weather model used (e.g., ECMWF reanalysis 5 (ERA5)) [164]. In this way, the presence of other clouds is taken into account. Subsequently, the contrail energy forcing is calculated by integrating

the radiative forcing of each contrail segment (RF′) multiplied by its length and width over the contrail segment's lifetime [14, 177, 186]. The humidity data of the ECMWF reanalysis 5 (ERA5) data scaling to in-situ measurements [317] is performed using the "exponential boost with latitude scaling" method [9]. Furthermore, radiative heating effects (i.e., the influence of radiative heating on the contrail plume and thus contrail lifetime) are taken into account [9].

4.2.2.2 Data

The operational requirements for the segregated supply of low contrail kerosene (section 4.2.2.1.1) were gathered by expert interviews as first-hand information from partners involved in the measurement campaign. The general requirements for the segregated supply (section 4.2.3.1) were derived based on these interviews and publicly available information on aviation kerosene handling requirements [335].

The CoCiP model is used with the aviation's kerosene hydrogen content as free variable and further datasets about the flight trajectories, performance data such as kerosene consumption and weather data (e.g., relative humidity at the aircraft's altitude).

Five different kerosene options are assumed (Table 4.2). As described in section 4.2.2.1.2, the hydrogen content is used as proxy for the respective kerosene composition.

Table 4.2 Kerosene types compared against each other

Name	Hydrogen content [m-%]	Description
"conventional low hydrogen"	13.8	First conventional (crude oil-based) kerosene assuming a comparatively high aromatics content / low hydrogen content. [10, 17, 20, 131, 191]
"conventional average"	14.10	Second conventional (crude oil-based) kerosene assuming an average aromatics content, based on data of [179]; an evaluation of kerosene certificates at Stockholm airport and Copenhagen airport indicates similar hydrogen contents for the conventional supplied at the time of the demonstration flights.
"blend uniform"	14.13	Kerosene blend based on 2 m-% neat synthetic kerosene and 98 m-% "conventional average" kerosene. 2 m-% corresponds to EU blending mandate in 2025. [205]
"blend demo"	14.34	Kerosene blend used in the demonstration flights, hydrogen content measured from kerosene batch.

"blend max"	14.7	Kerosene blend based on 50 m-% neat synthetic kerosene and 50 m-% "conventional average" kerosene. This reflects the current upper blending limit of the ASTM specification. [280]

- "Conventional average" denotes a kerosene resembling an average hydrogen content, based on World Fuel Survey Data, summarizing kerosene samples taken until 2013 [179].
- As the properties and composition of conventional (crude oil based) kerosene differ considerably, a second conventional kerosene option, "conventional low hydrogen" with a relative low hydrogen content is also included. It's hydrogen content corresponds to the conventional kerosene used during the ECLIF-2 flight measurement campaigns [17, 20].
- A blend of 2 m-% synthetic kerosene, corresponding to the EU's blending mandate in 2025 is assumed for "blend uniform". It represents a case where the renewably-sourced kerosene is uniformly distributed among all flights departing at a particular airport.
- The kerosene used during the demonstration flights is "blend demo", its hydrogen content was measured using the ASTM D7171 method.
- To incorporate a kerosene blend at the blending limit of 50 m-%, "blend max" is introduced with an estimated hydrogen content of 14.7 m-%. This hydrogen content is based on a blend of "conventional average" (hydrogen content 14.1 m-%) and neat synthetic kerosene (hydrogen content 15.3 m-% [16, 17, 131, 135]), but does not take into account the minimum aromatics content of 8 m-% for renewably-sourced kerosene blends.

Flight trajectories of the 84 demonstration flights between Stockholm airport and Copenhagen airport are based on Automatic Dependent Surveillance Broadcast (ADS-B) data from flightradar24 [336]. They contain temporal, latitudinal, longitudinal and flight altitude information subsequently resampled to a frequency of 1 min. Figure 4.11 shows the corresponding flight trajectories.

Performance data are derived from the flight trajectories, using geodesic functions (e.g., to calculate a flight's groundspeed) and the Eurocontrol Base of Aircraft Data (BADA) version 4.2 [189] (e.g., to calculate a flight's kerosene consumption).

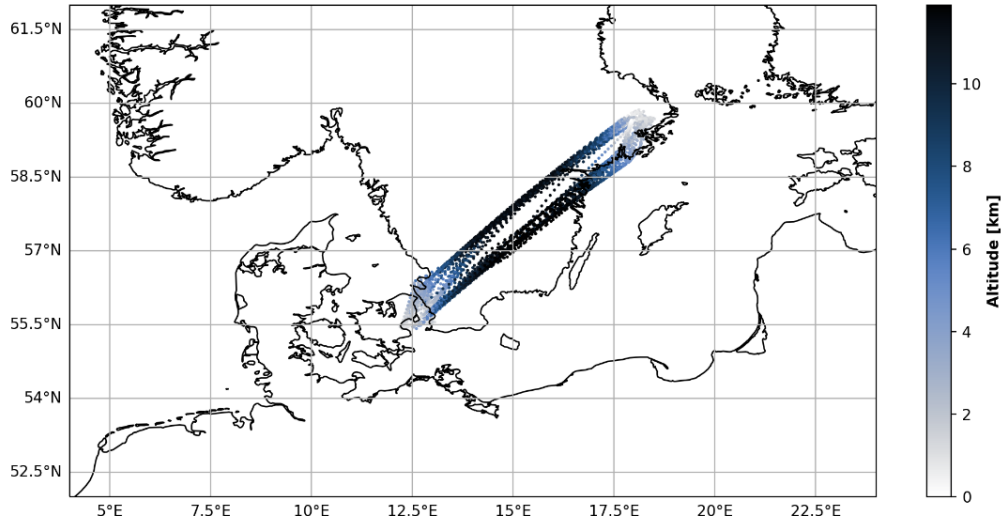


Figure 4.11 Flight trajectories of the demonstration flights from 17.01.2023 until 02.02.2023

The demonstration aircraft is a relatively new aircraft and its LEAP1A-26 engines were designed with so-called "lean-burn" combustion chambers. This design is expected to substantially lower soot particle emissions [31]. It is suspected that the emissions of those engines fall in the so-called "soot-poor regime" of $< 10^{13}$ particles/kg_{fuel}, whereas engines with previous designs emit in the so-called "soot-rich regime" ($> 10^{14}$ particles/kg_{fuel}) [337]. According to theory, within the "soot-poor regime" at ambient temperatures considerably below the Schmidt-Appleman temperature, the activation of ultrafine aqueous particles is enhanced [8]. This would counterbalance the linear relationship between soot particle emissions and nucleated ice crystal numbers assumed in the contrail cirrus prediction model (CoCiP). Thus, the representation of the LEAP1A-26 engine in this model is highly uncertain. For this reason, the simulations were performed assuming a similar aircraft equipped with CFM56-5B4 engines (turbines), a predecessor of the LEAP1A-26 engine. For an average kerosene hydrogen content of 14.1 m-%, the CFM56-5B4 emit about $6.5 \cdot 10^{14}$ particles/kg_{fuel} in the simulations for this study. In terms of ground handling and aerodynamical properties, both aircraft are almost identical and most likely also the operational efforts for their segregated supply with low contrail kerosene will be identical.

Weather data from the European Centre for Medium-Range Weather Forecast's fifth generation high-resolution reanalysis (ECMWF ERA5) are utilized [192], featuring a $0.25° \times 0.25°$ horizontal resolution across 37

pressure levels, with a temporal resolution of 1 h. Meteorological conditions for flights between these pressure levels are interpolated from the two closest pressure levels. Recent studies reveal a slight underestimation of RHI in ERA5 data at cruise altitudes [338, 339], which needs to be corrected. Therefore the ERA5 humidity fields are adjusted to in-situ observations using an exponential scaling with latitude correction. [317]

4.2.2.3 Model Uncertainties

The primary goal of the experiment was to demonstrate the feasibility of the segregated use of SAF on airport level. For this reason, the number of flights evaluated here is small (84 flights) compared to other studies on contrail-related climate forcing. This small sample size motivates a detailed analysis of the uncertainties of the Contrail Cirrus Prediction (CoCiP) model to estimate (a) an individual flight's absolute contrail climate forcing and (b) the effect of differing kerosene compositions on the resulting relative change in contrail climate forcing.

4.2.2.3.1 Contrail Climate Forcing of an Individual Flight

Uncertainties of the contrail climate forcing estimations have been evaluated in a broad range of studies, e.g., by comparing model results with in-situ measurements or remote sensing data from ground- or space-based cameras [25, 313, 314, 340–344]. In one study, a sample size of about 250,000 flights was evaluated using satellite images of the contiguous US with an automated detection and matching algorithm for a timeframe from 04th April 2019 to 04th April 2020 [314]. The algorithm matches flight trajectories from Automatic Dependent Surveillance Broadcast (ADS-B) data with linear-shaped, high-level ice clouds in the satellite image [313]. The resulting data are compared to CoCiP model results for the same flight dataset using ECMWF's ERA5 meteorological dataset. In this way, each contrail predicted by CoCiP is compared to satellite images. For the investigated weather and contrail model resolution, the study finds, however, a rather low agreement between the contrails predicted by the weather-contrail model and the contrails detected by the satellite-based detection algorithm [314] (about 15 % of the contrails predicted by ERA5 / CoCiP matched a contrail found on a Geostationary Observational Environmental Satellite (GOES) image and about 30 % of the contrails detected via satellite

images matched a contrail predicted by ERA5 / CoCiP). However, it remains unclear, to which extent the detection algorithm for the satellite images or the weather model input or the contrail model lack resolution or accuracy. Thus, a binary (yes / no) predictability of an individual contrail remains challenging. In addition to the validation of the respective climate forcing of individual flights not considered here.

In-situ measurements of contrails have been conducted since 1972 [340, 341, 344]. A large comparison study including most in-situ measurements and many remote sensing data indicates a large variation for both, measurement and CoCiP contrail simulation data [25]. Contrail evolution from initial formation stages to lifetimes of almost 3 h and a variety of local contrail parameters are assessed (e.g., ice particle numbers, ice water content, optical thickness). In general, a good agreement of the micro- and macro-physical properties of the modeled contrails has been reported over the contrail's lifetime within the measurement range of the various observations [25]. The physical processes reflected in the model align with the measurement data, indicating that the CoCiP model reflects the behavior of these processes [25]. A similar, earlier study also highlights a generally good agreement between satellite observations and the contrail model CoCiP [342].

The outgoing longwave radiation and reflected shortwave radiation used by CoCiP to calculate the radiative forcing of contrails has been compared to remote sensing retrievals by MSG and a general agreement has been found within the uncertainties during times of normal and reduced air traffic (e.g. the COVID pandemic) [14, 129, 193, 310]

With respect to the weather model input, many simulations use ERA5 weather data as input for contrail simulations. While the ERA5 weather data set is more accurate than many other weather model predictions, recent studies have demonstrated a humidity bias in the ERA5 data set particularly for high humidity in cirrus regions at cruise altitudes [343, 345, 346]. Measurement data by the In-flight service Aircraft for a Global Observation System (IAGOS) were also used to evaluate uncertainties of the weather input to the contrail simulations [343] and to develop correction functions for relative humidity [339] or AI based optimizations [338] with specific correction functions used in CoCiP [9, 10]. The general prediction quality of the integrated forecast system (IFS) of the ECMWF is supported by experiences

in using the IFS based CoCiP simulations for planning of contrail measurement campaigns [16, 17, 162, 347]. Still, the persistence of contrails (and thus their overall life cycle) is subject to uncertainties often related to the representation of relative humidity and ice supersaturation in weather models [338, 343].

Concluding, estimating the absolute contrail energy forcing especially for individual flights is still subject to relevant uncertainties, to a large extent due to uncertainties of the model input data (e.g., weather data) as well as caused by uncertainties in the contrail cirrus micro- and macro-physical as well as radiative properties [5]. For the relative change in contrail energy forcing, e.g., when comparing the contrail forcing of different kerosene options, weather and aircraft data are not varied and thus the uncertainties in weather and aircraft data are of minor importance. Instead, the effect of fuel composition in terms of aromatic and hydrogen content [10] plays a role for the contrail properties and radiative effect.

4.2.2.3.2 Contrail Climate Impact for different Kerosene Compositions

The effect of different kerosene compositions on the resulting contrail climate forcing is reflected in CoCiP by using the kerosene's hydrogen content. The various chemical component groups contained within kerosene being mainly n- and iso-alkanes, cycloalkanes and aromatic components vary characteristically in their hydrogen content (e.g., a typical hydrogen content of an alkane is ca. 15.3 m-%, of a cycloalkane about 14.3 m-% and of an aromatic component about 10.1 m-%) [281]. Thus, using the hydrogen content of a kerosene can serve as a proxy for its composition related to the various chemical component groups. However, such an approach might underestimate the case when certain components (e.g., polyaromatic molecules) are over-proportionally responsible for a kerosene's sooting tendency.

Soot particle emissions are modelled by CoCiP using data from the ICAO Aircraft Emissions Database [191], which provides soot particle emission values depending on the engine's thrust setting for 47 different engines (turbines), including the reference aircraft's engines. These data are based on engine manufacturer's reports during engine certification. While the emissions are calculated for changes in engine thrust settings, increasing soot particle emissions due to engine aging are not taken into account [191].

Subsequently, the emissions number is calculated for the respective kerosene hydrogen content with a thrust-setting dependent empirical relationship [10, 15, 18, 19, 136].

The number of initial ice crystals formed is modelled as a function of soot particle emissions, with a lower boundary of 10^{13} particles/kg_{fuel} considering the activation of organic volatile particles and ambient naturally occurring aerosols. Additionally, partial activation of soot particles for temperatures close to the Schmidt-Appleman threshold temperature is taken into account [186]. These interrelations are based on data from in-situ measurements comparing renewably-sourced and conventional (crude oil based) kerosene [17, 20, 22, 131, 326]. The physical relations after initial ice crystals have been formed are independent of the kerosene used.

Overall, the effects of differing kerosene compositions are depicted at great detail in the model and largely based on measurement data, at least for the engine models studied in ground- and flight experiments (e.g., CFM56-5B4). For this reason, a well validated engine is used in the simulations (CFM56-5B4) instead of the comparatively new LEAP1A-26 engines used for the demonstration flights. The omission of engine aging affecting soot emissions most likely increases the overall uncertainty. Again, the primary interest here is the relative change of contrail climate forcing for different kerosene options within an identical set of flights and meteorological data. As a result, it can be assumed that the engine aging of these flights is identical and thus the associated uncertainty does not affect the relative mitigation potentials. Overall, the absolute contrail climate impact for a single flight has substantial uncertainties, but relative changes in contrail energy forcing for different fuels – which are the focus of this study – are calculated with reasonable certainty.

4.2.3 Results and Discussion

This section qualitatively weights the operational efforts for a segregated kerosene supply with its potential climate benefits. First, operational efforts for targeting flights with the highest climate forcing and the general applicability of a targeted use concept are discussed (section 4.2.3.1). Then, the satellite detection of individual contrails is described (section 4.2.3.2) and associated potential contrail climate benefits are detailed for five different kerosene options (section 4.2.3.3).

4.2.3.1 Operational Efforts

The segregated supply of low contrail kerosene requires modifications of the fuel supply infrastructure and alterations to the current fueling operations at airports. The respective efforts to realize a segregated fuel supply are discussed below based on the experiences made by conducting the demonstration flights. The implications derived from the demonstration flights are transferred to an approach where flights with the highest climate forcing (instead of flights for a particular route) would be targeted (section 4.2.3.1.1) and the general applicability of such a targeted use concept is discussed in terms of operational and economic efforts (section 4.2.3.1.2).

4.2.3.1.1 Targeting Flights with the highest Climate Forcing

While the segregated supply of the measurement campaign aimed at flights for an individual aircraft flying a specific route ("segregated use"), the largest climate benefits from using low contrail kerosene could be achieved by targeting the flights with the highest contrail energy forcing first ("targeted use"). This approach would most likely require the fueling of various aircraft flying on different routes and thus might incur additional operational efforts.

First, a model to provide a list with the highest climate forcing flights to be targeted is required, in order to allocate the available volumes of low contrail kerosene to the respective individual flights. This would require the use of ex-ante weather data. Once the data on the most climate relevant flights are available, basically the requirements of the segregated use concept would apply. Presumably, several aircraft would need to be fuelled by refueller trucks at a remote stand and the segregated refueller trucks should be compatible to those aircraft types (e.g., in terms of fuel panel height).

The requirement to use refueller trucks creates further implications concerning space requirements for refueling and fueling times. In general, the fueling time is a crucial factor for airline operation, since airlines aim at minimizing the time on ground to save cost and increase an aircraft's economic productivity [232]. While a typical short- to medium-range aircraft like the demonstration aircraft has a tank capacity of about 21 t [348], large long-range aircraft have a tank capacity of up to 250 t [349]. At an approxi-

mate capacity of 6.4 to 8 t, more than 30 trucks would be required for fueling such a long-range aircraft. Assuming a typical turnaround time of about 90 min [232], in the short-term it seems practically unfeasible to fuel long-range aircraft by refueller trucks in due time.

For short to medium range flights, in terms of the fuel supply system, no major obstacles would result when changing from the segregated supply of an individual route towards a targeted supply of the flights with the highest contrail energy forcing.

4.2.3.1.2 Applicability of a Targeted Use Concept

Table 4.3 summarizes additional efforts for the demonstration flights (chapter 4.2.2.1.1), their rationale to which extent they would be required in general and lists potential economic implications. The fuel supply systems of individual airports differ considerably; e.g., some are supplied by various means of transport from different refineries across the globe while others are more or less directly connected to a specific refinery [135]. Thus, implications for a particular airport might differ to some extent from the general points described below.

Table 4.3 Additional efforts during the measurement campaign, their rationale and general necessity as well as potential cost implications for a dedicated supply with low-contrail kerosene

Additional Effort for demonstration flights	Rationale	Generally required for segregated supply	Potential cost implication
Segregated storage and supply lines at Gävle	Avoid commingling when transferring kerosene from tank to loading bridge	A segregated tank in any case, most likely also supply lines	+10 % land-side storage capacity
Transport from Gävle to Stockholm airport by road tanker	Segregated supply via pipeline to Stockholm airport's fuel depot not feasible without construction of a second pipeline	Individual supply line from land-side fuel storage to air-side fuel storage	10 % of annual fuel consumption supplied by road tanker
Fueling by refueller trucks instead of hydrant system and dispenser	Enable segregated supply	Required, provided that airport has single hydrant system	Modification of supply lines, designated fleet of refueller trucks
Draining and cleaning of road tankers and refueller trucks	Avoid commingling with residual kerosene volumes	Required due to comparatively large filter capacity (>800 L)	No additional cost, due to designated fleet of low-contrail kerosene refueller trucks

Draining of demonstration aircraft	Avoid commingling with residual kerosene volumes	Required in case of large volumes of kerosene remaining on board	Assumed to be negligible
Aircraft fueling at remote stand	Provide sufficient space for refueller truck	Depending on available space at contact stands	Assumed to be negligible

Almost all of the additional efforts within the measurement campaign would also be required for the general application of a segregated supply for individual flights. This particularly holds for the segregated storage and supply lines at Gävle, the transport from Gävle to Stockholm airport, and also the use of segregated refueller trucks instead of the airport's hydrant system.

Fuel supply standards advocate that only specification-compliant kerosene is delivered to an airport [335]. Since this has historically always been one fuel type, supply lines from the land-side storage to an airport's fuel storage will generally not be capable for a segregated supply of two different kerosene options; e.g., in the case of Stockholm airport a large portion of the transport is realized by tank wagon, which could physically segregate two different kerosene options, but the last part is realized by a pipeline where kerosene options would necessarily commingle. As a result, the construction of a second supply line would most likely be required to realize a segregated supply at most airports. Since 3 % of all flights are estimated to cause about 80 % of the contrail climate forcing [9], it is assumed that about 10 % (considering a safety margin) of the airport's fuel use would need to be provided by such an additional supply line. Presumably, these amounts are too small to justify the construction of a pipeline and would rather be transported by road tanker.

Typically, an airport's fuel storage contains several individual tanks. In principle, a subset of those tanks could be used for low contrail kerosene, provided that their supply lines allow the targeted supply of a kerosene batch to a specific tank and also supply of e.g., a refueller truck by a specific tank. Thus, at least the modification of supply lines at an airport's fuel storage would be required in general.

The closed-loop single line structure of most hydrant systems prevents the segregated supply of a particular kerosene to a specific flight via hydrant systems. In principle, a segregated supply of different kerosene types could be realized at airports where the hydrant system is composed of multiple

supply lines. However, this is rarely the case [278] and thus the use of a refueller truck is typically required. Presumably, a designated fleet of refueller trucks for low-contrail kerosene would be required to prevent commingling with conventional kerosene. At space-constrained airports, fueling at remote stands would be additionally required.

In principle, a hydrant system could be sequentially fuelled by different kerosene options (e.g., at day vs. at night or during different seasons). In this case, the segregated supply would be less specific; i.e., also flights without large contrail energy forcing would receive low contrail kerosene. The mitigation potential of such strategies is subject of ongoing studies [134]. Additionally, the restriction to refueller trucks would constrain the targeted use concept to short and medium range aircraft (chapter 4.2.3.1.1).

Some other additional efforts of the demonstration flights might not be strictly necessary for a general application of a segregated low contrail kerosene supply, but rather prevent commingling with smaller volumes of conventional (crude oil based) kerosene. This mainly relates to draining and cleaning of the road tanker, the refueller trucks and the demonstration aircraft itself. Provided that the remaining kerosene volume in each of them is small compared to the new load of low contrail kerosene, a certain extent of commingling with conventional (crude oil based) kerosene might be acceptable. Most likely, this would come at the cost of a slightly reduced kerosene hydrogen content and thus reduced climate benefits.

As a result, the economic implications for a segregated fuel supply are comprised of adding 10 % additional fuel storage at the airport's land-side, additionally supplying 10 % of the airport's fuel consumption by road tanker and procurement and operation of a dedicated fleet of refueller trucks. Since such infrastructure is usually commonly owned by the airport and fuel suppliers (at least for most European airports) [279], these changes would most likely increase the handling fees charged by the airports. Typically, such fees amount to less than 5 % of an airline's cost [232]. As a result, the segregated supply with low-contrail kerosene would most likely increase cost from an airline perspective by less than a few %-points. This increase seems rather small compared to current estimates for mitigating carbon dioxide-related climate impacts either by using renewably sourced kerosene [32, 91, 94] or liquefied hydrogen [350, 351]. However, a comprehensive economic analysis would be required for a sound compari-

son among the marginal abatement cost for reducing contrail-related climate impacts by a segregated fuel supply and the marginal abatement cost for reducing carbon dioxide-related climate impacts by renewably sourced kerosene or hydrogen. Such an investigation – while being beyond the scope of this study – is clearly an interesting area for further research. The implementation of a targeted use of low-contrail kerosene could be stipulated by economic incentives. As of now, only the carbon dioxide-related climate impact of aviation is considered in most mitigation policies [325], the European Union presently introduces a monitoring, reporting and verification scheme for aviation's non carbon dioxide-related climate impacts by 2025 [45]. Assuming that future mitigation policies will also aim at aviation's contrail-related climate impact and a broadly accepted methodology to determine the contrail climate forcing of individual flights will be implemented, also different economic approaches such as the inclusion in emissions trading schemes, subsidies or penalties for contrail-related climate impacts could be developed.

4.2.3.2 Satellite Detection of individual Contrails

For this study, the evolution of all 28 contrails simulated by CoCiP (out of 84 demonstration flights) were visually assessed and tracked during their evolution with corresponding images of the second generation EUMETSAT satellite (Figure 4.12).

To investigate the uncertainty in the ERA5 weather data input (mainly humidity and 3-dimensional wind velocities at cruise) the "Volcanic Ash RGB" color scheme [352–354] was applied. Most of the contrails on the satellite images (n = 21) were at least partially covered by other clouds, impeding a visual detection of the potential contrails. The remaining contrails (n = 7) are too few for a detailed statistical analysis. . Thus, a thorough validation of contrail mitigation strategies by satellite data would require substantially larger sample sizes and ideally also a multi-seasonal timespan. Such studies are part of current research projects (e.g., D-KULT [355]). Video files of all demonstration flights are available in the digital supplement.

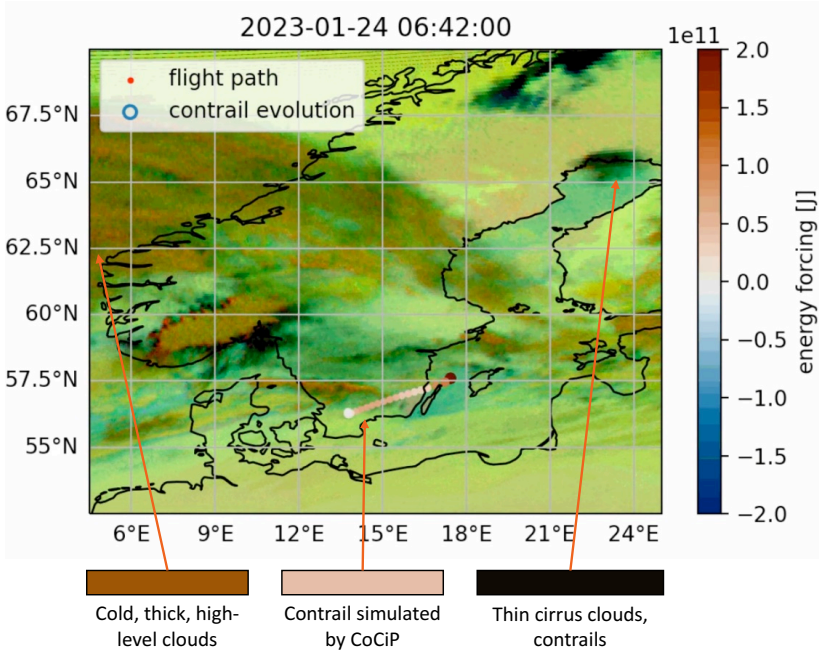


Figure 4.12 Contrail simulated by CoCiP and corresponding Volcanic Ash RGB image from EUMETSAT 2G satellite images for 24th January 06:42 UTC (all demonstration flights are available as videos via the digital supplement)

4.2.3.3 Contrail Climate Benefits

Figure 4.13 shows the resulting contrail energy forcing assuming the kerosene options described in section 4.2.2.3.2. The energy forcing of warming contrails is indicated by positive values (light orange) and cooling contrails are depicted as negative value (light blue). The net energy forcing (black) is clearly positive and decreases by increasing kerosene hydrogen content. In comparison to "conventional average", the contrail energy forcing of "conventional low hydrogen" increases by almost 13 m-%. The 2 m-% blend of "blend uniform" alters the contrail energy forcing only marginally (less than 2 -%), while the 35 m-% blend labelled "blend demo" (Table 4.2) and the 50 m-% blend named "blend max" (Table 4.2) lowers the energy forcing by about 10 % and 23 %, respectively.

The comparison of the two conventional (crude oil based) options highlights the uncertainty resulting from the conventional kerosene composition being here in the order of magnitude of 10 %. As a result, the difference between "conventional average" and "blend uniform" (Table 4.2) can hardly

be considered significant. Despite the large effect of the conventional kerosene's hydrogen content, only very limited data is publicly available [179]. Measuring or estimating the hydrogen content of the kerosene used for individual flights would substantially improve the estimation of their contrail energy forcing.

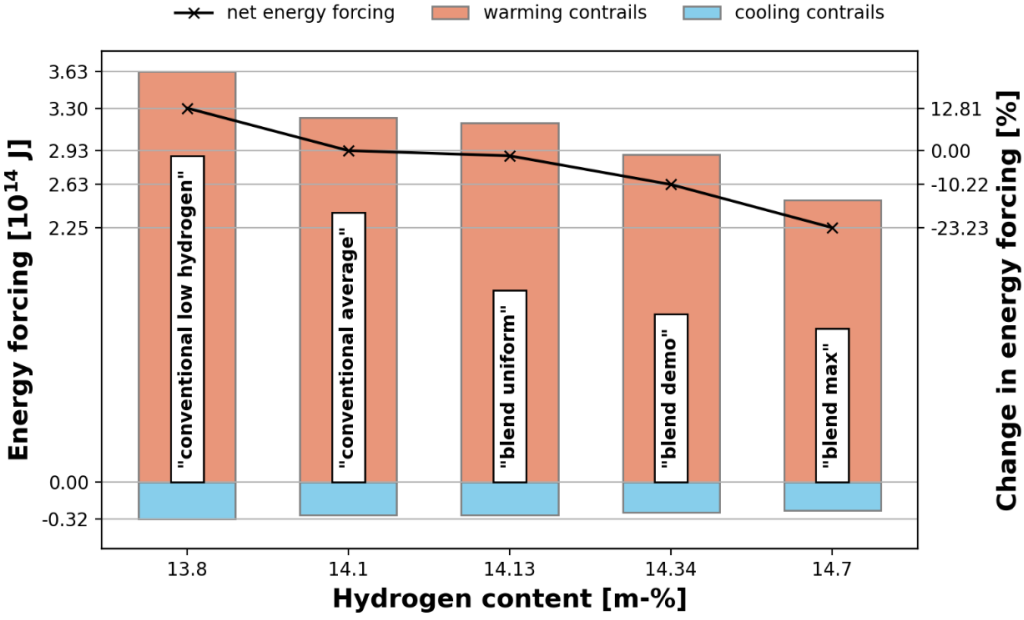


Figure 4.13 Contrail energy forcing of the simulated flights (n = 84) in absolute terms (left ordinate) and relative change (right ordinate) compared to the "conventional average" kerosene (Table 4.2)

Overall, for the aircraft-engine combination used in these simulations, the segregated use of low contrail kerosene reduced the associated contrail energy forcing by more than 10 %, compared to the "conventional average" kerosene (Table 4.2). This is broadly in line with previous mitigation potential estimates for this hydrogen content [281]. For the theoretically maximum blend share of 50 m-%, the mitigation potential would increase to about 20 %. These values are roughly in accordance with other investigations [281]. Simultaneously, kerosene specifications require certain amounts of aromatic molecules in a low contrail kerosene blend, while renewably-sourced kerosene typically do not contain any aromatic compounds. Hence, the conventional kerosene for such blends would require a comparatively high amount of aromatics [135]. This effect might in turn slightly reduce the mitigation potential of the 50 m-% blend.

In absolute terms, warming contrails largely outweigh cooling contrails for any of the fuels investigated. This can be explained by daily and seasonal variation. In theory, during daytime contrails typically exhibit a cooling climate forcing by reflecting incoming shortwave (solar) radiation to a larger degree than they absorb outgoing longwave (terrestrial) heat radiation. At night a contrail only absorbs outgoing longwave radiation and thus causes a warming climate forcing. Despite that, most demonstration flights take place between 06:00 am and 22:00 pm local time. Therefore, the fraction of cooling contrails has been small (cf. Figure 4.13). At Stockholm airport the difference between sunrise and sunset is only about 7.5 h in January, which is more than 10 h less than on 21st June. Since the demonstration flights took place in January and February, most likely their contrail climate forcing was substantially higher compared to a situation if they would have been realized in June or July. This effect will be less pronounced for regions at lower latitude, since the seasonal variation of sunrise and sunset times is lower for lower latitudes.

4.2.4 Conclusion

The targeted use of low contrail kerosene on particularly climate relevant flights has previously been discussed in various, simulation-based studies. This investigation derives the operational efforts for such a concept based on the segregated supply of low contrail kerosene to 84 flights between Stockholm airport and Copenhagen airport. The operational efforts are weighed against a simulation-based estimate of the demonstration flights' contrail climate benefits, assuming an experimentally validated aircraft-engine combination. Beyond the operational efforts for supplying the demonstration flights, implications for targeting flights based on their climate forcing are derived and a targeted use at large-scale is discussed.
The main results can be summarized as follows.

- For the current infrastructure, a segregated supply of low contrail kerosene can be realized for short to medium range flights, or in other terms any flight which can be fuelled by refueller trucks at an outside position. To realize such a concept, large parts of the supply chain (e.g., supply lines to and at airports) would need to be duplicated, incurring additional efforts and of course further costs. Targeting long-range flights with low-

contrail kerosene would most likely require a multiple line hydrant fueling system at airports, which would need to be constructed at most airports and thus incur additional cost and be available in the medium to long term only.

- A segregated supply of e.g., a particular flight route (as employed during the demonstration flights) and targeting flights with highest contrail energy forcing first are almost identical in terms of operational efforts. Primarily, it might be necessary to allocate several remote stands for a targeted use concept (instead of one). The general applicability of a targeted use concept, however, is highly airport specific; nevertheless, it is most likely that in most cases large sections of the kerosene supply infrastructure would need to be duplicated and / or an additional other fuel supply system would need to be installed.
- In terms of contrail climate benefits, the segregated supply of low contrail kerosene reduces the contrail energy forcing for the aircraft-engine combination with the 35 % blend assumed here by about 11 %. A higher blend share could increase these benefits towards a reduction of more than 20 %, specifically targeting flights with the highest contrail energy forcing could allow for even greater contrail climate benefits [10]. Additionally, the mitigation potentials for flights conducted at other latitudes will be altered by a different ratio of day- and night-time for different seasons.
- The coarse estimation of the cost implications for a segregated fuel supply indicates a cost increase due to the abovementioned infrastructure modifications. These cost seem to be smaller than the marginal abatement cost of e.g., renewably sourced kerosene or the direct use of hydrogen. For the development of incentive schemes to facilitate a targeted low-contrail kerosene supply, several prerequisites exist, such as the inclusion of aviation's contrail-related climate impacts in mitigation targets or an accepted and validated approach to determine the contrail climate forcing of an individual flight.

Estimating the absolute contrail energy forcing of individual flights is still strongly affected by the available input data (e.g., meteorological data), but these uncertainties do not affect the relative changes given here. Uncertainties in fuel composition data increase towards the highest hydrogen content fuels. Further uncertainties exist for new engine (turbine) models (e.g.,

lean-burn combustors), when ice activation on soot particles might be replaced by other processes. When comparing the use of different kerosene options for an identical set of flights, the meteorological uncertainties do not play a role for the relative changes in contrail forcing. As a result, the relative contrail benefits are subject to smaller uncertainties than the absolute values of the demonstration flights contrail energy forcing.

The study of those uncertainties highlights important areas of further research: Increasing the accuracy of atmospheric weather data at aircraft cruise altitude (especially humidity data) would allow for more reliable estimations of contrail evolution and associated contrail energy forcing. Also, more detailed information about kerosene properties (e.g., by using sensors during refueling) would improve the reliability of current models. The same holds for experimental data about modern engines and the implementation of engine aging in current contrail climate impact models.

Solutions for the infrastructure modifications are technologically and organizationally available. The primary barrier are the efforts and thus the costs for their implementation. Considering that several companies are aiming to develop a hydrogen fueled aircraft within the next decade [32, 78], cost due to infrastructure modifications for a targeted use concept appear comparatively small. Estimating the investment and operational costs of the discussed efforts would be an important step towards calculating the marginal abatement cost of a targeted use concept and thus to compare it against other mitigation strategies, which is partially envisioned as future work of the ALIGHT research project

Overall, by conducting the demonstration flights, a segregated supply of low contrail kerosene was successfully demonstrated in an experimental setting. Contrail climate benefits were quantified based on simulations. An insightful next step would be to compare the weighting between operational efforts and contrail climate benefits described here against other climate mitigation options for aviation.

4.3 Blending of Aviation Powerfuels

Zschocke, Alexander; Quante, Gunnar; Bullerdiek, Nils; Pechstein, Jan (2025): Blending of Aviation Powerfuels, in POWERFUELS: Status and prospects, [S.l.]: SPRINGER INTERNATIONAL PU, 2025, pp. 791–818.
Typesetting and formatting are slightly adjusted to ensure consistency within this thesis.

Abstract

As the global energy landscape evolves in response to anthropogenic climate change, there is an increasing focus on using sustainable alternatives to conventional fossil-based fuels. In aviation such an alternative is provided by drop-in synthetic fuels which can blended with fossil kerosene to produce a blend that is virtually indistinguishable from conventional kerosene and is fully compatible with existing infrastructure. However, for most of these fuels blending is a crucial part of the process as the fuels are not fully drop-in on their own. This topic is discussed in the following chapter, with a focus on powerfuels.

4.3.1 Introduction

As the global energy landscape evolves in response to anthropogenic climate change, there is an increasing focus on using sustainable alternatives to conventional fossil-based fuels. Yet, in sectors where end-use applications will continue to depend on liquid hydrocarbon fuels in the foreseeable future (e.g., in aviation, maritime sector), a mixing or "blending" of fossil-based fuels with renewably sourced ones, like Power-to-Liquid (PtL) hydrocarbons, may not only become necessary but also be beneficial when leveraging existing fuel infrastructure. Moreover, blending of different fuel types from renewable sources would ease infrastructural efforts. Thus, a thorough understanding of the implications of blending hydrocarbon fuels in general and powerfuels in particular is central for a smooth transition from fossil fuels towards renewable alternatives. In this context, various aspects related to the blending of renewable and conventional fuels are examined in this article using the example of synthetic kerosene in aviation. The overarching intention is to highlight different fuel properties critical for blending and explain how these properties influence permissible blending ratios of conventional and synthetic fuel components.

Therefore, first an overview of specifications for both conventional (fossil) and synthetic kerosene is provided, along with aspects of blending these kerosene types. Subsequently, for conventional kerosene and synthetic kerosene of relevant powerfuel conversion pathways, characteristic physical and chemical properties are described and their variations discussed. Based hereupon, conclusions towards maximum permissible blending shares are drawn from a present-day perspective. The chapter concludes with an outlook on potential future developments.

4.3.2 Kerosene Specifications and Blending

In this section, a concise overview of aviation (turbine) fuel specifications for both conventional and synthetic kerosene is presented and overall aspects on blending of both options in light of existing specifications are outlined.

4.3.2.1 Kerosene Specifications

Aviation fuel characteristics are determined by fuel specifications that primarily define performance, material, and manufacturing properties. Given that the air transport system is an international market, aviation fuel standards apply virtually global, with minimal regional political differences in fuel specifications (this uniformity is also the case in other sectors, such as maritime transport). The predominant aviation kerosene specifications in the Western world are the Jet A/A-1 specification administrated by the ASTM International and the Jet A-1 specification administered by the United Kingdom's Defence Standard (DefStan) organization. Both organizations coordinate their activities closely to harmonize their specifications to the greatest extent possible. Based on these prevailing aviation fuel specifications, kerosene can be categorized into conventional and synthetic types. The corresponding fuel specifications, or specific aspects thereof, are described in greater detail below.

Conventional kerosene (ASTM D1655 specification). For conventional kerosene, the central specification is known as ASTM D1655. The parameters and limits specified in ASTM D1655 are primarily based on historical reasons, stemming from experiences with kerosene derived from fossil crude oil, which has been the predominant feedstock. The properties of conventional kerosene vary significantly, depending on crude oil feedstock and refinery operation [39]. Even with the rigorous standardization of aviation fuels, ASTM D1655 does not prescribe an exact chemical composition for the fuel, such as specifying certain hydrocarbons. Rather, it sets out minimum and maximum requirements for performance, material and manufacturing properties [356]. This flexibility allows for a range of hydrocarbon compositions in the fuel, for example with regard to variations in contents of n- and iso-alkanes, cycloalkanes, and aromatics (owing to the fact that the properties of a kerosene fraction can differ, depending on the particular crude oil processed). Despite these permissible variations, the fuel properties must remain within the specified compliant range of performance, material and manufacturing properties, such as fuel density, freezing point, smoke point or aromatic content (Figure 4.14).

Synthetic Kerosene (ASTM D7566 specification). For synthetic kerosene, defined from a specification perspective as aviation fuel not produced from crude oil, ASTM is also the leading organization. The primary

ASTM specification for synthetic kerosene is ASTM D7566 with its respective annexes [280].[15] Each annex specifies the production pathway and the required properties of a particular specific synthetic kerosene option. As of October 2023 (at the time of writing) eight respective production pathways have been approved by ASTM and are included in the ASTM D7566 specification. These are presented in the following Table 4.4, together with two co-processing pathways (specified in ASTM D1655), which involves the joint refining of certain feedstocks or intermediates alongside with conventional crude oil in refineries.

Table 4.4 Approved production pathways for synthetic kerosene (at the time of writing; A: aromatics; AtJ: Alcohol-to-Jet; CH: Catalytic Hydrothermolysis; FT: Fischer-Tropsch; HC: Hydrocarbons; HEFA: Hydroprocessed Esters and Fatty Acids; HFS: Hydroprocessed Fermented Sugars; SIP: Synthetic Isoparaffins; SK: Synthetic Kerosene; SKA: Synthetic Kerosene with Aromatics; SPK: Synthetic Paraffinic Kerosene)

ASTM	Annex	Year of approval[a]	Process	Blending-Limit[b]
D7566	1	2009	FT-SPK	50 vol.-%
	2	2011	HEFA-SPK	50 vol.-%
	3	2014	HFS-SIP	10 vol.-%
	4	2015	FT-SPK/A	50 vol.-%
	5	2016	AtJ-SPK	50 vol.-%
	6	2020	CH-SK	50 vol.-%
	7	2020	HC-HEFA-SPK	10 vol.-%
	8	2023	AtJ-SKA	50 vol.-%
D1655	-	2018	Co-Processing of vegetable oils	5 vol.-% [c]
	-	2020	Co-Processing of FT-crude	5 vol.-%

[a] This refers to the initial approval. After the initial approval, approved processes were partially adapted, for example by increasing the maximum blending limit or by expanding the raw materials that can be used.
[b] Precautionary maximum blending limit of the synthetic kerosene component
[c] An increase of the blend ratio to 30 vol.-% is currently prepared for approval as ASTM. This increase will require that the co-processing includes a hydrocracking step.

The first ASTM D7566 pathway for synthetic kerosene was already approved in 2009, based on the Fischer-Tropsch technology. In the subsequent years since then, various other pathways have been added. The maximum blending limit for all these options is currently at 50 vol.-%, with some pathways having significantly lower limits in the range of 5 to

[15] ASTM specifications are available at the ASTM website (www.astm.org/products-services/standards-and-publications.html). Except where stated otherwise, references to ASTM D7566 in this paper refer to ASTM D7566-23a, which is the version in force at the time of writing. However, this specification is frequently updated, and at the time of printing a more recent version may well be in force.

10 vol. %. The subsequent section describes these aspects and the corresponding blending procedure in more detail.

4.3.2.2 Blending of Synthetic Kerosene

In the following, first, a general overview of blending is provided. Subsequently, the blending of synthetic and conventional kerosene is described in the context of the previously presented specifications.

Blending in General. Blending, as used in oil industry parlance, generally refers to the intentional mixing of two or more fluids with the intention of creating a blend meeting a defined specification. It is different from incidental commingling of fluids meeting the same specification, which routinely happens when crude oils or products come together in pipelines or common tank storage:

- Blending of fluids. Blending may involve two different batches of a product meeting the same specification, as for example if one parameter in one of the batches is marginal and needs to be improved by blending. But more typically, it involves blending of two or more different products. A well-known example is the blending of road gasoline with a certain percentage of bio-ethanol, where both the gasoline and the ethanol have to meet individual, but different, specifications. Another example is the supply of (renewable) synthetic kerosene for aviation, where a synthetic kerosene component compliant to one specification (ASTM D7566) is mixed with a (currently typically fossil-based) kerosene component compliant to another specification (ASTM D1655).
- Commingling of fluids. Comingling refers to mixing fuel batches of the same specification in an uncontrolled environment. In particular commodities (e.g., aviation or maritime fuels) are subject to comingling, since they are globally traded and thus undergo bulk transportation and storage. Especially the use of pipeline systems or large storage tanks cause comingling, which in turn can result in an averaging tendency of fuel properties. As in case of aviation only certified fuel is fed into the fuel distribution systems, commingling is considered uncritical. Therefore, it will not be addressed in this chapter in greater detail.

In blending, a complete mix of the blended fluids is aimed for, unlike in incidental commingling where mixing typically only occurs at the border zone

between two batches. Large-scale blending therefore typically involves the use of dedicated mixing equipment. This, however, is not a legal requirement, and small-scale blending of synthetic and conventional kerosene in early trials has involved more ad hoc methods, like repeatedly pumping around in a single tank or pumping between several tanks.

Blending of Conventional and Synthetic Kerosene. From an operational perspective, synthetic kerosene options are primarily designed to serve as "drop-in" fuels. This designation necessitates their seamless integration into the existing aviation fuel supply infrastructure and compatibility with current aircraft fleets alongside other specification-compliant aviation fuels. Consequently, to achieve this, they must adhere to the fuel requirements of ASTM D1655. Thus, they are not required to have a specific chemical composition, but, similar to ASTM D1655, they need to meet a certain prescribed set of performance, material, and manufacturing properties, as illustrated in Figure 4.14.

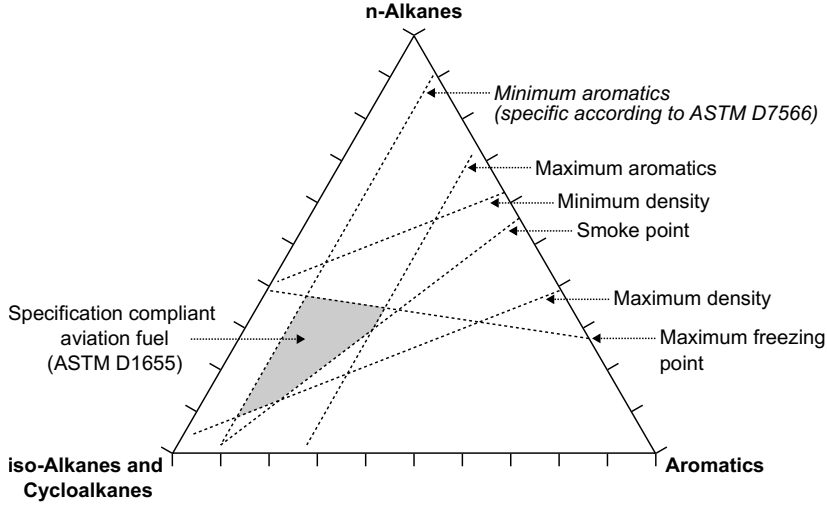


Figure 4.14 Relationship between aviation fuel composition and the synthetic kerosene fuel specification domain (Ar: aromatics; BC: branched alkanes and cycloalkanes, n: n–Alkanes; based on [74])

However, despite a multitude of nearly identical properties, (many of) the neat synthetic kerosene options produced in compliance with ASTM D7566 differ in some respects from typical ASTM D1655 Jet A/A-1 aviation fuel, for example in terms of their aromatics content. Therefore, to use the synthetic kerosene as aviation fuel and ensure adherence to the properties defined by ASTM D1655, so far an additional process step, namely blending, is re-

quired. In this blending process, the synthetic kerosene (synthetic blending) component is mixed with (conventional) ASTM D1655 aviation fuel. Therefore, ASTM D7566 not only contains the specification on synthetic kerosene in its respective annexes, but also the required properties of a blend between a conventional ASTM D1655 kerosene component and a synthetic blending component ("blend specifications"). This blending procedure and interplay of the aviation fuel specifications mentioned is schematically shown in Figure 4.15.

The ASTM D7566 specification defines a precautionary maximum blending ratio (as shown in Table 4.4) and defines properties for both the neat synthetic component as well as the blended fuel ("blending requirements"). These blend specifications cover the requirements of ASTM D1655 and some additional ones. The practically achievable blend ratio largely depends on the properties of the conventional blending component. Thus, a conventional blend component which is compliant with ASTM D1655 is not necessarily compliant with the ASTM D7566 blend specifications. If its properties are unfavorable (e.g. aromatic content), the allowable blending ratio must remain below the precautionary maximum. On the other hand, with particularly favorable conventional kerosene batches even higher blending ratios than currently approved (Table 4.4) would be achievable, if ASTM was to abolish the precautionary requirement. This is the reason, why also the properties of the conventional blending component need to be taken into account for fuel blending (section 4.3.3).

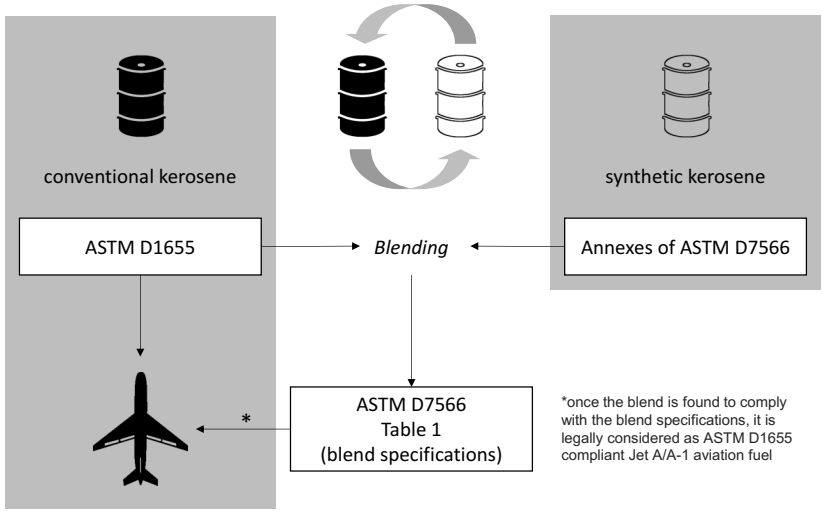


Figure 4.15 Specification and certification of conventional and synthetic kerosene

4.3.3 Conventional Kerosene

The classical petroleum fuels – gasoline, kerosene, and diesel – are conventionally produced by fractionated distillation of crude oil. Basically, they are defined by a certain boiling range. In case of kerosene this is approximately 170 to 270 °C [39]. The properties of conventional kerosene vary to a great extent. Hence, they also influence permissible blend ratio significantly. The most important properties directly result from the chemical composition, which, however, usually is not analyzed itself. This chapter will therefore provide a brief outline of the main constituents in kerosene with regard to the chemical composition in terms of hydrocarbon components, the aromatics content, the density as well as distillation curve characteristics.

In order to illustrate the variety of properties of conventional kerosene with regard to aromatics content, the density as well as distillation curve characteristics, a dataset of a study on German kerosene properties is used in the respective sections [135]. Other studies are available, e.g., the World Fuel Sampling Program and the Petroleum Quality Information Service (PQIS) in the UK [179, 180, 357]. However, to ensure comparability, the following section focusses on the dataset of Germany only. It contains data from ca. 2,000 fuel certificates representing the fuel used at 14 major airports in Germany.

4.3.3.1 Chemical Composition

Kerosene derived from conventional sources typically consists of thousands of different molecules that can be categorized into a few main types, mainly hydrocarbons. Their carbon numbers are normally distributed as depicted in Figure 4.16.

By far most molecules of conventional kerosene have a carbon number between C_8 and C_{16} [358]. However, compounds up to C_{19} may be detected [359]. The precise composition varies due to factors such as the type of crude oil used and the refining process. Overall, it is a complex mixture of various hydrocarbons. The main hydrocarbon components of aviation fuel include alkanes (paraffins) in the form of n-alkanes and iso-alkanes, cycloalkanes, and aromatics – as well as alkenes to very minor amounts:

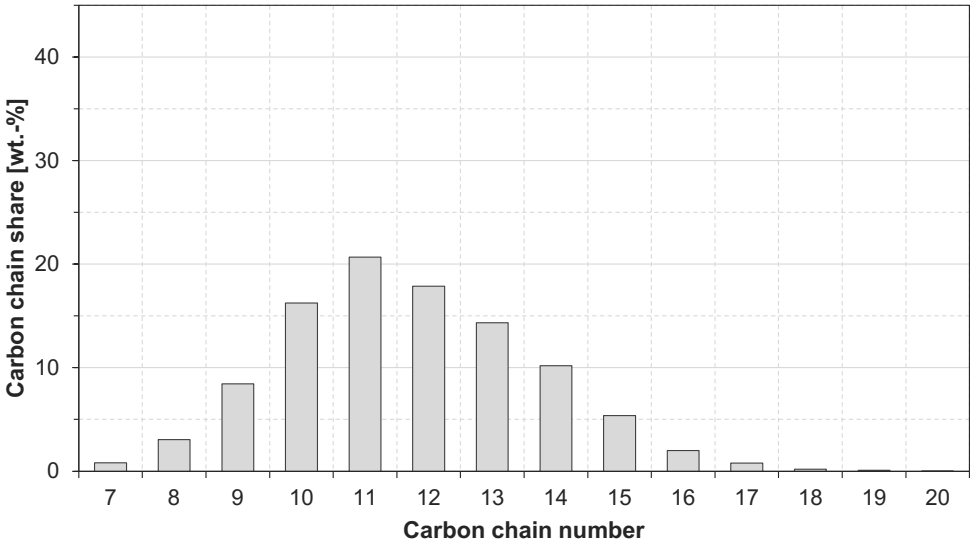
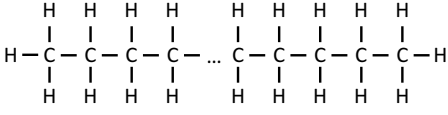


Figure 4.16 Carbon chain distribution of a sample Jet A kerosene from fossil-based crude oil[16]

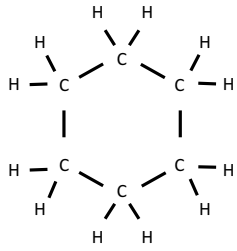
- **Alkanes (paraffins).** Alkanes, or paraffins, are straight or branched chain molecules. The straight / linear alkanes are commonly referred to as n-alkanes while the branched alkanes are referred to as iso-alkanes. As a general rule, the freezing point of iso-alkanes is lower than their corresponding n-alkane with the same carbon number. Alkanes are the major constituent in conventional aviation fuel. Among all hydrocarbons, they offer the largest hydrogen-to-carbon-ratio. Regarding the hydrocarbons found in aviation fuel, they burn cleanest and offer the highest net heat of combustion at the lowest density [18, 179]. Their composition conforms to Equation (1):



$$C_nH_{2n+2} \qquad (1)$$

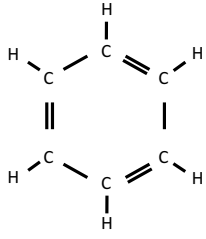
- **Cycloalkanes.** Cycloalkanes are saturated ring molecules with a slightly lower hydrogen-to-carbon ratio than alkanes. This results in a reduced heating value and an increased density in comparison to alkanes [358]. Their composition conforms to Equation (2):

[16] Data are for reference conventional kerosene in LanzaTech research report, Table A 3.1c.



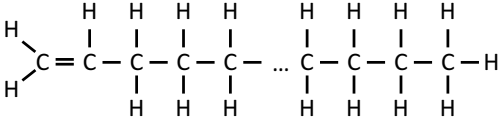
$$C_nH_{2n} \tag{2}$$

- **Aromatics.** Aromatics also are ring-shaped molecules but contain carbon double binds. They have the lowest hydrogen-to-carbon ratio resulting in the lowest heating value and the greatest density. When burned, aromatics act as soot precursor [15, 16, 18, 357]. Short hydrocarbon chains may be attached to the ring structure [39, 358]. The chemical composition of aromatics is described by Equation (3):



$$C_nH_{2n-6} \tag{3}$$

- **Alkenes (olefins).** Alkenes, or olefins, are unsaturated alkanes, i.e., at some point of the hydrocarbon chain is a double bound instead of a hydrogen atom. They are not chemically stable and therefore undesirable, hence their presence in kerosene is limited to minor amounts only. By far most of them originate from cracking processes within the refinery [179, 280]. Their composition conforms to Equation (4):



$$C_nH_{2n} \tag{4}$$

Saturated hydrocarbons (alkanes and cycloalkanes) account for approx. 72 to 88 vol.-% in aviation fuel [360]. Of these, cycloalkanes amount to approximately 30 vol.-% [179, 361]. When presuming that aromatics amount to ca. 18 vol.-% [135, 362] and alkenes do not exceed 1 vol.-% [280], a typical conventional aviation fuel may be approximated as shown in Figure 4.17.

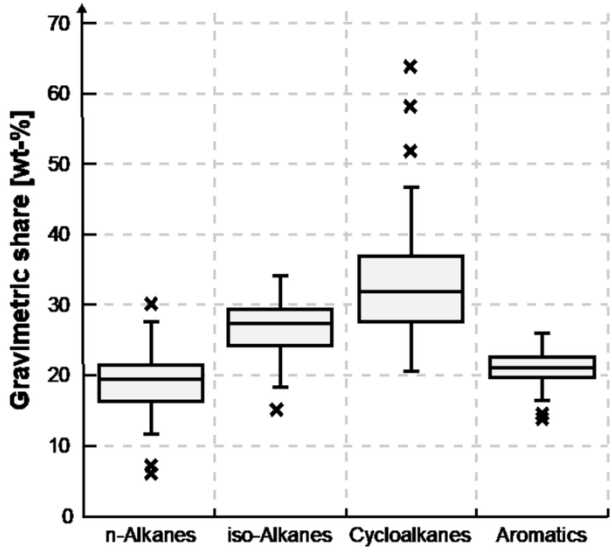


Figure 4.17 World Fuel Survey distribution of hydrocarbon types in aviation fuel [179]

Besides those components described above, conventional aviation fuel also contains non-hydrocarbons. From this group, sulfur is the most important representative. This element occurs either pure or in chemical compounds. In either form, it is corrosive and its presence is limited by specification to a maximum of 0.3 wt.-%. Usually 99 % of the sulfur is bound in thiophenes [39, 179] belonging to the group of heteroorganic compounds. These are molecules containing sulfur, nitrogen or oxygen. Even in very small amounts, they improve the lubricity and inhibit oxidation. But they tend to form deposits and degrade the ability of water separation (due to polarity).

Furthermore, naphthenic acids may be present in conventional aviation fuel as their boiling range is similar to kerosene. They are aggressive and therefore undesired. When reacting with certain metals they tend to form soaps. The described non-hydrocarbons can be removed by caustic washes or hydroprocessing in combination with clay filtering [179, 357]. The share of these compounds in conventional aviation fuel is variable. It may reflect the characteristics of the crude oil and is strongly influenced by the refinery technology used for kerosene production [179, 280]. As a rule of thumb, straight-run kerosene contains the highest amount of non-hydrocarbons. With increasing hydroprocessing severity, their number is successively reduced.

4.3.3.2 Aromatics Content

The specification limits for aromatics content of conventional kerosene are maximum 25 vol.-% if measured following ASTM D1319 and 26.5 vol.-% if measured in accordance with ASTM D6379. For the final aviation fuel blend, ASTM D7566 also requires a minimum aromatics content of 8 vol.-%. An exemplary aromatic content of aviation fuel batches when leaving the refinery is shown in the following Figure 4.18, based on data from the mentioned study at 14 major airports in Germany [135].

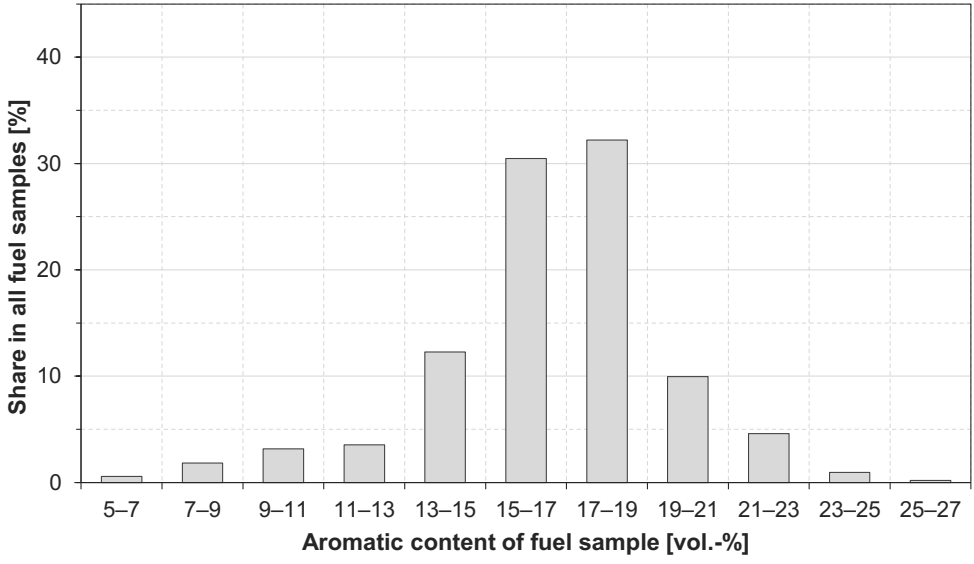


Figure 4.18 Aromatic content of aviation fuel batches when leaving the refinery [135]

The minimum aromatics content in the dataset of the study were 5.9 vol.-% and the highest 25.5 vol.-%. As shown in Figure 4.18, the modal values range from 15 to 19 vol.-%. This covers roughly 60 % of the corresponding samples in the dataset, while aviation fuel batches with lower and higher aromatics contents account for less than 40 %. Note that those values were obtained by ASTM D1319 and ASTM D6379. Both methods give similar results, but ASTM D6379 results in somewhat higher values.

When comparing the aromatic content of all samples with batches from tank farms and pipelines (Figure 4.19), a clear averaging tendency can be observed. The comingling of fuel batches in tanks and pipelines yields fuel properties closer to the average values, thus reducing extreme values.

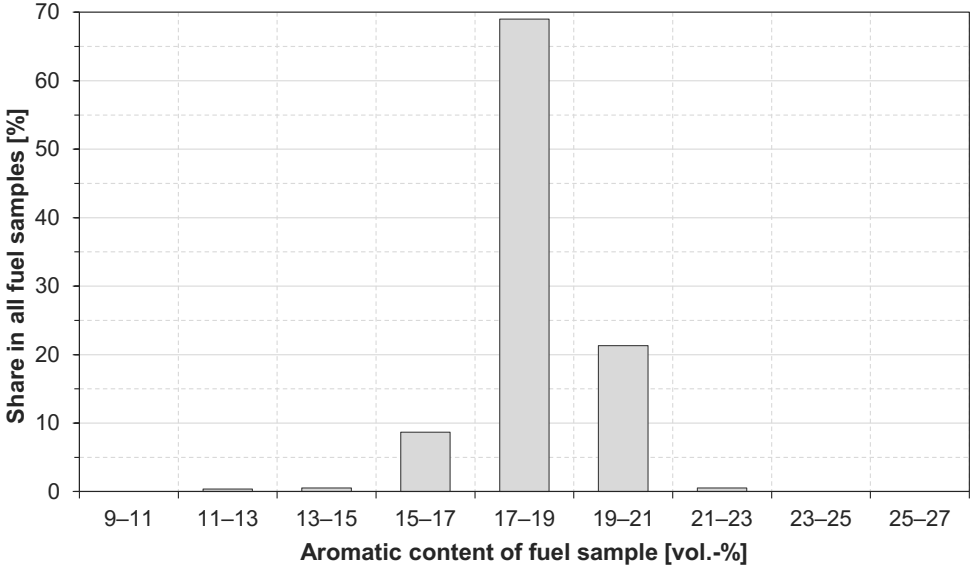


Figure 4.19 Aromatic content of aviation fuel batches from tank farms and pipelines [135]

Bearing in mind the current requirement of a minimum aromatics content of 8 vol.-% for synthetic kerosene blends, it is noteworthy that 15 of the German batches had an aromatics content lower than 8 vol.-%, as conventional ASTM D1655 kerosene is not required to meet the 8 vol.-% minimum. These batches were all produced by one refinery over a course of two months, and were delivered directly from the refinery to two airports, where this refinery was in one case the only and in the other case the major supplier. No adverse issues relating to the low aromatics content were observed at these airports while this low aromatics fuel was delivered and used.

4.3.3.3 Density

ASTM D1655 defines a density range from 775 to 840 kg/m^3. The minimum density found in the German dataset was 786.9 kg/m^3, and the maximum was 834.2 kg/m^3. As shown in Figure 4.20, the majority of the samples falls in the range between 795 and 805 kg/m^3. These account for approx. 67 % of the samples. In less than 10 % of the fuel batches sampled, densities were discovered to be lower than 790 kg/m^3 or higher than 815 kg/m^3. This indicates that such extreme density values were relatively rare occurrences within the sampled batches.

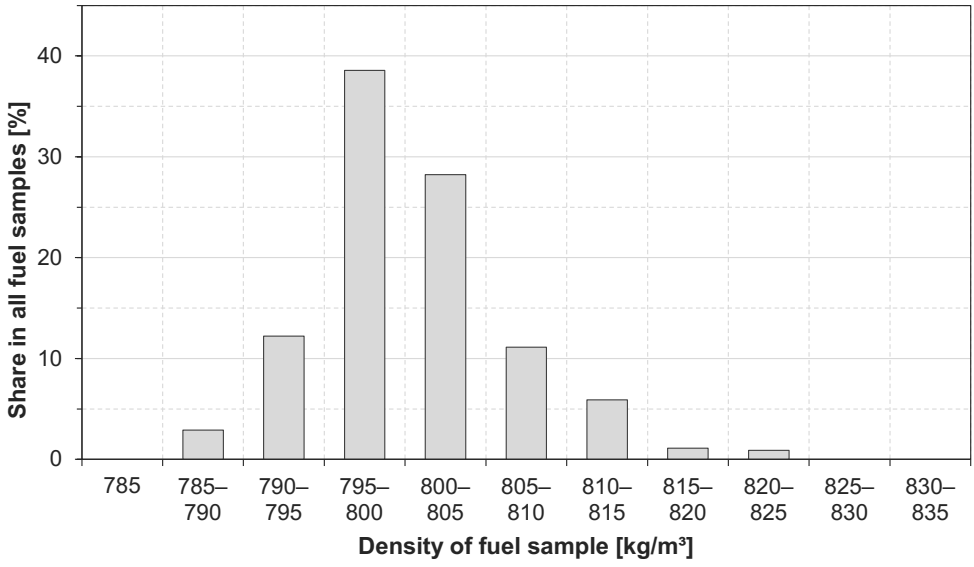


Figure 4.20 Distribution of density in conventional kerosene in Germany [135]

All values are well within the specification range. ASTM D7566 uses the same density range for the blend as ASTM D1655 requires for the conventional kerosene component, hence the density distribution of the conventional blend component seems generally well suited for blending.

4.3.3.4 Distillation Curve

The variety of hydrocarbons (in terms of carbon-chain lengths and molecular structure) of conventional kerosene (Figure 4.16) results in the phenomenon that during distillation certain components evaporate earlier than others. Thus, a part of components in conventional kerosene evaporates at lower temperatures (e.g., 150–180 °C) while others need substantially higher temperatures for evaporation (ca. 240–260 °C). As per ASTM D1655, one temperature for the recovery of 10 vol-% (205 °C) is defined to control the fuel's volatility and ease of evaporation. This temperature is referred to as "T10" and is important for engine start performance. In turn, the final boiling point (maximum 300 °C) prevents undesired heavy fractions (alkanes beyond C_{16}, poly-aromatics) from being incorporated in the fuel [280]. Figure 4.21 illustrates that the distillation slopes of the conventional aviation fuel in Germany are very similar [98]. A share of 90 % of the samples remain within a spread of less than 36 °C.

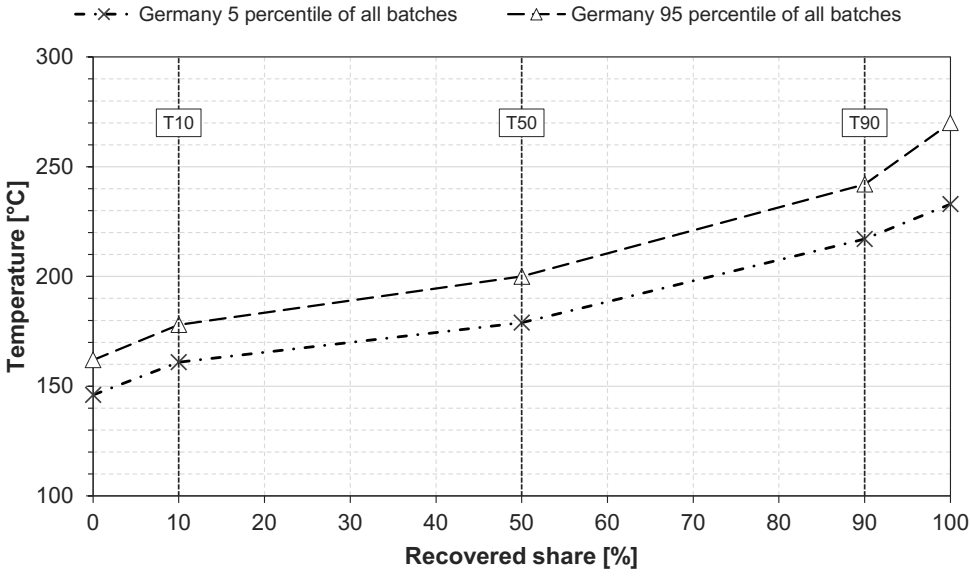


Figure 4.21 Distillation curve gradient range for conventional kerosene in Germany [135]

In order to replicate this behavior, ASTM D7566 requires the synthetic kerosene (blend) to show a similar behavior [280]. In addition to the maximum limits for T10 and the final boiling point, a minimum temperature rise of 15 °C is required between the 10 % recovery temperature and the 50 % recovery temperature (T50-T10). From 50 % recovery to 90 % recovery (T90-T50) an increase in temperature of at least 40 °C is mandatory.

ASTM D1655 (conventional kerosene) does not specify a certain minimum gradient. Thus – as for aromatics – there may be conventional batches that do not conform with ASTM D7566 (blend specification). Actual requirements towards distillation gradients are under investigation [280].

4.3.4 Synthetic (Powerfuel) Kerosene

None of the ASTM D7566 annexes are specific to synthetic kerosene that can be produced by Power-to-Liquid (PtL) production pathways. Rather, the production pathways specified in the annexes typically start from an intermediate product and describe the conversion of the intermediate product to a kerosene blending component. For example, the Alcohol-to-Jet (AtJ) SPK pathway describes the conversion of either ethanol or iso-butanol to a synthetic Alcohol-to-Jet (AtJ) SPK blending component, regardless of how the alcohol itself has initially been produced. Such alcohol can possibly be

the result of a Power-to-Liquid (PtL) process, but can equally result from biomass conversions or by using industrial off-gases. As long as the conversion pathway of the specific ASTM D7566 annex is followed, the resulting fuel will be a specification compliant, valid kerosene blending component, both legally and chemically.

There are basically three production pathways that start with an intermediate product, which can potentially be produced based on Power-to-Liquid (PtL) pathways, namely Fischer-Tropsch (FT), Ethanol-to-Jet (EtJ)[17] and AtJ-SKA. The approval process for Methanol-to-Jet (MtJ) is ongoing at the time of writing [302, 363]. The other pathways listed in Table 4.4 start from intermediate products based on vegetable oils, animal fats or sugar, which currently cannot be replaced by Power-to-Liquid (PtL). A discussion of Power-to-Liquid (PtL) kerosene blending can therefore be limited to blending of these three pathways.

Within the Alcohol-to-Jet (AtJ) pathway, so far, ethanol and iso-butanol are the only applicable synthetic Alcohol-to-Jet (AtJ) kerosene feedstock options. However, the approval of methanol as an alcohol feedstock for the kerosene production is ongoing at the time of writing. Since a corresponding approval for the Methanol-to-Jet (MtJ) pathway and the AtJ-SKA pathway is expected in the next years [302, 363] and since a kerosene production based on methanol is already considered to play an important role in future, the Methanol-to-Jet (MtJ) pathway is also discussed here.

With regard to aviation fuels, most of the specification requirements only indirectly refer to the fuel composition (except for specific aspects like acidity, aromatics content, mercaptan sulfur content and total sulfur content) [137, 181] . Therefore, the connection between fuel composition and its' specification compliance is complex and conclusions about specification compliance based on fuel composition are very challenging. A more pragmatic approach is to study kerosene blends empirically and derive critical properties for blending by testing the resulting blends for specification compliance. This has been done in the past, e.g., in the High-Biofuel-Blends in Aviation (HBBA) study [135]. This study examined a broad range of synthetic types, all certified by ASTM D7566. Fuel density, aromatics content and the distillation curve gradient were found to be critical characteristics

[17] ASTM D7566 refers to this process as Alcohol-to-Jet (AtJ) SPK. To allow for a more transparent distinction between the feedstock ethanol and methanol, the expressions Ethanol-to-Jet (EtJ) and Methanol-to-Jet (MtJ) are used. AtJ SPK may also be produced from isobutanol or isobutene, but these feedstocks have so far not been discussed in connection with PtL.

for some aviation fuel blends, partially resulting in permissible blending ratios well below the precautionary blending limit. In the following section, different powerfuel production pathways, namely the Fischer-Tropsch (FT) pathway and Alcohol-to-Jet (AtJ) pathway are described, the resulting fuel properties are discussed and conclusions regarding permissible blending ratios and overall blending characteristics are drawn.

4.3.4.1 Fischer–Tropsch Kerosene

The Fischer-Tropsch (FT) pathway was the first alternative kerosene blending component pathway to be approved and is covered in Annex 1 of ASTM D7566. The approval process for this pathway was chiefly promoted by Sasol, with a view to the FT-conversion of coal to kerosene. However, the approved pathway is feedstock independent, and any feedstock that can be converted into FT-synthesis gas (syngas) is suitable in principle. In this case, the syngas primarily consists of a mixture of hydrogen and carbon monoxide in a ratio of about 2 to 1. In addition to coal, feedstocks for the production of FT syngas can be for example natural gas, biomass, municipal waste but also hydrogen and carbon dioxide that represent the two core components for Power-to-Liquid (PtL) processes.

Work on approval of the Fischer-Tropsch (FT) pathway took some ten years, from 1999 to 2009, not counting prior work by Sasol on an approval specific to their fuel [200]. This was partly due to this being the first ASTM approval of a production pathway for an alternative, synthetic kerosene blending component, but also because there is much potential flexibility in the design of the production process for FT liquids.

4.3.4.1.1 Chemical Composition

The direct result of the Fischer-Tropsch (FT) process is not a usable product, but a so-called syncrude consisting of hydrocarbon chains ranging from C_1 to well over C_{30}, i.e. from gases to waxes [356]. The distribution of the chain lengths of the syncrude is typically lognormal, but as Figure 4.22 illustrates, both the range and the shape of the ultimately resulting kerosene chain lengths distribution vary depending on the kind of FT reaction (e.g. type of catalyst, type of reactor, operating parameters). This FT syncrude must then be subject to a refining process to be converted into usable products, and again there is scope to vary this refining process. As a result, there

are potentially many ways to shape the kerosene resulting from the FT process, and much effort was spent to determine what was acceptable, and what was not.

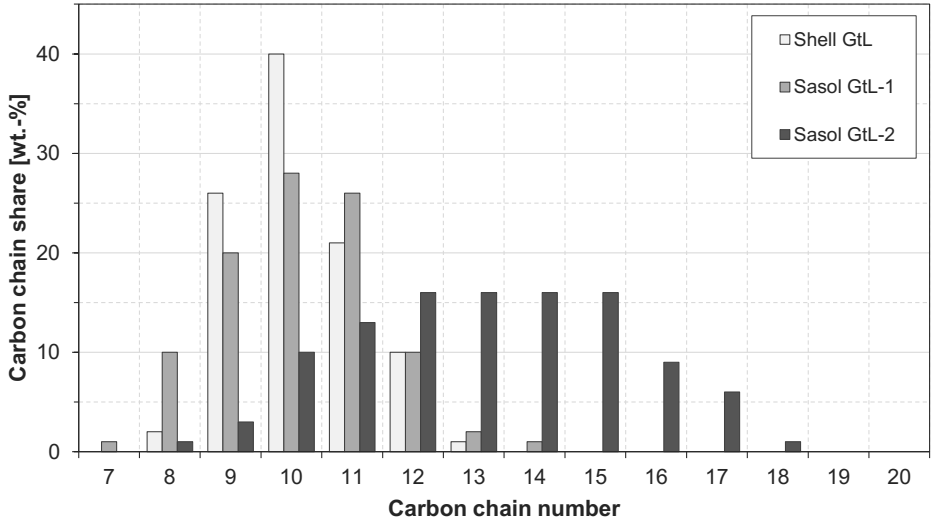


Figure 4.22 Carbon-chain distributions for various Fischer–Tropsch synthetic kerosene (GtL: Gas-to-Liquid; based on [73])

In the end, it was found that a blend of conventional kerosene and FT kerosene meeting the requirements of the standard ASTM D1655 specification can be used for aviation purposes, except in those cases where the FT kerosene is extremely concentrated at a few carbon chain lengths, leading to a very spiky distribution of the blend. To control this factor, minimum limits were introduced for the difference between certain points of the distillation curve.

4.3.4.1.2 Aromatics Content

The Fischer-Tropsch (FT) pathway does not comprise an aromatisation step, hence the resulting fuel does not contain aromatic components. ASTM D7566 Annex 1 is therefore known as FT synthetic paraffinic kerosene (SPK) – or FT-SPK – pathway annex, as the hydrocarbons in the fuel are all paraffins (alkanes). Aromatics burn worse than paraffinic components, and hence increase undesirable soot emissions. However, they also cause the seals and valves in an aircraft's fuel system to swell, and thus to remain tight. Aircraft trials with neat FT kerosene showed that fuel with no

aromatics increases the risk of fuel leaks. Consequently, blends with alternative fuel components are required to have a minimum aromatics content of 8 vol.-%. This limit is another constraint, which may only permit blend ratios well below 50 vol.-%.

4.3.4.1.3 Density

The practical aspects of blending conventional and Fischer-Tropsch (FT) kerosene were investigated in the HBBA study [135], which particularly looked at limiting factors. Although the HBBA study was about blending limits for biokerosene, the FT blending component used was provided by Sasol and produced from coal, as no biomass-based FT material was available. The lack of aromatics in Fischer-Tropsch (FT) SPK results in a lower density than conventional kerosene, in the case of the sample used in the HBBA study 761.2 kg/m^3. This is because aromatics are heavier than paraffins (alkanes), and their absence results in a fuel of a lower density. Density is therefore another constraining factor. However, the HBBA study found this constraint only becomes relevant for FT kerosene at blend ratios beyond 50 vol.-%.

4.3.4.1.4 Distillation Curve

For distillation curve gradients, the most limiting factor identified in the HBBA study was T50-T10. The T50-T10 of the FT blendstock was only 8 °C. As a result, the T50-T10 of the conventional kerosene used for blending was a crucial factor for permissible blend ratios. For conventional kerosene itself having a very flat distillation curve, the HBBA study found that adding even a few percent of the FT blendstock resulted in the blend not meeting the specification requirements. Conventional kerosene with a steep distillation curve, on the other hand, permitted blending up to 50 vol.-%.

It needs to be emphasised, however, that to a certain extent these results only apply to the specific sample analysed in the HBBA study. The sample was in line with other samples described in literature, but as discussed above there is a considerable variation for FT blendstock, which potentially can be used to ease blending constraints.

4.3.4.2 Alcohol–to–Jet Kerosene

The Alcohol-to-Jet (AtJ) SPK pathway was first approved in 2016, with the respective annex becoming Annex 5 of ASTM D7566 [280]. This annex initially only covered synthetic kerosene produced from iso-butanol, a C_4 alcohol, and was produced based on biomass. Later on, ethanol was also certified as potential alcoholic feedstock, and in 2023 iso-butene was approved as another feedstock. The ASTM certification of methanol is currently ongoing. Ethanol and methanol can both be provided based on synthesis gas and thus pose potential powerfuel intermediate feedstock. In the case of ethanol, this would be possible via synthesis gas fermentation, while in the case of methanol, it is possible via a thermochemical conversion.

4.3.4.2.1 Chemical Composition

Ethanol based Alcohol-to-Jet (AtJ) kerosene. In 2018, annex 5 was expanded to also permit Alcohol-to-Jet (AtJ) from ethanol, based on a production pathway developed by LanzaTech [364]. With the inclusion of ethanol as feedstock, the maximum blending limit in annex 5 was increased from 30 to 50 vol.-%, for both Alcohol-to-Jet (AtJ) from ethanol and from iso-butanol [280]. Ethanol is a C_2 alcohol, and the resulting carbon chain distribution is comparatively close to the one of conventional kerosene (Figure 4.23). The distribution ranges from C_8 to C_{17} which is essentially the same as for conventional kerosene. In contrast to conventional kerosene, the carbon chain distribution of Alcohol-to-Jet (AtJ) SPK shows two distinct modal values at C_{10} and C_{12}. As expected, for Alcohol-to-Jet (AtJ) SKA from mixed alcohols only one modal values is recognizable, due to the range of alcohols used feedstock for the oligomerization.

Alcohol-to-Jet (AtJ) SPK from ethanol was only certified after the HBBA study was finished, and hence was not included in the study. Apparently, no other research on the blending of Alcohol-to-Jet (AtJ) SPK from ethanol has been performed, hence any statement on limiting factors needs to be based on the known properties of the fuel rather than any experimental verification. Aromatics content and fuel density are likely to play a similar role to what is the case for Fischer-Tropsch (FT) SPK (i.e., relatively low density of synthetic blending component and high aromatics content required in the conventional blending component). The reason is that both fuels are SPKs containing no aromatics. The boiling curve of Alcohol-to-Jet (AtJ) SPK from

ethanol is essentially linear, which gives the fuel a sufficiently large T50-T10 and T90-T10 for these factors not to be a constraint [364].

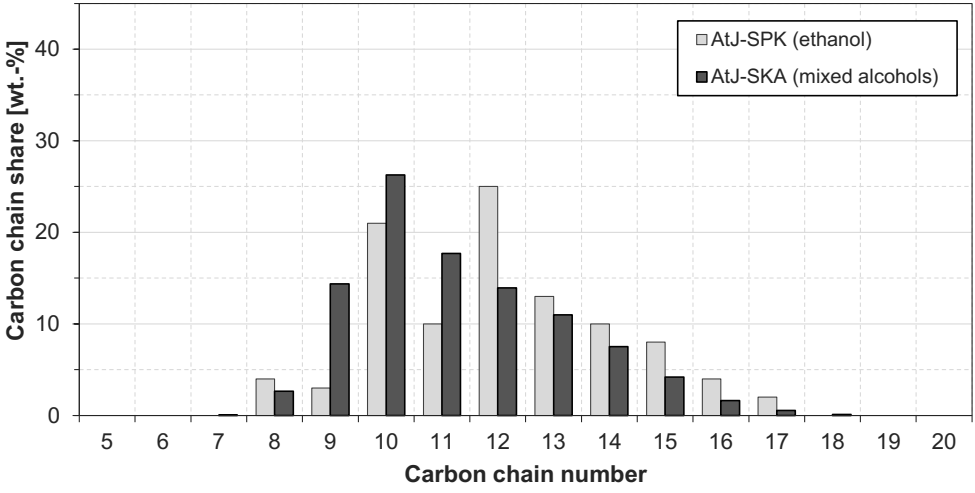


Figure 4.23 Carbon chain distribution of Alcohol-to-Jet (AtJ) SPK from ethanol and Alcohol-to-Jet (AtJ) SKA from mixed alcohols (SKA: synthetic kerosene with aromatics; SPK: synthetic paraffinic kerosene; based on [364])

Methanol based Alcohol-to-Jet (AtJ) kerosene. Several players have announced projects to produce Alcohol-to-Jet (AtJ) SPK based on methanol [302, 363], and an approval process is currently ongoing, with a Task Force established by ASTM in December 2022. Again, this process will produce negligible (if any) quantities of aromatics, meaning that again the same implications as for Fischer-Tropsch (FT) SPK can be assumed (i.e., relatively low density and high aromatics content required in the conventional blending component). If AtJ-SPK from methanol shows a similar, linear boiling curve like ethanol, T50-T10 and T90-T10 would most likely be large and probably not a constraint. Other challenges, specific to AtJ-SPK from methanol cannot be ruled out, as at the time of writing no study on the blending behaviour of this fuel type is available.

4.3.4.2.2 Aromatics Content

By definition, none of the synthetic kerosene production pathways contain an aromatisation step, and the fuels therefore are also synthetic paraffinic kerosenes (SPKs), like Fischer-Tropsch (FT) blendstock. Therefore, both the requirement for a minimum aromatic content of 8 vol.-% and the fuel density are further constraining factors identified by the HBBA study. Still,

in most cases these factors only become binding at blend ratios close to 40 vol.-% or above [135].

However, very recently the company Swedish Biofuels has received approval for an AtJ-SKA pathway – where "SKA" stands for synthetic kerosene with aromatics. The Swedish Biofuels kerosene is designed to correspond to conventional kerosene in every respect except burning cleaner, with almost no contaminants. Due to the similarity, the carbon chain distribution of this fuel therefore corresponds to that for conventional kerosene. This process is feedstock flexible, with all alcohols from C_2 to C_5 possible, either as single alcohols or as mixtures. Approval is for a blend ratio of 50 vol.-% at first, with approval as a 100 vol.-% fuel to be pursued as a second step. Blending with conventional kerosene is expected to be easiest for the Swedish Biofuels pathway, as the blending component is designed to correspond to conventional kerosene. As a rule, it should be possible always to blend up to the limit of 50 vol.-% [303].

4.3.4.2.3 Density

Like Fischer-Tropsch (FT) SPK, neat AtJ-SPK does not contain aromatics and thus its density is lower compared to conventional kerosene (in the HBBA study the density amounted to 757.1 kg/m3, which is substantially below the specification minimum of 775 kg/m3). The dependency of density on blend ratio is again linear for blends of conventional and synthetic kerosene and therefore the resulting density of the blend can be calculated from initial values of the blend components. For the fuels investigated in the HBBA study, the limits range from ca. 40 to 70 vol.-%. For AtJ-SKA this will not be a problem.

4.3.4.2.4 Distillation Curve

In the HBBA study, T50-T10 and to a lesser extent T90-T50 was identified as a possible obstacle to higher blend ratios of 70 vol.-% or more, as the sample supplied had relatively low T50-T10 and T90-T10 values and did not on its own meet target values for the blend.[18] However, the HBBA study used AtJ-SPK from iso-butanol which has a different carbon-chain distribu-

[18] HBBA study, page 77.

tion than AtJ-SPK from ethanol, for instance. Using iso-butanol (C_4) as feedstock results in high modal values for C_{12} and C_{16} molecules, as the oligomerization step primarily generates integer multiples of the feedstock. These modal values are likely to result in a rather flat distillation curve. In contrast, in the kerosene range (C_8–C_{16}) there are more integer multiples for ethanol (C_2). Accordingly, the carbon distribution is most likely rather linear and thus the resulting distillation curve gradient could be closer to the specification limits. The AtJ-SKA production pathway uses a process that is independent of the chain length distribution of the initial alcohol, and therefore can produce a fuel with a carbon chain length distribution corresponding to that of fossil kerosene, independent of the feedstock alcohol [303]. Early versions of this fuel still had unsatisfactory values for T50-T10 [135], but in its current form the distillation curve is not a limiting factor. The Methanol-to-Jet (MtJ) pathway involves a conversion into olefins of different chain lengths as an interim step [303], hence the resulting product should also be well-distributed [365].

4.3.5 Blending Properties

As described in section 4.3.2, an unfavorable combination of a conventional and synthetic blending component might yield a fuel blend which does not comply with the ASTM D7566 blend specification or at least the maximum allowable blending ratio may not be achievable. Accordingly, synthetic and conventional fuel batches for blending – and thus also in case of the production of synthetic blending components by power-based or powerfuel production pathways – should be matched carefully in the future aviation fuel supply chain (Table 4.5). From a technical point of view, even blending ratios beyond the current precautionary limit could be possible, if two favorable batches were chosen.

According to ASTM D7566, blending is considered manufacture of Jet A or Jet A-1, respectively. In Europe an explicit requirement demands that it shall be conducted upstream of the airport storage [334]. In the US, such a requirement does not exist. However, in practice, general quality assurance standards can be expected to rule out blending at the airport [137]. Three analyses have to be performed before a fuel blend may be used in commercial aviation:

- an ASTM D1655 analysis of the conventional kerosene before blending,

- an ASTM D7566 analysis of the neat synthetic kerosene before blending,
- an analysis of the blend, which is described in ASTM D7566, but in practice, is an analysis of the ASTM D1655 parameters, plus some additional ones.

Table 4.5 Comparison of properties relevant for the blending of conventional and synthetic kerosene types (properties critical for blending are marked bold; data based on [135]; AtJ: Alcohol-to-Jet; FT: Fischer-Tropsch; SPK: Synthetic Paraffinic Kerosene)

Characteristic	Conventional	FT-SPK	AtJ-SPK
Carbon-distribution	normal	log-normal	linear (consisting of integer-multiples of C-number of the alcohol used)
Composition	alkanes (n- and iso-), cycloalkanes, aromatics, heteroatoms	alkanes (n- and iso-)	alkanes (n- and iso-)
Density	reference	usually reduced (lack of cyclic hydrocarbons)	usually reduced (lack of cyclic hydrocarbons)
Aromatics content	up to 25 vol.-%	max 0.5 wt.-% (as per ASTM D7566)	max 0.5 wt.-% (as per ASTM D7566)
Distillation curve	reference	strongly depends on feedstock and process conditions	strongly depends on feedstock and process conditions
Lubricity	There is no general correlation between blend ratio and lubricity. In blends the component with the better lubricity usually positively influences this parameter.		
Freezing point	As long as both individual blend components meet the specification, also the freezing point of the blend was found to be compliant with the specification.		
Smoke point	The smoke point primarily depends on the aromatics content of a fuel. Therefore, blends with aromatic free synthetic fuels / blend components (FT-SPK, AtJ-SPK) show an improved smoke point.		
Flash point	Flash point is mainly influenced by the presence of volatile fuel components. In blends this property strongly depends on the blend component with the lower flash point. For all blends investigated in the HBBA study, flash point was not an issue.		

An entire ASTM D1655 analysis requires ca. 20 labor hours and the use of specialized, expensive equipment. These incur high cost, usually in the range of thousands of Euros. For the first two analyses these costs are independent of the blend ratio and will usually be performed for large batches of thousands of tons, yielding comparatively low specific (per ton) costs in the range of a few Euros. This is not the case for the analysis of the blend, since the cost impact per ton of powerfuel is crucially dependent on the blend ratio. For single-digit blend ratios, the cost for the analysis will be incurred for selling only a few tons of powerfuel, leading to very high costs per ton. However, for high blend ratios these costs will not be an issue. Furthermore, using low blend ratios implies that large volumes of conventional kerosene have to be transported to the blending point, inducing complex and expensive logistics, and in particular potentially increase the transport distances and thus related emissions [135].

This is why the maximum allowable blend ratio holds significance for powerfuel producers and blenders, even in the early stages of the market. It will also be relevant for governments and communities involved in the planning of logistics and blending capacities [135].

Regarding the actual blending process, currently ASTM D7566 only permits binary blending. This means, a conventional component meeting specification ASTM D1655 and an alternative, synthetic kerosene blending component as specified in any individual annex to ASTM D7566 may be blended. The resulting blend can be regarded acceptable as an aviation kerosene if it meets the requirements defined in the body of ASTM D7566 for a target blend. Such a blend may then again be blended with a blending component defined in an annex to ASTM D7566.[19] However, simultaneous blending of two or more alternative, synthetic kerosene blending components with conventional kerosene – so-called "multiblends" – is not covered by ASTM D7566 yet, and hence not permitted. Against the background of increasing production volumes, a broader variety of synthetic kerosene types and the opportunity to achieve desirable fuel properties by multi-blending, this can become a practical problem in the future. An ASTM task force is working on also permitting the production of multiblends. However, as of now only binary blends are permitted.[20]

[19] See section 1.2.2 of ASTM D7566-21 [280].

[20] For a discussion, see DEMO-SPK report, section 6.1.4 and 6.4 [262].

4.3.5.1 Aromatics Content

In general, a high aromatics content leads to soot and carbon deposit formation during combustion. For this reason, the maximum content of aromatics in kerosene is restricted to 25 vol.-% (or 26.5 vol.-%, depending on test method). Yet, fuels without any aromatics are neither desirable, as aromatics contribute to a swell and mass gain of certain elastomer seals and thus prevent leakage in the aircraft's fuel system [137]. This chiefly affects nitrile butadiene rubber, a common elastomer in aviation. When in contact with aromatic-free fuel after having been exposed to highly aromatic fuel beforehand, the seal shrinks significantly [135]. Consequently, a minimum aromatic content of 8 vol.-% (8.4 vol.-%, depending on test method) has been introduced in ASTM D7566. However, this is only applicable to Jet A or Jet A-1 containing synthetic kerosene.

Figure 4.24 shows the relationship between aromatic content of the conventional kerosene and the resulting maximum share of synthetic kerosene, to remain within the lower limit for the aromatics content in the blend.

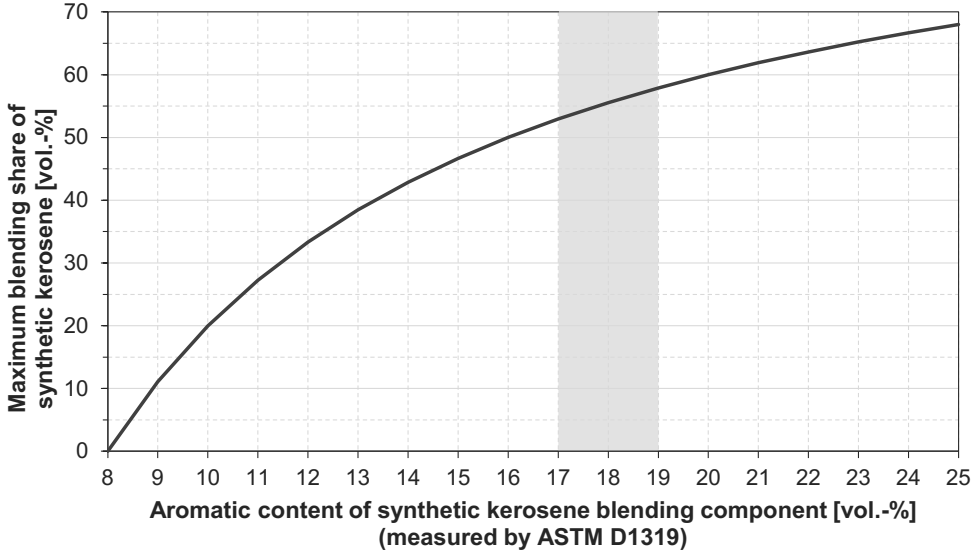


Figure 4.24 Maximum share of synthetic kerosene as a function of aromatic content in conventional blending component (grey area indicates a representative value range for fuels leaving pipeline systems or airport tank farms in Germany; adopted from [137])

The grey area indicates a representative value range for aviation fuels leaving pipeline systems or airport tank farms in Germany. It shows that most likely for the majority of conventional fuel in use, blend ratios of at least

50 vol.-% of synthetic kerosene can be achieved. Still, at batch level, the variation of aromatics content is substantially larger (Figure 4.18), thus for blending individual batches the permissible blend ratio might be substantially lower.

4.3.5.2 Density

Density describes the ratio of a fuel's mass per its volume. According to ASTM D1655 and ASTM D7566 the density of Jet A and Jet A-1 must be between 775 and 840 kg/m^3. Consequently, the density of the fuel and the tank volume of an aircraft defines the maximum fuel mass available on board and hence its maximum range. In general, the lack of aromatics in the discussed aviation powerfuels results in a reduced fuel density. For example, the fuel densities for neat Fischer-Tropsch (FT) SPK and Alcohol-to-Jet (AtJ) SPK measured by the HBBA study were about 760 kg/m^3.

Figure 4.25 shows the maximum permissible blend ratio for different densities of the synthetic blend component (x-axis) and the conventional blend component (y-axis). Exemplarily, the density for both fuel types of the HBBA study is also indicated. Assuming a mean density of the kerosene in Germany of 800 kg/m^3 [135] blend ratios of about 60 % seem feasible. However, this will strongly depend upon the individual conventional fuel batch.

There is a notable distinction between density as mass per volume and energy density as energy per mass or per volume. Even though the lack of aromatics reduces a fuel's density, the energy content increases due to the improved combustion behavior of straight-chain hydrocarbons compared with cyclic hydrocarbons. A higher energy density is generally preferable, as the same amount of mass stored as fuel leads to a higher energy stored on board of an aircraft and consequently, the amount of fuel that an aircraft needs to carry for flight operations can be reduced, resulting in a decrease in the aircraft's fuel consumption.

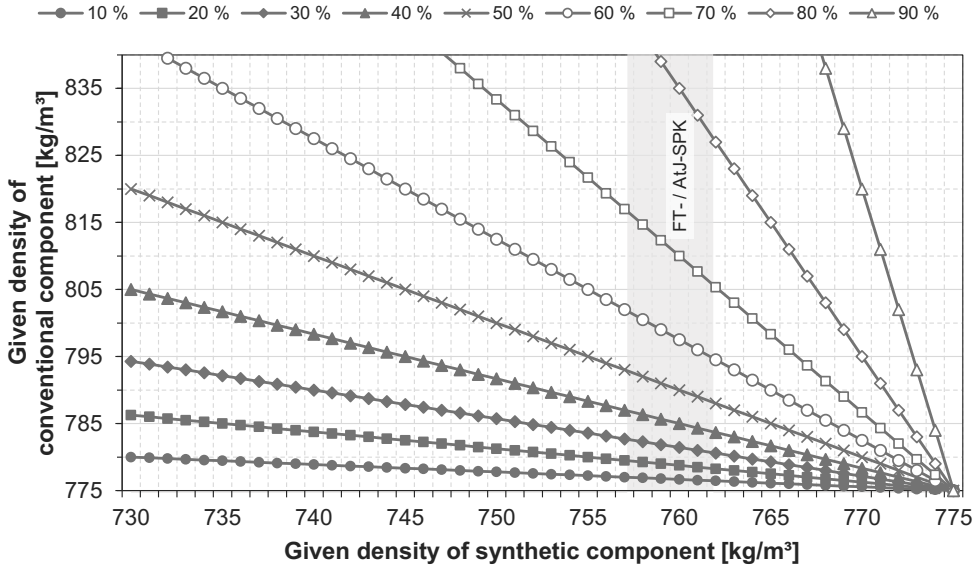


Figure 4.25 Maximum share of synthetic kerosene as a function of aromatic content in conventional blending component, the grey bar indicates the density of Fischer–Tropsch (FT) SPK and AtJ–SPK measured by the HBBA study [135](adopted from [137])

4.3.5.3 Distillation Curve

ASTM D7566 states that the volatility and ease of evaporation are controlled by the distillation requirement. The 10 % recovery temperature guarantees engine start performance by ensuring that volatile compounds are present [137]. In turn, the final boiling point prevents undesired heavy fractions (alkanes beyond C_{16}, poly-aromatics) from being incorporated [137]. However, the introduction of synthetic kerosene affects the aviation fuel's composition. As a precautionary measure minimum distillation gradients have been specified resembling the typical behavior of conventional aviation fuel. Between the 10 % recovery temperature and the 50 % recovery temperature (T50 to T10) a minimum temperature rise of 15 °C is required, while from 50 % recovery to 90 % recovery (T90 to T50) an increase in temperature of at least 40 °C is mandatory.

Figure 4.26 shows the distribution of distillation curve gradients for German kerosene batches and – as illustrative data – the distillation curve for a single hydrocarbon molecule ($C_{15}H_{32}$) and Alcohol-to-Jet (AtJ) SPK and Alcohol-to-Jet (AtJ) SKA as well as Fischer-Tropsch (FT) SPK. For conventional kerosene, ASTM D1655 only requires to determine the 10 % recovery

temperature and the final boiling point. It does not specify a certain minimum gradient. Thus – as for aromatics – there may be conventional batches that do not conform to ASTM D7566. As conventional kerosene contains a broad range of different hydrocarbons with various chain lengths, the distillation curves commonly show a distinct slope. This would not be the case if the fuel would consist only of one molecule type. For example, farnesane ($C_{15}H_{32}$; grey line with circles) has a boiling point of 274 °C. Thus, it would entirely vaporize at this temperature and its distillation curve would be horizontal.

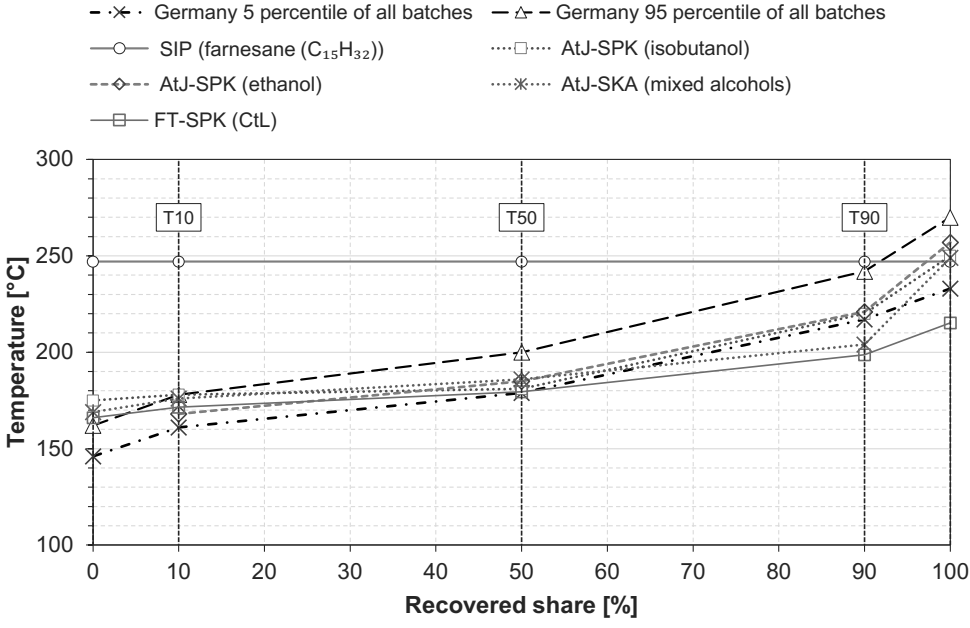


Figure 4.26 Distillation curves for conventional kerosene (black lines) and indicative curves for a single hydrocarbon molecule ($C_{15}H_{32}$) and Alcohol-to-Jet (AtJ) SPK from isobutanol and ethanol, Alcohol-to-Jet (AtJ) SKA from mixed alcohols and Fischer-Tropsch (FT)-SPK; (SKA: synthetic kerosene with aromatics; SPK: synthetic paraffinic kerosene; based on [135, 303]

As it is composed primarily of three different alkanes, the distillation curve of AtJ-SPK from iso-butanol is extraordinary flat (dashed grey line with boxes). This is particularly pronounced below the 50 % recovery point. Special attention must therefore be paid to the conventional blending component. It must have a very steep gradient for compensation [135]. However, AtJ -SPK from ethanol shows a broader range of alkanes and accordingly

their distillation curve gradient is slightly steeper (dashed grey line). A similar behavior can be observed for Alcohol-to-Jet (AtJ) SKA, which is produced from mixed alcohols.

A similar situation can be observed for Fischer-Tropsch (FT) SPK. The distillation curve of the sample investigated in the HBBA study was also fairly narrow (T_{50} to T_{10} = 8 °C). Consequently, the conventional blending component needs a substantially steeper slope in order to compensate for it [135]. However, this is not necessarily the case for all Fischer-Tropsch (FT) SPK batches, as reaction products are highly dependent on reaction conditions (Section 4.3.4.1) Thus, for blending Fischer-Tropsch (FT) SPK, the distillation characteristics require special attention; some conventional kerosene might not be suitable for blending at all [135].

4.3.6 Conclusion and Outlook

In sectors like aviation and maritime, where dependence on liquid hydrocarbon fuels will most likely persist in the foreseeable future, blending conventional and renewable fuels, such as Power-to-Liquid (PtL) hydrocarbons, offers both a necessary path and an opportunity to leverage existing infrastructure. Thus, a thorough understanding of powerfuel blending requirements and implications is important. In this context, this article provides an overview of blending these fuels, using the example of aviation fuels and examining the respective physical and chemical properties of conventional and synthetic kerosene options for all presently approved aviation powerfuel production pathways.

In this context, it can be concluded that physical and chemical properties of synthetic and conventional kerosene options vary considerably. Attention needs to be paid to the specific properties of each blending component, to ensure that the resulting blend complies with fuel specifications. Fuel density, aromatics content and the distillation curve gradient were found to be critical for some blends, potentially resulting in permissible blending ratios well below the precautionary blending limit laid out in the fuel specifications.

As synthetic paraffinic kerosene (SPK) fuels contain no aromatics, the conventional component needs to contain at least enough aromatics that the blend still achieves the minimum aromatics content of 8 vol.-%. The lack of aromatics also results in a rather low density, which again needs to be

compensated for by the conventional kerosene component. In terms of distillation curve gradient, the results are less specific. As the distillation curve gradient of the neat synthetic kerosene strongly depends on process conditions (AtJ-SPK, FT-SPK) and the (intermediate) feedstock used (AtJ-SPK), a simple conclusion cannot be drawn. In general, a broader distribution of carbon-chain lengths appears to be beneficial for this specification requirement.

The main goal of the blending procedure as discussed in this article is to produce a specification compliant blend from a conventional and a synthetic kerosene component. However, in future, with increasing synthetic kerosene market shares, a more targeted approach towards blending might be beneficial. i.e. targeted blending might be used to achieve a high fuel energy content or low aromatics content. In the nearer term, permitting the use of 100 % synthetic kerosene will permit the use of potentially fully greenhouse gas (GHG) neutral kerosene, which is not possible with the current limitation to a 50 % blend ratio. Similarly, a fully synthetic kerosene, in particular one with reduced aromatics content and thus improved combustion properties would be beneficial for other impacts besides GHG emissions, namely contrail climate impact and local air quality [17].

In the near future, inclusion of 100 % synthetic fuels in ASTM D7566 can simplify the production process and potentially enable the use of fully GHG neutral kerosene. Such 100 % synthetic fuels can either be fuels like AtJ-SKA, where the aromatics production is part of the pathway, or blends of SPKs with synthetic aromatics. At the same time, research is required on the blend properties for powerfuel SPKs based on ethanol and / or methanol. In the longer term, the potential of “designing” fuels more specifically to utilize potentials towards improved local air quality and climate impact should be investigated.

4.4 Simulation-Based Analysis of the Potential of Alternative Fuels towards Reducing CO_2 Emissions from Aviation

Kieckhäfer, Karsten; Quante, Gunnar; Müller, Christoph; Spengler, Thomas; Lossau, Matthias; Jonas, Wolfgang (2018): Simulation-Based Analysis of the Potential of Alternative Fuels towards Reducing CO_2 Emissions from Aviation. In Energies 11 (1), p. 186. DOI: 10.3390/en11010186.
Typesetting and formatting are slightly adjusted to ensure consistency within this thesis.

Abstract

The mid-term framework of global aviation is shaped by air travel demand growth rates of 2–5 % p.a. and ambitious targets to reduce aviation-related CO_2 emissions by up to 50 % until 2050. Alternative jet fuels such as bio- or electrofuels can be considered as a potential means towards low-emission aviation. While these fuels offer significant emission reduction potential, their market success depends on manifold influencing factors like the maturity of the production technology or the development of the price of conventional jet fuel. To study the potential for adoption of alternative jet fuels in aviation and the extent to which alternative fuels can contribute to the reduction targets, we deploy a System Dynamics approach. The results indicate that the adoption of alternative fuels and therefore their potential towards low-emissions aviation is rather limited in most scenarios considered since current production processes do not allow for competitive prices compared to conventional jet fuel. This calls for the development of new production processes that allow for economic feasibility of converting biomass or hydrogen into drop-in fuels as well as political measures to promote the adoption of alternative fuels.

4.4.1 Introduction

Today, air transport accounts for approximately 12 % of transport-related and 2 % of all human-induced CO_2 emissions [366]. Due to the expected growth of air travel demand of 2–5 % p.a. [367, 368], CO_2 emissions from aviation are projected to triple by 2050 compared to today's level unless substantial efforts are made to reduce the environmental impact of aviation [369]. For that reason, the International Air Transport Association (IATA), for instance, strives to improve fleet-wide fuel efficiency by 1.5 % p.a. from 2009 to 2020, cap net emissions from 2020 (carbon-neutral growth) and reduce net emissions by 50 % until 2050, relative to 2005 levels [366, 369]. As a consequence, airlines are forced to modernize their fleet either by replacing old aircraft or by retrofitting new fuel-efficient airframe and engine technologies (e.g., blended winglets, geared turbofan) into existing aircraft of the fleet [153, 370]. However, fulfilling the emission reduction targets solely by fleet modernization will not be possible and even approaching them would be a substantial economic burden for airlines as long as aircraft are purely powered by conventional jet fuels [153, 369–371].

Alternative jet fuels produced from biomass or hydrogen from electrolysis powered by renewable electricity have received considerable attention as a potential means towards low-emission aviation [371–373]. For biofuels, five different production pathways have already been certified for use in current aircraft engines by the American Society for Testing and Materials (ASTM) International as drop-in alternative fuels. The resulting variety of feedstock (e.g., corn grain, soybean oil, cellulosic biomass) and conversion processes affect the mitigation potential of these alternative fuel types significantly. Biofuels that are based on cellulosic biomass, for instance, allow for a reduction of lifecycle CO_2 emissions by up to 80 % compared to petroleum-derived fuels [371, 374]. However, the large land areas that are required to grow biomass as well as additional resources such as water and fertilizer pose an obstacle for the rise of biofuels in aviation. Electrofuels are a promising alternative to resolve these issues since they only rely on renewable electricity, water, and CO_2 that can be obtained from concentrated sources or extracted from the air as main constituents. Over the entire life cycle, the CO_2 mitigation potential of electrofuels from renewable electricity and CO_2 is estimated to range between 70 % and 87 % compared to petroleum-derived fuels [371, 375–377].

In contrast to operational and technological improvements, alternative jet fuels are not yet available on a commercial scale since production costs are much higher than those for conventional jet fuels [92, 372]. One of the main challenges to ensure the market success of alternative jet fuels is thus to allow for an economically feasible conversion of biomass or hydrogen from electrolysis into drop-in alternative fuels. For that, the maturity of the production technology, the available production capacities, the price development of conventional jet fuel, as well as the air travel and jet fuel demand can be considered as main determinants. Due to these manifold influencing factors, understanding the forces of successfully introducing alternative fuels in aviation is a complex challenge. To this end, a model that allows for adequately investigating the evolution of the market share of alternative jet fuel is required. Such a model must depict the behavior of the different actors of the air transport system (ATS), i.e., passengers, airlines, airports, aircraft manufacturers, and fuel producers. Moreover, the structure of the ATS including all relevant influencing factors, interdependencies, and feedback loops that affect the adoption of alternative jet fuels have to be taken into account.

System Dynamics is a simulation approach that allows for the study of dynamic complex systems such as the ATS. In the past, several System Dynamics models have been developed to simulate the aggregated and endogenous behavior of the ATS. Causes and strategies to manage aviation's cyclical behavior are examined by Pierson and Sterman [146], Liehr et al. [378], and Weil [379]. Lyneis and Glucksman [380] evaluate the inclusion of feedback for simulation-based forecasts and Kleer et al. [381] study different pricing strategies for aviation. Pfänder et al. [382] focus on trade-offs between fleet technology and policy alternatives. Urban et al. [383]study the development of the air transport demand as well as the required fleet size under consideration of the main interactions between passengers, airlines, airports, and aircraft manufacturers. Only one System Dynamics model by Sgouridis et al. [149] evaluates alternative jet fuels as a means to reduce aviation emissions. However, this model assumes an exogenous development of alternative jet fuel availability instead of integrating the development of the production technology into the modeling approach. In addition to these System Dynamics models, several techno-economic studies have been carried out to assess the potential of alternative jet fuels [306,

372, 375, 376].These studies only consider the production costs of alternative fuels and neglect important factors of the ATS that affect the adoption of alternative fuels in the aviation sector and their potential towards low-emission aviation.

The objective of this paper is thus to thoroughly investigate the adoption of alternative jet fuels and assess their potential towards low-emission aviation from the perspective of the ATS. In particular, we are interested in answering the following two questions: (1) What is the potential for adoption of alternative jet fuels in aviation? (2) To which extent can alternative fuels contribute to the air transport industry's reduction targets?

To answer these questions, we deploy a System Dynamics model of the ATS. Based on existing simulation models, we develop a novel approach that includes the main actors of the ATS, namely passengers, airlines, aircraft manufacturers, as well as producers of alternative jet fuels. Uncertainties inherent to our study are addressed by defining alternative future scenarios for the development of the the ATS and conducting sensitivity analyses as well as Monte Carlo simulations. The contribution of our work is twofold. First, we extend existing System Dynamics models from the literature by integrating feedback loops related to the production of alternative jet fuels, resulting in a novel System Dynamics model of the ATS. Second, by applying the model, a better understanding of possible obstacles for the introduction of alternative fuel types as well as the potential of alternative fuels towards low-emission aviation is gained taking into account relevant endogenous system behavior. This facilitates, amongst others, the development of suitable policy measures to accompany the introduction of alternative jet fuels for decision makers from policy. The remainder of the paper is organized as follows: We describe the concept and mechanisms of the System Dynamics model in Section 4.4.2, continue by specifying the database, validating the model, and presenting and discussing the results of our simulation in Section 4.4.3 and finally summarize our findings and give directions for further research in Section 4.4.4.

4.4.2 Modeling Approach

The System Dynamics model of the ATS consists of four modules, namely air travel demand, airline industry, aircraft manufacturer, and alternative fuel producers. Between these modules several interdependencies exist, which mainly determine the endogenous behavior of the ATS and thus also

the adoption of alternative jet fuels in aviation. Moreover, the behavior is influenced by several exogenous parameters (cf. Figure 4.27).

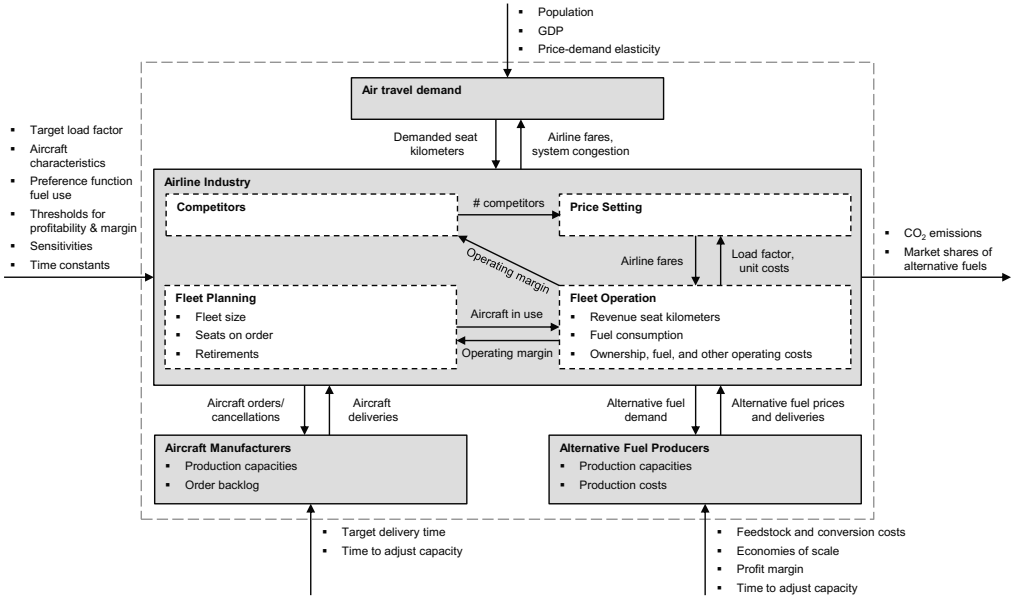


Figure 4.27 Concept of the simulation model

In a nutshell, air travel demand depends on the external development of the gross-domestic product (GDP) and population as well as endogenous effects due to price elasticity of demand and system congestion. Based on the development of travel demand, the airline industry adjusts the necessary fleet sizes (long-term decision) as well as the airline fares (short-term decision). Decisions on the fleet size are additionally influenced by the operating margin, which is determined under consideration of aircraft ownership, fuel, and other operating costs. The operating margin also has an impact on the number of competitors entering or exiting the market. In turn, the number of competitors exhibits an influence on the price setting. The same holds true for the load factor and the unit costs of operating the aircraft fleet per revenue seat kilometer. In order to adjust the fleet size, aircraft orders can be placed. These orders are fulfilled by the aircraft manufacturers taking into account production capacities and delivery delays in the supply chain. Together with the average fleet age, the fleet size constitutes the central determinant for fuel consumption and thus aviation's CO_2 emissions. The CO_2 emissions further depend on the market shares of alternative jet fuels and their mitigation potential. The adoption decision of the airline industry is influenced by the price difference between alternative and conventional jet

fuels as well as supply capacities and mandatory drop-in quotas. The price and production capacities for alternative jet fuels are adjusted by the alternative fuel producers due to changes in fuel demand as well as feedstock and conversion costs.

In the following, the four modules are described in detail. Thereby, the modules depicting the customer demand, the behavior of the airline industry, and the aircraft manufacturers are in particular based on previous work by Pierson and Sterman [146]. This work is extended by taking into account dynamic manufacturing capacities for aircraft, a detailed breakdown of aircraft costs, the influence of competition on airline fares, and decisions regarding the production and adoption of alternative jet fuels.

4.4.2.1 Air Travel Demand

The module depicting the air travel demand is based on the work of Pierson and Sterman [146]. Air travel demand $D(t)$ depends on the population size $P(t)$, a reference demand per capita D^{REF}, which corresponds to the initial demand per capita, the gross domestic product per capita $E^{GDP}(t)$, the airline fares $E^{AF}(t)$, and the system congestion $E^{CG}(t)$:

$$D(t) = P(t) \cdot D^{REF} \cdot E^{GDP}(t) \cdot E^{AF}(t) \cdot E^{CG}(t) \tag{5}$$

While the population is exogenously given, effects of gross domestic product, airline fares, and system congestion are determined within the model. The effect of system congestion $E^{CG}(t)$, modeled by the load factor, is accounted for by comparing the current load factor $LF(t)$ to the perceived load factor $PLF(t)$. Since passengers perceive the current load factor with a delay τ^{CG}, a first-order smooth function is used. Additionally, the ratio of perceived to reference load factor is smoothed to take into account that passengers change their flying habits due to congestion with some delay. The effects of gross domestic product $E^{GDP}(t)$ and airline fares $E^{AF}(t)$ are captured similarly, albeit without smoothing.

$$E^{GDP}(t) = \left(\frac{GDP(t)}{GDP^{ref}}\right)^{\gamma^{GDP}} \tag{6}$$

$$E^{AF}(t) = \left(\frac{AF(t)}{AF^{ref}}\right)^{\gamma^{AF}} \tag{7}$$

$$E^{CG}(t) = \left(smooth\left(\frac{LF(t)}{PLF(t)}, \tau^{CG}\right)\right)^{\gamma^{CG}} \quad (8)$$

$$PLF(t) = smooth\,(LF(t), \tau^{PLF}) \quad (9)$$

γ^{GDP}, γ^{AF} and γ^{CG} indicate the sensitivities of demand to gross domestic product, airline fares, and congestion, respectively.

4.4.2.2 Airline Industry

The modeling of the order behavior of airlines is based on a standard stock management structure and similar to the model used by Pierson and Sterman [146]. Both stocks (aircraft orders $SO(t)$ and fleet capacity $AU(t)$ are measured in seats, assuming a constant flight distance per seat. Airlines place aircraft orders at the order rate $OR(t)$. Aircraft in use $AU(t)$ are discarded after a fixed lifetime τ^{AL}. The indicated order rate $IOR(t)$ is based on the desired acquisition rate $DAR(t)$, the supply line adjustment $SLA(t)$, expected growth rate $SLA^G(t)$, and aircraft returning into service $RS(t)$

$$OR(t) = \max\,(0, IOR(t)) \quad (10)$$

$$IOR(t) = DAR(t) + SLA(t) + SLA^G(t) - RS(t) \quad (11)$$

The desired acquisition rate $DAR(t)$ is the sum of retirements $RT(t)$, adjustments for capacity $CA(t)$, and capacity growth adjustment $CA^G(t)$. The adjustment for capacity $CA^G(t)$ is given by the difference between the desired capacity $DC(t)$ and the aircraft in use $AU(t)$ divided by the time to adjust capacity τ^{CA}. The desired capacity is based on estimated demand $ED(t)$ taking into account the airlines' target load factor LF^{REF}

$$DAR(t) = RT(t) + CA(t) + CA^G(t) \quad (12)$$

$$CA(t) = \frac{DC(t) - AU(t)}{\tau^{CA}} \quad (13)$$

$$DC(t) = \frac{ED(t)}{LF^{REF}} \quad (14)$$

Similarly to the adjustment for capacity, the adjustment for supply line $SLA(t)$ is given by the difference between the desired supply line $DSL(t)$ and seats on order divided by the time to adjust supply line τ^{SL}. The desired supply line is estimated using Little's Law by multiplying estimated delivery time τ^{ED} and desired acquisition rate $DAR(t)$ [145]

$$SLA(t) = \frac{DSL(t) - SO(t)}{\tau^{SL}} \quad (15)$$

$$DSL(t) = \tau^{ED} \cdot DAR(t) \tag{16}$$

A desired acquisition rate $DAR(t)$ solely considering current demand and supply line delays would yield a steady state error in the case of exponential growth [146]. In the present study, airlines are assumed to consider demand growth, which is taken into account by two growth adjustment factors, $SLA^G(t)$ and $CA^G(t)$. They are calculated by the product of seats on order $SO(t)$ or aircraft in use $AU(t)$, estimated growth rates $EGR(t)$, and a weighting factor W^G

$$SLA^G(t) = SO(t) \cdot EGT(t) \cdot W^G \tag{17}$$
$$CA^G(t) = AU(t) \cdot EGR(t) \cdot W^G \tag{18}$$

The constant W^G allows for partial consideration of demand growth rates. Estimated growth rates $EGR(t)$ are calculated by a standard trend function [145].

The standard stock management structure is extended by order cancellations and the possibility to store aircraft. Aircraft seat orders $SO(t)$ are canceled at rate $CX(t)$ if the indicated order rate $IOR(t)$ falls below zero. The cancellation rate $CX(t)$ is the minimum of the indicated order rate $IOR(t)$ and the seats on order $SO(t)$ divided by the time to cancel an order τ^{CX}

$$\frac{d}{dt}SO(t) = OR(t) - DR(t) - CX(t) \tag{19}$$

$$CX(t) = \begin{cases} \min\left(IOR(t), \frac{SO(t)}{\tau^{CX}}\right) if\ IOR(t) < 0 \\ 0 \end{cases} \tag{20}$$

Airlines can shift seats between the stocks aircraft in use $AU(t)$ and aircraft in storage $AS(t)$ at the rates into storage $IS(t)$ and return into service $RS(t)$. The rate into storage $IS(t)$ is given by the minimum of the indicated order rate $IOR(t)$ and the aircraft used divided by the time it takes to store an aircraft τ^{ISTO} if $IOR(t)$ is below zero and the operating margin $OM(t)$ is below the reference margin OM^{REF}. The return rate into service is similarly given by the aircraft used $AU(t)$ divided by the time it takes to put an aircraft into service again τ^{ISER} if the indicated order rate $IOR(t)$ is above zero.

$$\frac{d}{dt}AU(t) = DR(t) + RS(t) - IS(t) - RT(t) \tag{21}$$

$$IS(t) = \begin{cases} \min\left(IOR(t), \frac{AU(t)}{\tau^{ISTO}}\right) if\ IOR(t) < 0\ and\ OM(t) < OM^{REF} \\ 0 \end{cases} \quad (22)$$

$$RS(t) = \begin{cases} \frac{AU(t)}{\tau^{ISER}} if\ IOR(t) > 0 \\ 0 \end{cases} \quad (23)$$

Airline unit costs are broken down into three different components: aircraft ownership costs, fuel costs, and other operating costs. Aircraft ownership costs represent cost components independent of the aircraft utilization, e.g., depreciations and insurances. Fuel costs relate to the sales prices of conventional and alternative jet fuels. Other operating costs sum up remaining cost components related to, e.g., flight crews, landing fees, and administrative costs. The development of these cost components is modeled using coflow structures [145]. This allows for differentiation between cost components that depend on the number of aircraft in use $AU(t)$ (fuel and other operating costs) and cost components that depend on the total number of aircraft, regardless of whether these aircraft are used or stored.

The fleet's fuel use per kilometer $FU^{FLE}(t)$ increases with deliveries $DR(t)$ of new aircraft and decreases with retirements of used aircraft $RT(t)$. Thereby, the fuel consumption of new aircraft $FU^{NA}(t)$ is set to a reference value FU^{REF} at the start of the simulation and assumed to decrease over time due to technology improvements $TI(t)$. In order to derive the annual fuel use of the airlines $FU^{ANN}(t)$, the fleet's fuel use $FU^{FLE}(t)$ is divided by the average yearly flight distance per seat DPS.

$$\frac{d}{dt}FU^{FLE}(t) = FU^{NA}(t) - \frac{FU^{FLE}(t)}{AU(t)} \cdot RT(t) \quad (24)$$

$$FU^{NA}(t) = FU^{REF} \cdot TI(t) \quad (25)$$

$$FU^{ANN}(t) = \frac{FU^{FLE}(t)}{DPS} \quad (26)$$

The airlines' decision behavior with regard to use of alternative fuels relies on a cost comparison. For both fuel types, the sales price is calculated on a per liter basis and compared. As soon as alternative fuels provide a cost advantage against conventional jet fuels, they are preferred. In reality, the sales prices of fuels will differ for each airline due to regional price differences. This effect is included by using a table function which represents a continuous change in the preference function for one fuel type instead of a

binary step ("either-or", [145]). Figure 4.28 depicts the effect of relative price difference on the target share of alternative fuels $AFS^{TAR}(t)$.

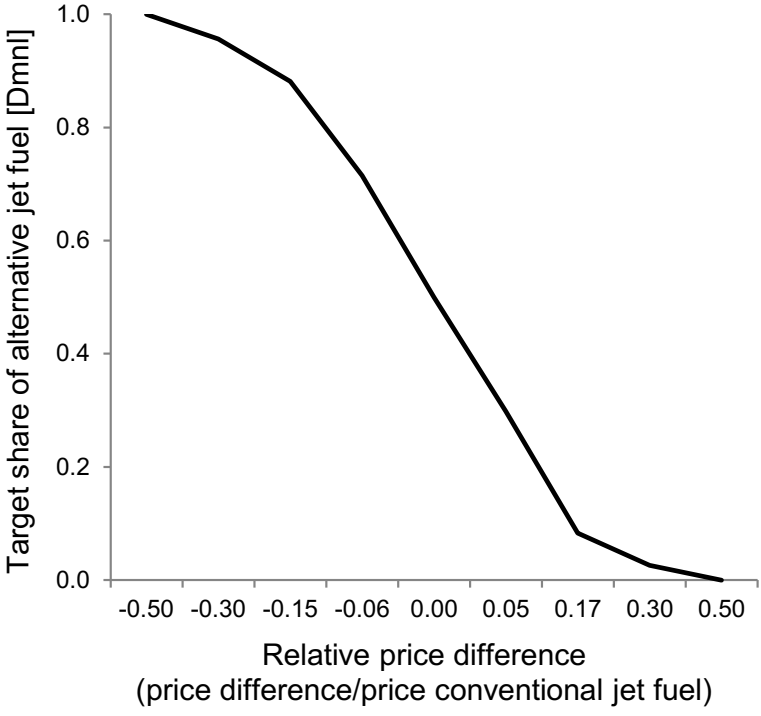


Figure 4.28 Table function for the effect of relative price difference between conventional and alternative fuel on target share of alternative jet fuel

Based on the total annual fuel consumption $FU^{ANN}(t)$, the target share of alternative fuels $AFS^{TAR}(t)$, a predefined drop-in quota for alternative fuels AFQ, and the available production capacity for alternative fuels $PC(t)$, the annual consumption of alternative jet fuels $AFU^{ANN}(t)$ is determined. From this, the annual emissions $E^{ANN}(t)$ are computed, taking into account the mitigation potential of alternative jet fuels MP and an emission index for conventional jet fuels EI.

$$AFU^{ANN}(t) = \min\left(\min(AFS^{TAR}(t), AFQ) \cdot FU^{ANN}(t), PC(t)\right) \quad (27)$$

$$E^{ANN}(t) = (FU^{ANN}(t) - AFU^{NN}(t) \cdot MP) \cdot EI \quad (28)$$

Also, the modelling of the airline industry's pricing mechanism is closely related to the work by Pierson and Sterman [146]. We assume that airlines use an anchoring-and-adjustment heuristic to determine appropriate fares [145, 384]. The airline fares $AF(t)$ adjust to a reference level $AF^{REF}(t)$ as a goal-seeking process with adjustment time τ^{AF}.

$$\frac{d}{dt}AF(t) = \frac{AF^{REF}(t) - AF(t)}{\tau^{AF}} \tag{29}$$

Current airline fares $AF(t)$ form the anchor to estimate the reference airline fares $AF^{REF}(t)$. The fares are adjusted to cost changes, competition, and load factors. The adjustment for cost changes $A^{UC}(t)$ calculates a minimum airline fare by correcting unit costs $UC(t)$ for a minimum profitability PR^{MIN} and the perceived load factor $PLF(t)$. The latter is included to consider that it takes airlines some time to measure the actual load factor. The adjustment factor for competition $A^{C}(t)$ describes how airline fares change if the number of airline competitors $NC(t)$ changes compared to an initial reference value NC^{REF}. We assume that fares are reduced if the number of competitors increases and vice versa. The adjustment factor for load factors $A^{LF}(t)$ captures the behavior of airlines to increase the load factor by means of yield management. That is, if the perceived load factor $PLF(t)$ is below the target value LF^{REF}, airline fares are reduced in order to increase the load factor. The parameters γ^{UC}, γ^{C} and γ^{LF} indicate the sensitivities of airline fares to unit costs, competition, and load factors, respectively.

$$AF^{REF} = AF(t) \cdot A^{UC}(t) \cdot A^{C}(t) \cdot A^{LF}(t) \tag{30}$$

$$A^{UC}(t) = \left(\frac{UC(t)}{AF(t)} \cdot \frac{1 + PR^{MIN}}{PLF(t)}\right)^{\gamma^{UC}} \tag{31}$$

$$A^{C}(t) = \left(\frac{NC(t)}{NC^{REF}}\right)^{\gamma^{C}} \tag{32}$$

$$A^{LF}(t) = \left(\frac{PLF(t)}{LF^{REF}(t)}\right)^{\gamma^{LF}} \tag{33}$$

The change of the number of competitors $NC(t)$ can be described by the airline market entries or exits $AME(t)$, which depend on the effect of the operating margin $E^{OM}(t)$ and the time to launch or close an airline τ^{E}. The effect of operating margin consists of the ratio of the current operating margin $OM(t)$ and a reference margin $OM^{REF}(t)$ above which airlines are expected to enter the market. The parameter γ^{OM} represents the sensitivity to the effect of operating margin. Since it is greater than zero, operating margins $OM(t)$ above the reference margin $OM^{REF}(t)$ will cause higher competition and vice versa.

$$\frac{d}{dt}NC(t) = AME(t) \tag{34}$$

$$AME(t) = \frac{E^{OM}(t)}{\tau^{E}} \tag{35}$$

$$E^{OM}(t) = \left(\frac{OM(t)+1}{OM^{REF}(t)+1}\right)^{\gamma^{OM}} - 1 \tag{36}$$

4.4.2.3 Aircraft Manufacturer

The aircraft manufacturer module depicts how the manufacturing capacity for new aircraft evolves over time in response to sudden changes of aircraft order backlogs as they occur frequently. In our model, we assume that these sudden changes significantly influence aircraft manufacturing capacity $AMC(t)$ leading to shifts in aircraft delivery times. $AMC(t)$ is modeled as a goal-seeking process in which aircraft manufacturers seek to achieve a certain target delivery time τ^{DT}. Hence, the target manufacturing capacity $TMC(t)$ can be estimated by dividing the actual backlog $SO(t)$ by the target delivery time τ^{DT}. The difference between current manufacturing capacity $AMC(t)$ and target manufacturing capacity $TMC(t)$ divided by the time to adjust manufacturing capacity τ^{MC} yields the manufacturing capacity change rate.

$$TMC(t) = \frac{SO(t)}{\tau^{DT}} \tag{37}$$

$$\frac{d}{dt}AMC(t) = \frac{AMC(t) - TMC(t)}{\tau^{MC}} \tag{38}$$

4.4.2.4 Alternative Fuel Producers

One of the main challenges for alternative jet fuels is the economic feasibility of converting biomass or hydrogen from electrolysis into drop-in alternative fuels in order to ensure low costs [92, 372].Currently, production capacities are too low to supply relevant amounts of fuel and production costs are too high to compete with conventional jet fuel. If production capacities increase, economies of scale reduce the costs of alternative fuels. This effect is depicted by the module of the production of alternative fuels. The production capacity $PC(t)$ of alternative fuels is modeled by first-order goal-seeking behavior, which adjusts to a target production volume $PC^{TAR}(t)$. This target volume is equal to the demand for alternative fuels. The time to

adjust production capacity τ^{PC} causes a constant delay, which takes into account the time required to install or expand capacities for the production of alternative fuels.

$$\frac{d}{dt}PC(t) = \frac{PC(t) - PC^{TAR}(t)}{\tau^{PC}} \tag{39}$$

Economies of scale $S(t)$ depend upon the ratio of the initial production capacity $PC^{REF}(t)$, which is taken as a reference value, the current production capacity $PC(t)$, and the degression exponent n, which aggregates effects due to capital costs, learning, and plant operation and depends on the used technology [376, 377].

$$S(t) = \min\left(\left(\frac{PC^{REF}(t)}{PC(t)}\right)^{n}, 1\right) \tag{40}$$

The costs of alternative fuels are subdivided into conversion and resource costs $CC(t)$ and $RC(t)$, respectively. Conversion costs comprise costs of components due to plant installation and operation while resource costs comprise the costs of the feedstock used. Thus, only conversion costs are subject to economies of scale. Both fuel types are influenced by the consumer price index $CPI(t)$ in order to account for inflation. The sum of conversion and resource costs subtracted by financial incentives per liter $AFI^{l}(t)$ constitutes production costs $PCO(t)$. Based on the profit margin PM, the sales price of alternative fuels $AFP(t)$ can be determined.

$$PCO(t) = CC(t) + RC(t) - AFI^{l}(t) \tag{41}$$
$$CC(t) = S(t) \cdot CPI(t) \cdot CC^{REF} \tag{42}$$
$$RC(t) = CPI(t) \cdot RC^{REF} \tag{43}$$
$$AFP(t) = PCO(t) \cdot (1 + PM) \tag{44}$$

4.4.3 Validation and Computational Results

4.4.3.1 Data Base and Simulation Set Up

The system of ordinary differential equations described in Section 4.4.2 is implemented in the software Vensim DSS 6.2 (Ventana Systems, Harvard, MA, USA). Since the high shares of international and intercontinental flights create difficulties in defining consistent regional boundaries, a global framework is chosen for the simulation experiments. All simulation runs

start in 1991 because no structural changes to the ATS have been indicated since liberalization took place in the early 1990s. In order to capture each of the IATA targets, simulations end in 2050. Alternative jet fuels are assumed to become available on a commercial scale from 2020 onwards. For the numerical integration of the differential equations, Euler-integration method with a time step of 0.015625 years is applied.

The data base for the simulation experiments is compiled from publicly available sources. Airline unit costs are estimated by means of an approach described by Liebeck et al. [385]. Their development is determined under consideration of improvements in operational and fuel efficiency as well as the development of the CPI and the price for conventional jet fuels. The improvement rate for operational and fuel efficiency is set to 1.5 % per year according to the IATA reduction targets and in line with historic improvement rates [92]. Time series data related to the development of conventional jet fuel price, population, GDP per capita, and CPI is based on information from the Energy Information Administration (Washington, DC, USA) [268], United Nations (New York, NY, USA) , and World Bank (Washington, DC, USA) [386, 387], respectively. Moreover, many parameters of the model are calibrated as these parameters are either not directly observable or cannot be obtained from scientific literature with sufficient accuracy. To this end, time series of demand taken from Boeing (Chicago, IL, USA) [388–390], of load factors taken from ICAO (Montreal, QC, Canada) [391], of operating margins taken from Sgouridis [392], and of aviation emissions taken from IATA (Montreal, QC, Canada) [393] are used.

Calibration followed a two-step procedure. First, data ranges were obtained from scientific literature wherever possible. The parameters were then calibrated within these ranges to minimize the differences between historic data and model output by means of maximum-likelihood estimation. For this step, a timeframe from 1991 to 2007 was chosen, which allows for the inclusion of an ex-post forecast during validation. Six variables were used for calibration, i.e., aircraft in use, annual aviation emissions, demand, load factor, operating margin, and airline fares. The resulting set of parameter values can be considered to be consistent with other studies, causes plausible model behavior, and does not interfere with physical laws. For that reason, we believe that the calibrated values are appropriate for the purpose of our study.

In order to take into account uncertainties when investigating the adoption of alternative jet fuels and assess their potential towards low-emission aviation, the following input parameters are systematically altered in the simulation model: feedstock costs of alternative jet fuels, conversion costs of alternative jet fuels, time to adjust production capacity for alternative jet fuels, mitigation potential of alternative jet fuels, drop-in quota for alternative jet fuels, and growth factor of conventional jet fuel prices. Biofuels as well as electrofuels are considered. Table 4.6 gives an overview of all relevant parameters and value ranges.

Conversion and feedstock costs for biofuels were derived from Schäfer et al. [306]. The feedstock costs depend on the biomass used for the production of alternative jet fuels, ranging from low-cost biomass waste to expensive plantation wood. Also, the mitigation potential of biofuels differs amongst the alternative feedstock as indicated by the German Environment Agency [371]. For electrofuels, the cost factors stem from Moser et al. [394]. Here, feedstock costs are heavily influenced by the energy prices, which are assumed to range between 0.0 €/L (excess energy free of charge) and 0.15 €/L. Regarding the mitigation potential of electrofuels, it is assumed that production fully relies on renewable energies. The drop-in quota is based on several types of alternative fuels that have been certified according to ASTM D7566 (standard specification for aviation turbine fuels) [371]. The time to adjust production capacity for alternative jet fuels is derived from a production start-up schedule for renewable jet fuels given in de Jong et al. and varied in order to take into account uncertainties [91]. Similarly, uncertainties related to the development of conventional jet fuel prices are taken into account by varying prices to grow at different growth rates of their past average. The System Dynamics model including the required data file is provided in the Supplementary Materials.

Table 4.6 Selection of parameters related to the adoption of alternative jet fuels that are altered in the simulation experiments.

Parameter	Value range for biofuels	Value range for electrofuels
Conversion costs [€$_{2012}$/L]	0.79	0.83
Feedstock costs [€$_{2012}$/L]	[0.096, 0.84]	[0.17, 3.92]
Mitigation potential [-]	[0.35, 0.8]	1
Drop-in quota [-]	0.5	0.5
Time to adjust capacity [a]	[3, 7]	[3, 7]

Growth factor of conventional jet fuel prices [-]	[0.8, 1.2]	[0.8, 1.2]

4.4.3.2 Model Validation

Several validation tests following procedures suggested by Forrester and Senge [395] and Sterman [145] were performed. Based on tests of the model structure, we ensured that the structure of the model corresponds to its real-world counterpart and that system boundaries are chosen adequately. This is in particular given since the structure follows existing model structures of the ATS (cf. Section 4.4.2) that can be found in the scientific literature. Relevant feedback loops and influencing factors related to the adoption of alternative jet fuels are modeled at an appropriate aggregation level. The same holds true for the model parameters and parameter values. For each parameter a real-world correspondence can be identified and the values are in line with findings reported in literature and what is known from industry (cf. Section 4.4.3.1). Moreover, the model is consistent with regard to its dimensionality, it shows plausible behavior for extreme conditions, and it was is successfully tested against integration errors.

Regarding the model behavior, the model allows to reproduce modes of behavior that can be observed in the ATS. For instance, the model exhibits cyclical behavior when disturbed from equilibrium state by a sudden demand decrease of 25 %. Cyclical dynamics are a very typical characteristic of the ATS [378]. Moreover, the model is able to reproduce historic system behavior that is of particular interest for the purpose of our study. That is, the ex-post timeframe from 2007 to 2016 of the variable used for calibration (cf. Section 4.4.3.1) is consistent with historic data (cf. Figure 4.29). For these variables, we additionally applied Theil inequality statistics [145] to identify the sources of error when comparing the historic data with the model behavior from 1991 to 2016. The results of this test reveal that most of the error is rather unsystematic with regard to the model purpose. Only the statistics for CO_2 emissions indicate a higher degree of systematic error (cf. Table 4.7). This error, however, is of minor importance for the model purpose since the simulated emissions reveal the same trend as the historic data.

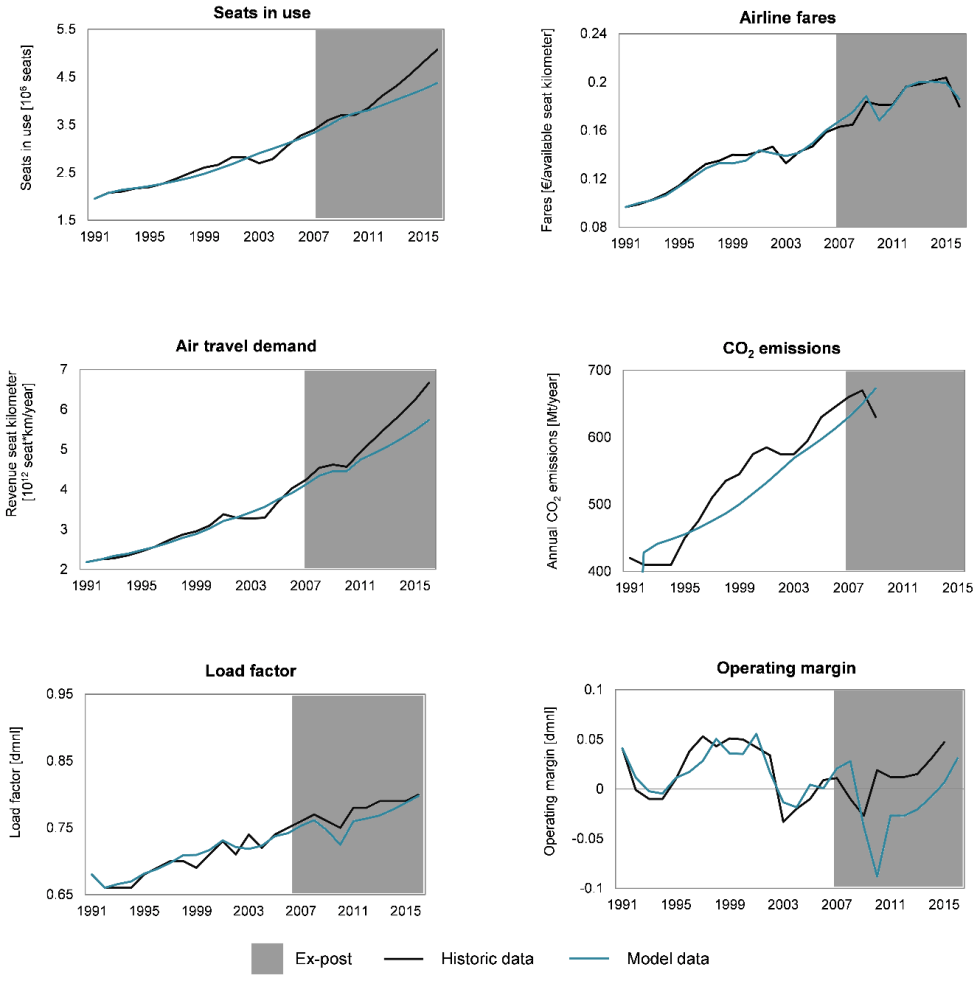


Figure 4.29 Comparison between model behavior and historic development for aircraft in use, airline fares, air travel demand, CO_2 emission, load factor, and operating margin.

Because alternative jet fuels have not been produced and used at a commercial scale so far, the corresponding model variables cannot be obtained by means of model calibration methods. Additionally, the long-term horizon of this simulation study leads to high uncertainties with regard to the development of important exogenous influencing factors. For that reason, we also conducted sensitivity analyses. The results indicate that especially external factors such as economic growth rates, feedstock costs and the mitigation potential of alternative fuels, as well as the time required to adjust fuel production capacities have a substantial influence on the model behavior. Overall, the model reveals a high degree of numerical sensitivity, while it can be considered robust in terms of behavior mode sensitivity [396]. The

high uncertainty regarding the future development of the ATS is also reflected by other studies, e.g., the CONSAVE scenarios (Constrained Scenarios on Aviation and Emissions) [397]. Thereby, our simulation results regarding the development of emissions and demand levels in the ATS lie within the range of forecasts of these studies.

Based on the conducted validation tests, we are confident that the model can be used to gain new insights with regard to adoption of alternative jet fuels and their potential towards low-emission aviation. In order to take into account the uncertainties associated with the development of external influencing factors, we will make use of Monte Carlo simulation and sensitivity analyses in the following simulation experiments. Moreover, different scenarios of the development of the ATS will be analyzed.

Table 4.7 Theil inequality statistics to compare model behavior with historical data between 1991 and 2016.

Variable	Fraction of mean square error due to		
	bias	unequal variation	unequal covariation
Aircraft in use	0.005	0.001	0.993
Airline fares	0.044	0.027	0.929
Air travel demand	0.002	0.014	0.984
CO_2 emissions	0.303	0.243	0.453
Load factor	0.026	0.166	0.808
Operating margin	0.001	0.225	0.744

4.4.3.3 Simulation Experiments and Discussion

Various simulation experiments are carried out in order to answer the two research questions raised in the introduction. The first question addresses the potential for adoption of alternative jet fuels in aviation while the second question is concerned with the extent to which alternative fuels can contribute to the CO_2 emissions reduction targets for the aviation sector. First, a Monte Carlo simulation with 1000 runs is conducted. During the Monte Carlo simulation, the values of feedstock costs, mitigation potential, time to adjust capacity, and the growth factor of conventional jet fuel prices are varied within the ranges reported in Table 4.6. The values for biofuels are varied using a uniform distribution. For electrofuels, time to adjust capacity and the growth factor of conventional jet fuel prices are also varied using a uniform distribution while a triangular distribution (with a peak at 1.67 $€_{2012}$/L [394] is used to vary feedstock costs. The mitigation potential

of electrofuels is not varied, assuming that electricity from renewable sources is used and thus no emissions are caused by production (cf. Section 4.4.3.1).

As outlined in Section 4.4.1, several institutions and organizations have set ambitious targets to mitigate CO_2 emissions from air transport such as a reduction of net emissions by 50 % until 2050, relative to 2005 levels as proposed by IATA. The results of the Monte Carlo simulation in Figure 4.30 indicate that achieving this target will require further mitigation measures since alternative fuels, if at all, only allow for decoupling air travel demand and CO_2 emissions for a limited time span. Even the largest reduction of CO_2 emissions, observed for the case of biofuels in our simulation study, only allows to reduce emissions to approximately 710 Mt/year between 2030 and 2035, which is still an increase of approximately 13 % compared to 2005 emissions (630 Mt/year), followed by an increase to 2014 levels until 2050. The increase in emissions is due to an increase in demand of 280 % between 2016 and 2050, which is in line with forecasts from the CONSAVE scenarios (cf. Section 4.4.3.1). One of the main reasons for the limited mitigation potential is the drop-in quota of alternative fuels, which is limited to 50 % and thus restricting the possible market share. In order to improve the mitigation potential, options to increase the drop-in quota should be explored by engine manufacturers as well as certification authorities.

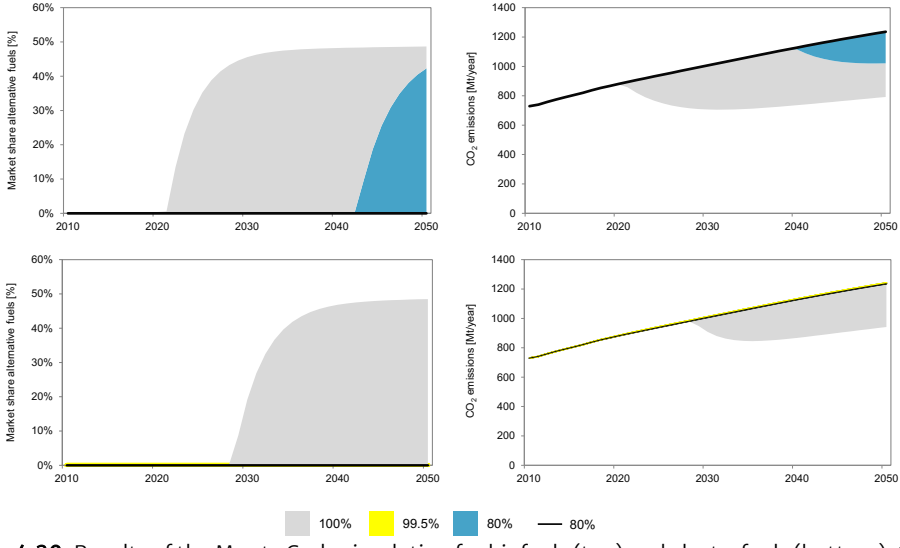


Figure 4.30 Results of the Monte Carlo simulation for biofuels (top) and electrofuels (bottom). Grey areas indicate 100 %, yellow areas 99.5 %, and blue areas the 80 % of simulated values, which are closest to the median (black line)

When comparing the adoption for the two investigated types of alternative fuel, it can be seen that biofuels have an advantage over electrofuels, i.e., biofuels gain market shares more often and also at an earlier point in time than electrofuels. This is mainly due to the lower feedstock costs of biofuels compared to electrofuels. Current production processes for electrofuels require significant amounts of electricity and are therefore highly dependent on the electricity price. Even moderate increases of the electricity price lead to significant cost benefits of biofuels over electrofuels. In order to exploit the higher mitigation potential of electrofuels, new production processes that are more energy-efficient should be developed. The relevance of such processes is further underlined as electrofuels do not rely on biomass that requires large areas of land and has to be transported to the production facilities. Instead, hydrogen from water electrolysis can be supplied easily for the production of electrofuels. Thus, especially in areas where biomass has to be transported over long distances or the area to cultivate biomass is very limited, electrofuels are a promising alternative, provided that economically feasible production processes exist.

Since the results of the analysis suggest that biofuels provide a higher potential towards low-emission aviation, this fuel type is further investigated. To this end, three different scenarios are defined, namely a baseline scenario, a scenario favoring alternative fuels (pro alternative) and a scenario favoring conventional fuel (pro conventional). The scenarios differ in the values of the mitigation potential of biofuels, the growth factor of conventional jet fuel, the time to adjust capacity, and the feedstock cost, as reported in Table 4.8.

Table 4.8 Parameter values that define the three scenarios considered in the analysis of biofuels.

Parameter	Pro alternative	Baseline	Pro conventional
Feedstock costs [€$_{2012}$/L]	0.096	0.47	0.84
Mitigation potential [-]	0.8	0.5	0.35
Time to adjust capacity [a]	3	5	7
Growth factor of conventional jet fuel prices [-]	1.2	1.0	0.8

The pro alternative scenario is the only setting where biofuels gain market shares (cf Figure 4.31). Thus, a contribution of alternative fuels towards reducing CO_2 emissions from aviation can only be achieved if the general conditions favor biofuels significantly.

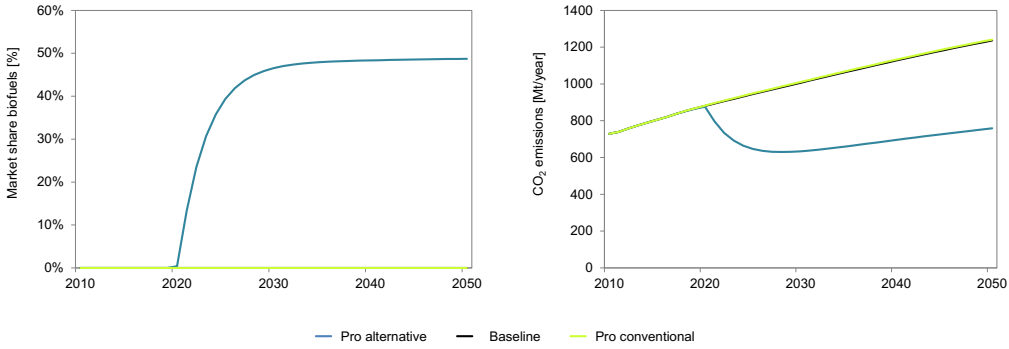


Figure 4.31 Market shares and CO_2 emissions for biofuels for the baseline (black), pro alternative (blue), and pro conventional (green) scenario.

This requires very low feedstock costs that can only be realized if biomass is obtained from waste and if the available amount of biomass from this source suffices to satisfy fuel demand from the aviation sector. Additionally, a high growth rate of the price of conventional jet fuel is necessary for biofuels to gain substantial market shares. Provided that market shares are gained, the reduction of CO_2 emissions as shown in Figure 4 can only be realized if the mitigation potential of biofuels is high. Since the adoption of biofuels requires them to be produced from waste to ensure low feedstock costs, a high mitigation potential can be achieved.

In order to trigger demand for biofuels in a less favorable setting, incentives are required. To study the effect of incentives on market shares of biofuels and CO_2 emissions from aviation, we introduce an incentive on the production costs (incentive level in €/L) of biofuels for a predefined time period (incentive duration) in the baseline scenario. A full factorial simulation experiment is conducted to study all combinations of incentive level (step size of 0.05 €/L) and duration (step size of 1 year). The results of this experiment are shown in Figure 4.32.

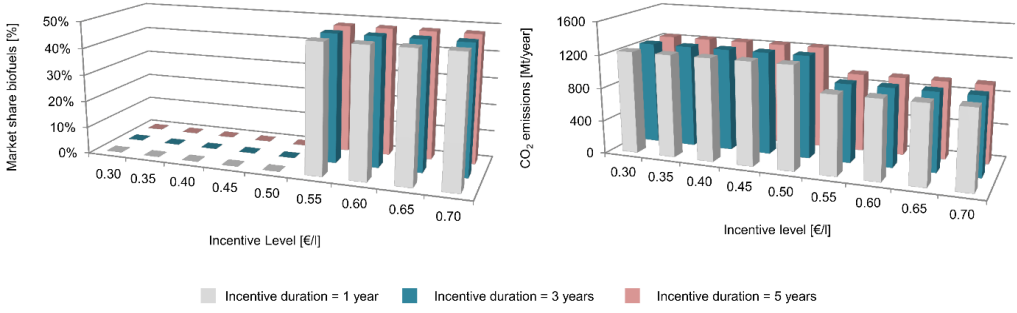


Figure 4.32 2050 levels of market shares and CO_2 emissions for biofuels for different incentives levels and an incentive duration of one year (grey) three years (blue) and five years (red), respectively.

It can be seen that an incentive level of 0.55 €/L is required to trigger demand for biofuels. A further increase of the incentive does not result in additional demand in 2050. The same holds true for the incentive duration. An incentive that supports biofuels for one year is sufficient as an extension of the duration does not result in additional market shares. This underlines the importance of political measures to steer the development of the aviation sector. Such measures are currently explored (e.g., Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA) as proposed by IATA or already implemented (e.g., inclusion of the European aviation sector in the European Emission Trading System (ETS)).

4.4.4 Summary

In this paper, a System Dynamics model of the ATS has been developed in order to investigate the adoption of alternative jet fuels in aviation and their potential towards low-emission aviation. Real-world data is used to calibrate the model by means of maximum-likelihood estimation methods, to thoroughly validate the model, and to conduct Monte-Carlo simulations as well as scenario and sensitivity analyses. Based on the simulation experiments, we show that the adoption of alternative fuels is rather unlikely for the currently certified production pathways. These pathways do not allow for competitive prices compared to conventional jet fuel, which holds especially true for electrofuels. In contrast, high growth rates of conventional jet fuel prices, short durations to increase production capacities, and monetary incentives are identified as the main drivers for the adoption of alternative jet fuels. Even if alternative jet fuels are adopted, their potential to achieve long-term reduction targets for aviation is limited, which is especially due to existing restrictions regarding the blend of alternative jet fuels with conventional jet fuel. The results emphasize the need for the development of new production pathways that allow for a more efficient conversion of biomass or hydrogen into drop-in fuels. Additionally, the application of policy measures seems to be a promising measure to promote the adoption of alternative fuels.

One limitation to our study is that we do not take into account constraints on the availability of the feedstock, which is especially important for biofuels. The same holds true for the impact of an increase in biofuel demand on land use changes and transport distances between biomass sources and conversion facilities. Including these results would most likely

further limit the adoption of alternative jet fuels and their potential towards low-emission aviation. Future research should investigate these effects in more detail. Integrating aspects of fuel availability at the airports would be another way to extend the model. Additionally, the decisions of fuel producers concerning the deployment of production facilities for alternative jet fuels, of airlines concerning the adoption of alternative jet fuels, and of policymakers concerning the application of policy measures could be modeled and analyzed in more detail. With regard to the passengers, the influence of more sustainable fuels on the willingness to pay and, thus, overall demand for alternative jet fuels might be a promising way to extend the scope of the model.

4.5 Synthesis – System Integration

The previous sections cover aspects of integrating alternative fuels into the air transport system, with regard to climate forcing and integration complexity. These sections are now summarized and discussed against other measures to transform the commercial air transport system towards a lower climate forcing. Consequently, different measures to integrate the fuel-related mitigation measures into the commercial air transport system are described and discussed first (*Research Question 4*, section 4.5.1) and then main influential factors for their successful system integration (*Research Question 5*, section 4.5.2) and their climate forcing (*Research Question 6*, section 4.5.3) are described and discussed, respectively. Lastly, potential trade-offs and interdependencies among these mitigation measures are discussed in the overall synthesis (section 4.5.4).

4.5.1 Options for System Integration

In this first part, different options for the integration of alternative fuels into the air transport system are summarized (section 4.5.1.1). Subsequently, other, not fuel-related transformations of the air transport system to reduce its climate forcing are discussed (section 4.5.1.2).

4.5.1.1 Synthesis

Three different fields of action concerning the system integration of kerosene with a potentially lower climate forcing compared to conventional kerosene are studied, namely the targeted use of paraffinic kerosene, blending requirements of current fuel specifications and system studies for market-based measures to stimulate demand for alternative aviation fuels with a reduced climate forcing.

The targeted use of paraffinic kerosene aims at maximizing the climate-forcing mitigation potentials of a given amount of paraffinic kerosene (section 4.1). Kerosene mainly consisting of such paraffinic components can significantly reduce contrail-related climate forcing compared to conventional kerosene, since it causes lower soot emissions due to its very low content of aromatic components (section 4.1.1 [18, 84–86, 131]). In principle, paraf-

finic kerosene could be provided from renewable feedstock or from hydroprocessed crude oil-based kerosene. However, it is currently scarcely available on global markets (section 3.2.4.1 [240]).

Only a small fraction (< 10 %) of the commercial flights worldwide cause the large majority (> 80 %) of the contrail climate forcing [9, 10, 177]. Moreover, contrails are typically formed during a small portion of the entire flight distance [317]. Targeting flights or even flight segments causing a high contrail climate forcing with paraffinic kerosene could result in substantial climate forcing mitigation potentials [10]. But such a concept would require a new, segregated infrastructure to supply paraffinic kerosene for particularly climate relevant flights and – for the segment-specific allocation – also modifications of the aircraft in use (section 4.1.2.1.1). Both demands result in additional operational and partly even infrastructural efforts.

Based on the experiences made during a demonstration experiment to study the effects on local air quality from using renewably sourced kerosene (section 4.2.2.1.1), such efforts are described and differences between the demonstration flights and a targeted use concept as well as a potential large-scale application are discussed (section 4.2). Large parts of the supply chain (e.g., supply lines to and at airports) would need to be duplicated, incurring additional costs. A segregated supply of paraffinic kerosene by fuel tanker trucks appears realistic for short- to medium-range aircraft. Long-range aircraft, however, are equipped with substantially larger fuel tanks (about ten times) requiring by far higher fuelling rates for the given short turnaround times (section 4.2.2.1.1). As a result, fuelling long-range aircraft during routine operations depends in most cases on a hydrant system, for which the introduction of a segregated supply would be truly challenging (section 4.2.3.1).

The current requirements defined by the respective ASTM standards for fuel blending limits carbon dioxide and contrail-related climate mitigation potentials (section 4.3). Implications from blending renewably sourced kerosene show that fuel density, content of aromatic components and the distillation curve gradient are relevant factors for the permissible blend ratio, due to their strict limits in the present ASTM specifications (section 4.3.6 [135–137, 181, 280]). For blends of conventional and renewably sourced kerosene, also the variation of conventional kerosene's properties should be considered (section 4.3.3).

The study of the air transport system's dynamics (section 4.4) indicates central levers for the market ramp up of renewably sourced kerosene, namely the cost differential between conventional and renewably sourced kerosene, the air transport system's growth rate and the lead times ("delay") for the ramp up of renewably sourced kerosene production capacities (section 4.4.3). Currently, a large difference exists between the cost of conventional and renewably sourced kerosene; this is particularly true for renewably sourced kerosene from non-biogenic feedstock (section 4.4.4). The main reason of this cost differential is that the cost of conventional kerosene occurring during their use (e.g., cost to recover from more extreme weather events, additional pressures on health systems from deteriorated local air quality, higher dams due to a rise in sea water level) are covered by the global society as a whole instead of solely the users of conventional kerosene.

4.5.1.2 Discussion

Measures to transform the commercial air transport system for lower climate forcing mostly affect flight operations and infrastructure, such as airports and airspace structures [304]. The measures discussed here are flight route modifications to lower contrail-related climate impacts, more efficient flight operations and the harmonization of airspace structures; they are listed in Table 4.9.

Table 4.9 Exemplary climate forcing mitigation measures and implications of their system integration into the air transport system

Measure	Description
Flight route modifications for contrail avoidance	Avoid ice-super-saturated regions to reduce contrail-related climate forcing
More efficient flight operations	Modify flight profile and operations to lower fuel required for flight, e.g., by more continuous descends, direct routings, taxiing with fewer engines)
Airspace harmonization	Modify airspace structures to allow for more direct flight routings

The modification of flight routes could lower contrail-related climate forcing [29, 177, 355]. Persistent contrails form in ice-super-saturated regions typically characterized by a limited geographical extent [29, 177]. Therefore, deviating flights around such ice-super-saturated regions might be possible for a comparatively small trade-off in terms of flight time and fuel

consumption (and thus additional greenhouse gas emissions) [29, 177, 355]. Measures to increase the efficiency of flight operations typically refer to modifications of flight profiles to reduce the fuel consumption of individual flights, e.g., by continuous descends, more direct flight routings or taxiing with fewer running engines [153, 306]. Similarly, the harmonization of airspaces aims at allowing for more direct routings and thus a reduced fuel consumption by avoiding conflicting borders of controlled airspace [30].

4.5.2 System Integration

In the following, important factors for a successful integration of the fuel-related measures and of other transformations of the air transport system are discussed. Ergo, at first implications for the system integration of fuel-related measures are described (section 4.5.2.1) and then discussed against implications for further adoptions of the air transport system (section 4.5.2.2).

4.5.2.1 Synthesis

For the targeted use concept, the strategies “uniform allocation”, “flight-specific allocation” and the “segment-specific allocation” do not only differ in terms of their climate mitigation potentials, but also in their implications for a successful system integration. The system integration of a uniform allocation is comparatively simple, because no actions are required up to blend shares of about 50 %. Therefore, this measure is considered to be already available by now (section 4.2.3.1).

Aircraft are either fuelled via refueller trucks (smaller airports) or via a hydrant system (larger airports) [279]. Targeting individual flights via a single line hydrant fueling system is practically not feasible; therefore, for most of the current infrastructure available at airports, a segregated supply can only be realized using refueller trucks (section 4.2.3.1). Due to their high fuel demand, long-range aircraft typically cannot be fuelled by such trucks during the available turnaround time within the given economic constraints (section 4.2.3.1 [279]). Thus, a viable targeted use concept for long-range flights appears only possible in the medium-term, including sufficient lead time for the respective (significant) infrastructure modifications (e.g., the construction of an additional supply line in existing hydrant systems).

Instead, a segregated fueling of short- and medium-range flights by refueller trucks appears feasible, potentially even in the short-term (section 4.2.3.1). This holds particularly true for airports where the fuel is delivered by trucks anyway.

Targeting segments of flights would not only require the infrastructure modifications mentioned above, but also modifications of the aircraft's internal fuel system to allow for an in-flight fuel switching (section 4.2.3.1). Due to the long development and certification duration of new aircraft technologies, this measure would probably be available only in the medium-term. A potential advantage of such a strategy might be that also for long-range aircraft smaller amounts of paraffinic kerosene would be required. This could in turn enable its supply by refueller trucks while the majority of the flights' fuel demand is supplied via a hydrant system (section 4.2.3.1); as a result, this might enable the "segment-specific allocation" even for long-haul flights.

Current fuel specifications are defined in a way that blends of renewably sourced kerosene and conventional kerosene can be used in the same way as neat conventional kerosene (section 4.3.2). Accordingly, in terms of blending requirements, the system integration of alternative fuels cannot be simplified any further. To enable the use of neat synthetic kerosene, mostly the content of aromatic components is often considered critical for blending [135]. However, several further fuel properties (such as fuel density and distillation curve gradient) are (in)directly affected by blending renewably sourced and conventional kerosene [135, 137]. The lack of aromatic components reduces the density of a kerosene type, which might fall out of the permissible range defined by ASTM and thus needs to be compensated for by the conventional kerosene component (section 4.3.5 [135, 137]).

The system dynamics study of the air transport system provides insights about key levers affecting the system integration of renewably sourced kerosene. It identifies the air transport system's growth rate, the delay for the ramp up of renewably sourced kerosene and the cost difference between conventional and renewably sourced kerosene as key levers for a successful market ramp up of renewably sourced kerosene. However, from a present-day perspective some noteworthy limitations of the study are recognizable, e.g., a short delay for capacity ramp up and most likely strong scale effects for renewably sourced kerosene.

The commercial air transport system's growth rate almost directly affects the change in the air transport system's energy and thus fuel demand. Higher growth rates would require greater amounts of renewably sourced kerosene and thus a steeper increase in their production capacities, while less or even no growth of the air transport system would reduce the efforts for replacing the majority of aviation's current fossil fuel-based energy use demand by renewably sourced kerosene and thus facilitate the mitigation of aviation's climate impact (section 4.4.3.3). Similarly, the shorter the delay for the ramp up of renewably sourced kerosene production facilities (i.e., the faster the corresponding facilities can be planned and constructed), the greater would be the extent to which such fuels can support the reduction of aviation's climate forcing (section 4.4.4). The cost difference between conventional and renewably sourced kerosene could be overcome by either adequately allocating the use cost of conventional kerosene to its users (e.g., by carbon pricing mechanisms, section 4.5.1) or by incentivizing the use of renewably sourced kerosene (section 4.4.3).

4.5.2.2 Discussion

The main influential factors for the measures to adopt the air transport system for lower climate forcing are summarized in Table 4.10. In the following, key influential factors facilitating or hindering the respective measures' system integration are discussed as basis for a comparison with the system integration implications for the fuel-related measures discussed in the previous section.

Table 4.10 Exemplary climate forcing mitigation measures and main influential factors for their system integration

Category	Measure	System Integration
Operations and Infrastructure	Flight route modifications for contrail avoidance	Uncertain, due to uncertain marginal abatement cost and presently missing incentive schemes
	More efficient flight operations (continuous descent, direct routing, single-engine taxi)	Facilitated by reduction of airline operational cost
	Airspace harmonization	Facilitated by reduction of airline operational cost but hindered by political complexity

Due to the large effect of fuel cost on airline operating cost, a strong demand signal exists for reducing fuel consumption of engines and aircraft in general [232, 306]. This clearly facilitates the introduction of measures to reduce fuel consumption and thus carbon dioxide-related climate forcing such as more efficient flight routings and the harmonization of airspaces [306]. A prominent example for airspace harmonization is the EU's "Single European Sky" initiative, which has been delayed for a long period of time due to its political complexity [398].

Flight route modifications to reduce contrail-related climate forcing are currently not clearly associated with an economic benefit. As of now, the marginal abatement cost for mitigating contrail-related climate impacts by flight route modifications have not yet been investigated at depth. First studies indicate only a comparatively small increase in operating cost due to an increased fuel consumption [177, 399].

In light of these factors, it appears that measures to lower the air transport system's fuel consumption are already largely incentivized by the airlines' pressure to lower operational cost. For the system integration of measures to reduce contrail-related climate forcing, such climate effects would need to be reflected economically similar to carbon dioxide-related climate forcing. Thus, including all climate effects of aviation in economic systems, e.g., via emissions trading schemes, could create an incentive for the introduction of mitigation strategies such as the targeted use of paraffinic kerosene or flight route modifications for contrail avoidance, for which some studies indicate a high mitigation potential at comparatively low operational cost [177, 399].

4.5.3 Climate Forcing Mitigation Potentials

Now, the climate forcing mitigation potentials of the different system integration options of the fuel-related measures and of other transformations of the air transport system are discussed. Initially, the climate forcing mitigation potentials of the fuel-related measures are described (section 4.5.2.1) and then discussed against mitigation potentials of further air transport system adoptions (section 4.5.2.2).

4.5.3.1 Synthesis

The targeted use concept studied in chapter 4 assumes that 5 % of the overall kerosene consumption can be provided as neat paraffinic kerosene. Compared to no use of paraffinic kerosene, a uniform allocation to all 844 364 flights in the dataset used here would reduce the contrail energy forcing by about 4 %. If only the flights with the highest warming contrail forcing receive neat paraffinic kerosene, the contrail energy forcing would be lowered by 36 %. In this case, about 10 % of the flights with a net warming contrail energy forcing would receive paraffinic kerosene. Furthermore, when only the segments of flights which are responsible for the most warming contrails are targeted, the contrail energy forcing would even be lowered by 55 %. Here, about 62 % of the flights with a net warming contrail energy forcing would receive paraffinic kerosene.

Inter-annually (when comparing the years 2017, 2018 and 2019 against each other), estimated mitigation potentials are rather robust. However, on shorter time-scales, seasonal and meteorological variations strongly affect contrail-related climate forcing and thus also the associated mitigation potentials (section 4.1.3.1.3).

Provided that the envisioned ramp up of renewably sourced kerosene materializes, market shares of paraffinic kerosene would gradually increase. In this case, the advantages of a segment-specific over a flight-specific allocation diminish at market shares of about 25 % (section 4.1.3.1.2). Thus, the segment-specific allocation appears only beneficial for a transitional period.

Since the contrail-related climate forcing of the aircraft used for the demonstration flights are subject to large uncertainties, the associated mitigation potentials of the segregated supply were estimated using the previous model of the same aircraft family (section 4.2.2.1.1). From a flight operational perspective, both aircraft are very similar since the main difference among them is the engine type. The contrail energy forcing of the demonstration flights with a 35 % renewably sourced kerosene blend was about 11 % lower compared to a case where conventional kerosene would have been used. By using a 50 % blend, these mitigation potentials might be increased to more than 20 % in terms of contrail energy forcing (section 4.2.2.3.2).

The system dynamics model used here assumes that a blend limit of 50 % remains in place until 2050. Based hereupon, model simulations achieving a renewably sourced kerosene market share of 50 % reach similar carbon dioxide emissions level by the year 2050 as in 2019. In this case, the carbon dioxide emission reductions in 2050 are counterbalanced by the assumed commercial air transport system's growth rate (section 4.4.3.3). This underlines the importance of a specification for neat, renewably sourced kerosene on the one hand and the significant effect of the expected commercial air transport system's growth rates on the other.

4.5.3.2 Discussion

The main influential factors on the climate forcing mitigation potential for the measures to adopt the air transport system are summarized in Table 4.11. These factors are used as basis for a comparison with the main influential factors on the climate forcing mitigation potential for the fuel-related measures discussed in the previous section.

For flight route modifications to lower contrail-related climate impacts, a simulation study shows a mitigation of almost all warming contrail energy forcing for a fuel penalty of less than 1 % of the overall fuel consumption [29]. Similar results were found by an experimental demonstration of rerouting flights to avoid contrail formation [399]. However, several questions remain as to the applicability of such concept in high density airspace (e.g., above Europe), airspace with high separation minima (e.g., the North Atlantic flight corridor) and the reliability of contrail climate forcing forecasts.

Table 4.11 Exemplary climate forcing mitigation measures and influential factors affecting their system integration); ? – unknown mitigation potential, low – less than 10 %, medium – up to 50 %, high – up to 100 %

Category	Measure	Climate forcing mitigation potential (contrail- / carbon dioxide-related)
Operations and Infrastructure	Flight route modifications for contrail avoidance	**High** (high / low)
	More efficient flight operations (continuous descent, direct routing, single-engine taxi)	**Low** (low / low)
	Airspace harmonization	**Low** (low / low)

Typical measures to reduce fuel consumption in terms of flight operations or airspace harmonization are expected to reduce carbon dioxide-relate climate forcing by less than 5 % [153, 306]. Reductions in contrail-related climate forcing can hardly be expected [153, 306].

In light of these factors, flight route modifications and the targeted use of paraffinic kerosene appear as most promising options to lower contrail-related climate forcing. Measures to adopt the commercial air transport system for lower carbon dioxide-related climate forcing show a rather limited mitigation potential.

4.5.4 Overall Synthesis

Figure 4.33 shows a comparison of the measures concerning their system integration complexity and overall climate forcing mitigation. For most cases, the change in climate forcing and implications for system integration seem to be correlated – large mitigation potentials can mainly be achieved for a more complex system integration. Particularly promising measures would yield a comparatively large mitigation potential at rather low implications for technology and system.

The targeted use of paraffinic kerosene illustrates this relationship. The integration of a uniform allocation of paraffinic kerosene into the air transport system would be simpler than targeting specific flights or even segments of flights. However, a uniform allocation would also only allow for a minor mitigation of aviation's overall climate forcing. A flight-specific allocation to short- and medium-range flights appears feasible in the short-term and would allow for a clearly larger mitigation in climate forcing at the expense of a slightly more complex system integration. A segment-specific allocation or targeting long-range flights, however, appears rather to be feasible in the medium-term.

In comparison, flight route modifications for contrail avoidance appear particularly promising. For a seemingly simpler system integration than, e.g., targeting specific flights, they might yield major climate forcing reductions by mitigating a large fraction of contrail-related climate impacts. Measures to reduce fuel consumption either by more efficient flight operations or by airspace harmonization would only yield minor changes in climate forcing, but would require notable changes in the air transport system in some cases (e.g., airspace harmonization).

For this reason, understanding synergies among the targeted use of paraffinic kerosene and modifications of flight routes could reveal further insights. For example, paraffinic kerosene could be used on routes where the avoidance of ice-super-saturated regions is either impossible or counterbalanced by a substantially increased fuel consumption. Airspaces with high traffic densities (e.g., Central Europe) or large aircraft separation minima (e.g., the North Atlantic region) might impede the diversion of flights for contrail avoidance. Alternatively, in cases where the avoidance of such regions induces a high fuel penalty (e.g., by deviating from the most economic flight altitude or by substantially increased flight distances), the use of paraffinic kerosene might be suitable as well.

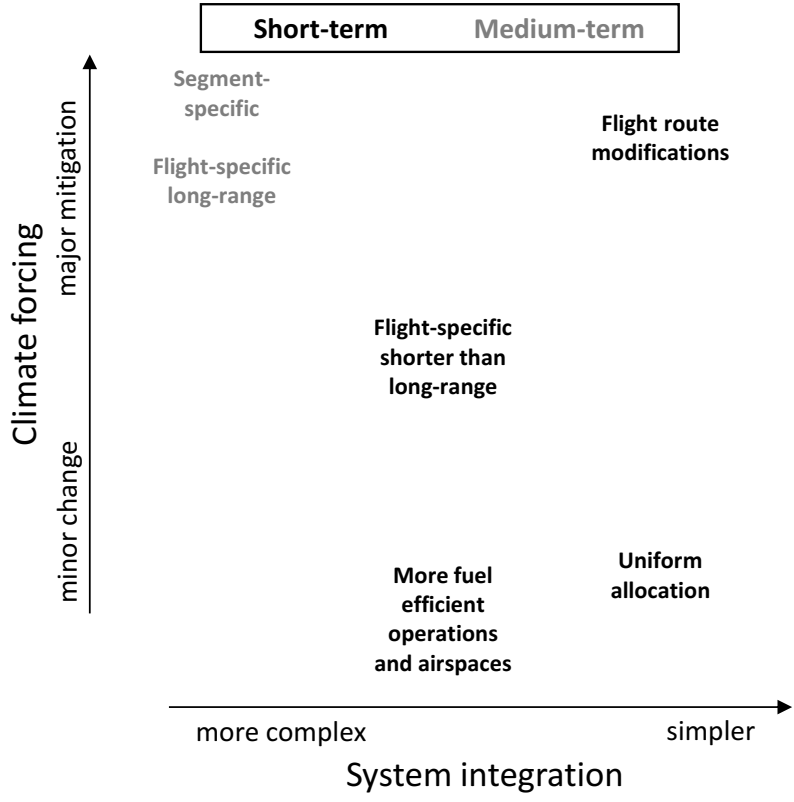


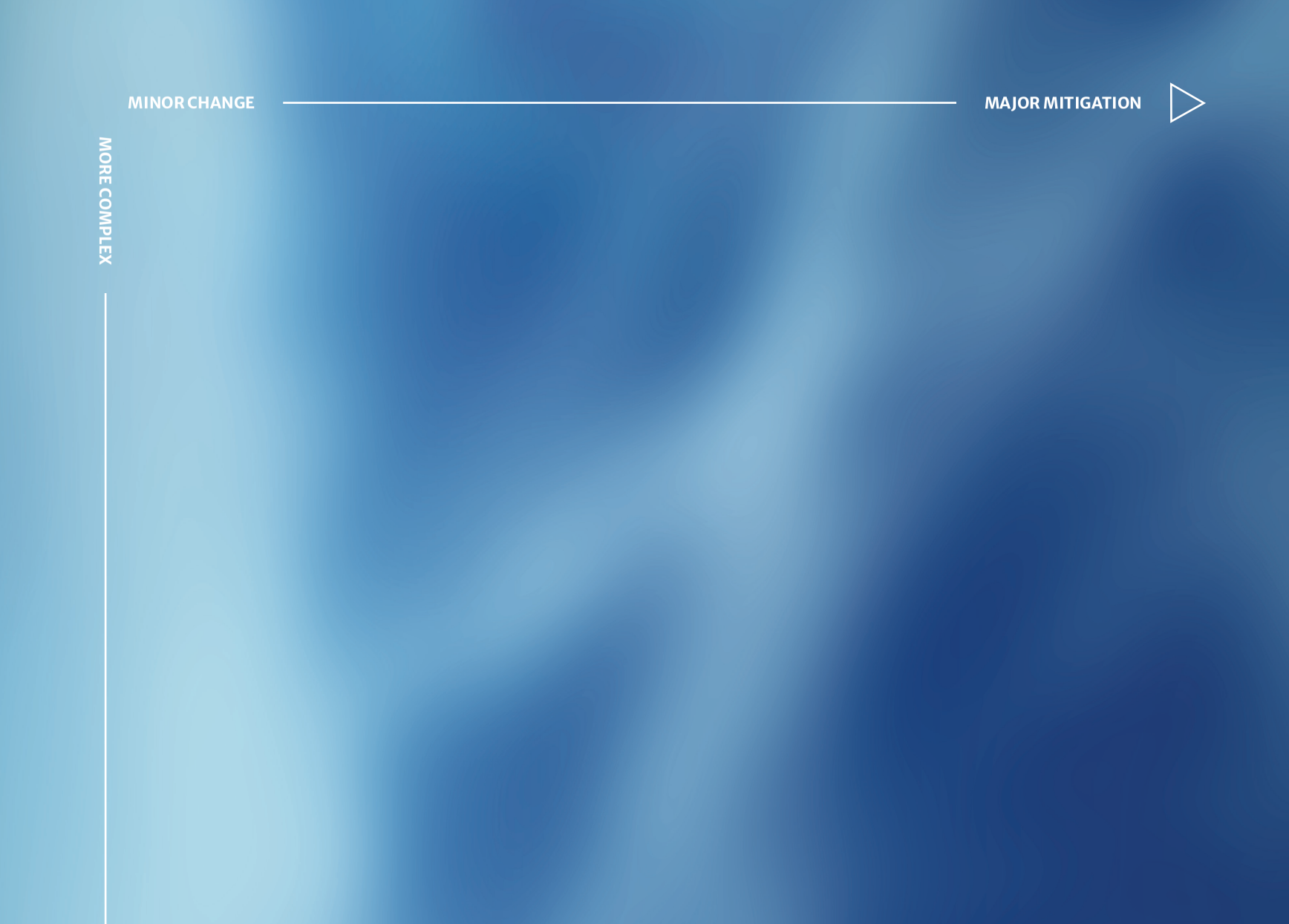
Figure 4.33 System integration and climate forcing mitigation potentials of the system integration measures discussed in this section

Assessing the mitigation cost of additional hydroprocessing against the mitigation cost of flight route modifications could indicate their respective

marginal abatement cost. This would provide further information on the economic efforts required for their realization.

The commercial air transport system's dynamics are presently characterized by an incomplete economic representation of the social and environmental / ecological costs of using fossil crude oil-based energy carrier. This results in a large cost differential between conventional, i.e., fossil fuel-based kerosene and renewably sourced kerosene. Since cost of climate damages incurred by the extensive use of fossil energy carrier are not included in the present economic system based on the current legal framing, their use is currently clearly favored. This holds true for contrail- and carbon dioxide-related climate impacts. A more accurate representation of these effects and all further climate impacts of aviation in economic systems (e.g., by including them in emissions trading schemes), could incentivize the use of renewably sourced kerosene or measures to lower contrail-related climate forcing, such as the targeted use of paraffinic kerosene or flight route modifications.

In summary, the comparative discussion of fuel-related mitigation measures with other mitigation measures indicates two particularly promising mitigation measures. These are the targeted use of paraffinic kerosene and flight route modifications to lower contrail-related climate forcing. The use of renewably sourced kerosene to lower carbon dioxide-related climate forcing in turn, might be stipulated by more adequately including the cost of using fossil energy carrier in economic systems. Furthermore, interactions among a targeted use concept and flight route modifications to lower contrail-related climate impacts might be of particular interest. For example, flights for which flight route modifications are not possible could be targeted with paraffinic kerosene.


MINOR CHANGE
MAJOR MITIGATION
MORE COMPLEX

5 SUMMARY AND OUTLOOK

5 Summary and Outlook

This chapter summarizes the results in terms of fuel provision (chapter 3) and system integration (chapter 4) and draws overall conclusions for the role of fuel-related mitigation measures to mitigate climate forcing of aviation. In the end, an outlook on potential further research developments is provided.

5.1 Summary

The primary goal of this thesis is to contribute towards a better understanding about the role of fuel-related measures to mitigate the climate forcing of commercial aviation. Both aspects, the availability of a technology to provide alternative aviation fuels and the integration of such fuels into the air transport system determine the climate forcing mitigation potential of any fuel-related measure. Hence, this thesis examines these two aspects, namely the provision and system integration of fuel-related measures to mitigate the climate forcing of aviation. Moreover, due to the time-critical nature of anthropogenic climate change, the duration to implement such fuel-related mitigation measures is considered as well.

Figure 5.1 shows the fuel-related measures in terms of fuel provision and system integration classified by contrail- / carbon dioxide-related climate forcing reduction and climate forcing reduction / system integration, respectively. The temporal availability of the different measures is indicated by black font for measures available in the short-term (until the year 2030) and grey font for measures available in the medium-term (between the years 2030 and 2050). Since the potential of measures available in the long-term (i.e., after the year 2050) is highly uncertain, they are not shown in this figure.

In the short-term, i.e., until the year 2030, mild hydroprocessing of conventional kerosene and blended renewably sourced kerosene appear to be realistic options for fuel provision. Mild hydroprocessing of conventional, crude oil-based kerosene would mainly lower contrail-related climate forcing by about 20 % (in terms of energy forcing) for the assumptions taken in section 3.1, but also imply a very small increase in carbon dioxide-related climate forcing. The use of blended renewably sourced kerosene would moderately lower carbon dioxide-related climate forcing (by up to 50 % depending on their specific lifecycle carbon dioxide emissions and global market shares). Regarding the system integration, a uniform allocation of paraffinic kerosene or targeting short- and medium-range flights appear feasible. While a uniform allocation could presumably only achieve a minor climate forcing mitigation, targeting short- and medium-range flights would allow for a larger climate forcing mitigation (up to 36 % in terms of contrail energy forcing) at the expense of a moderately more complex system integration.

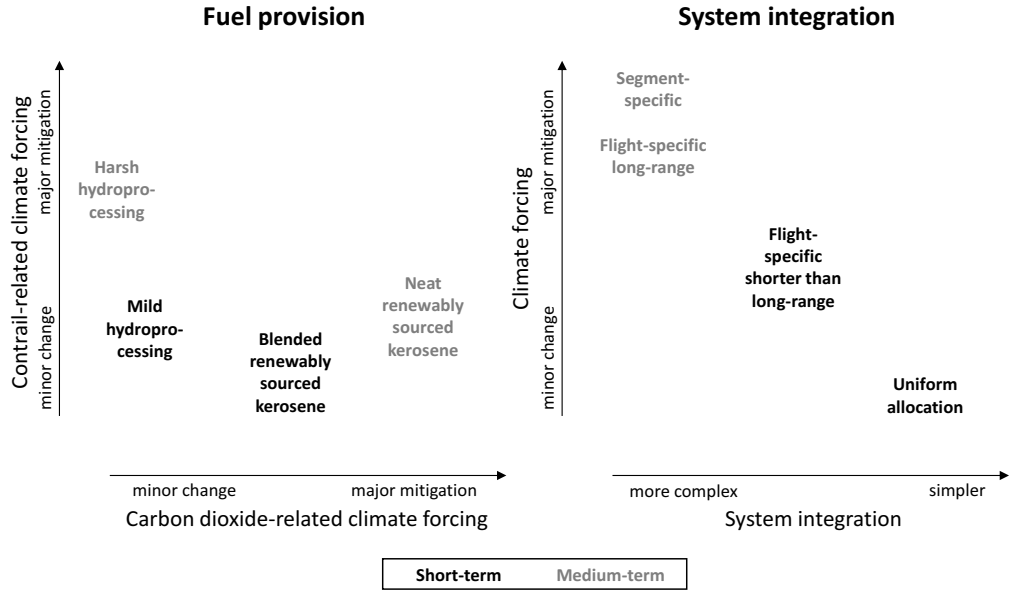


Figure 5.1 Fuel-related measures to mitigate the climate forcing of aviation and their effect on climate forcing and system integration; short-term – until the year 2030, medium-term – between the years 2030 and 2050

In the medium term, i.e., between the years 2030 and 2050, the development of fuel standards for neat paraffinic and / or renewably sourced kerosene might enable the utilization of harsh hydroprocessing and neat renewably sourced kerosene. Harshly hydroprocessing the majority of the conventional kerosene would lower contrail energy forcing by about 33 %, while already considering the small carbon dioxide trade-off from fuel processing. Neat renewably sourced kerosene could largely mitigate carbon dioxide-related climate forcing by up to 100 %, depending on its specific lifecycle carbon dioxide emissions and global market shares. The contrail-related mitigation potential of renewably sourced kerosene strongly depends on the allocation strategy employed. By then, further system integration measures could potentially be employed, such as a segment-specific allocation strategy and / or targeting of long-range flights with paraffinic kerosene.

In the long-term, i.e., after the year 2050, the majority of aviation fuel in use should originate from renewable sources of energy to achieve the globally agreed mitigation targets. In this case the additional benefits of a targeted use of paraffinic kerosene would be substantially smaller compared to the present situation.

Based on these results, the following conclusions about the role of fuel-related measures to mitigate the climate forcing of aviation can be drawn.

- For a transitional period, hydroprocessing of crude oil-based kerosene can further reduce aviation's contrail-related climate forcing. This holds true even when considering additional carbon dioxide emissions from hydrogen provision required for additional hydroprocessing.
- Renewably sourced kerosene is essential to mitigate aviation's carbon dioxide-related climate forcing, because it substitutes the currently used fossil fuel-based kerosene and thus allows for the mitigation of in principle all lifecycle carbon dioxide emissions from using kerosene. Additionally, depending on its system integration (i.e., uniform or targeted to flights with high contrail-related climate forcing), renewably sourced kerosene can additionally mitigate contrail-related climate forcing.
- The targeted use of paraffinic kerosene (either from renewable sources of energy or hydroprocessed crude oil-based kerosene) can substantially mitigate large contrail-related climate forcing. However, depending on the allocation strategy (flight or segment-specific) and the aircraft types affected (short- and medium-range or long-range), the system integration might become increasingly complex.

Overall, fuel-related measures play an important role in mitigating the overall climate forcing of aviation. In terms of carbon dioxide-related climate forcing, they constitute the only option to entirely mitigate lifecycle carbon dioxide emissions. For contrail-related climate forcing, hydroprocessing of conventional kerosene and allocating paraffinic kerosene to flights with high contrail-related climate forcing provide opportunities for further substantial climate forcing mitigation.

5.2 Outlook

After summarizing the role of fuel-related mitigation measures from a present-day perspective in the previous section, this section turns towards future research developments. Potential steps for the introduction of fuel-related measures are discussed in the interaction with other measures, sorted by their temporal availability.

5.2.1 Short-term

In the short-term, i.e., until the year 2030, the use of blended renewably sourced kerosene, mild hydroprocessing, a uniform fuel allocation and potentially targeting short- and medium-range flights with kerosene characterized by a reduced content of aromatic components appear feasible. However, a deeper understanding as well as the assessment of the broad variety of possible implications from the introduction of such measures and interdependencies with other mitigation measures require further investigation.

In this regard, the exploration of the extent of lowering the maximum permissible content of aromatic components contained in conventional fossil fuel-based kerosene can facilitate the introduction of mild hydroprocessing. For example, a content of aromatic components below the current average of about 18 m-% [180] could mitigate contrail-related climate forcing while being in line with existing fuel specifications and could thus be introduced without any infrastructure and / or aircraft modifications within the commercial air transport system (cf. section 3.1).

For a timely mitigation of aviation's carbon dioxide-related climate forcing, the production and use of renewably sourced kerosene should be ramped up rapidly. For this, the specific design of an appropriate economic representation considering the use cost of fossil energy carrier should be investigated. Instead of allocating these costs to society as a whole, these costs could be solely allocated to the users of fossil fuel-based energy carrier. This would reduce the price differential of conventional and renewably sourced kerosene and in turn stimulate demand for renewably sourced kerosene (cf. section 4.4).

Furthermore, it should be evaluated how political and industrial targets as well as incentive schemes could widen their focus on aviation's entire climate forcing instead of carbon dioxide emissions alone. The recent introduction of a monitoring, reporting and verification scheme for non-carbon dioxide-related climate forcing within the EU Emissions Trading Scheme [400] can be considered as an initial step towards this direction. The inclusion of non-carbon dioxide-related climate impacts, and thus also contrail-related climate impacts, could also further support the introduction of contrail-related climate forcing mitigation measures.

As long as market shares of renewably sourced kerosene remain far below market shares of conventional kerosene – which is very likely in the

short-term [154, 167, 205, 206] – allocating paraffinic kerosene to flights with high contrail-related climate forcing could provide additional mitigation potentials (cf. section 4.1). Such an approach would benefit from a valid estimation of the contrail climate forcing of individual flights. Several measures could potentially improve present models. An online monitoring, e.g., by sensors during refueling, might provide valuable information about the actual properties of kerosene used for specific flights and thus could reduce uncertainties about a fuel's content of aromatic components / hydrogen content. The effects of engine wear on soot particle emissions could be considered based on real-world measurements instead of model data, e.g., by measuring emissions during maintenance events. Humidity data at aircraft cruise altitude could be augmented by integrating humidity sensors in aircraft or at least in a part of the global aircraft fleet. Furthermore, the contrail formation of modern engines with lean-burn combustors could be validated by flight measurements and subsequently included in contrail climate forcing models. By investigating these options in greater detail, the uncertainties in the contrail-climate forcing estimation of individual flights could be reduced further.

To maximize the contrail-climate forcing mitigation from a targeted use concept, flights / flight segments with particularly high contrail-related climate forcing could be targeted with neat paraffinic kerosene, i.e., kerosene containing hardly any aromatics. It should be evaluated, if the use of neat paraffinic kerosene could be viable for a certain share of flights. Provided that, e.g., each 10^{th} flight of an aircraft can be approved to use neat paraffinic kerosene, this might allow for a large reduction of contrail-related climate forcing, while avoiding a costly re-certification of the aircraft. Alternatively, a new specification for neat paraffinic kerosene could be developed, and at least new aircraft types could be certified for its use.

Beyond the measures discussed in-depth here, other mitigation measures might complement fuel-related measures. Strategies for flight route modifications to avoid ice-supersaturated regions indicate a large contrail-related mitigation potential but might be limited by the size of such regions and airspace congestion. Flights could be targeted with paraffinic kerosene where the vertical extent of the en-route ice-supersaturated region causes a high fuel penalty for its circumnavigation. Similarly, a targeted use of paraffinic kerosene could be applied for flights in congested airspaces where avoidance is not possible due to aircraft separation minima.

5.2.2 Medium-term

In the medium term, i.e., from the year 2030 onwards, the approval of neat renewably sourced kerosene, harshly hydroprocessed kerosene and targeting long-range flights might allow for further mitigation potentials. In this period, the ramp up of renewably sourced kerosene plays a decisive role for achieving the global climate change mitigation goals. In parallel, hydroprocessing of conventional kerosene and a targeted use concept are required for the mitigation of aviation's climate forcing.

Provided that market shares of renewably sourced kerosene remain low even beyond 2030, hydroprocessing of conventional fossil fuel-based kerosene and the targeted use of paraffinic kerosene could potentially support the mitigation of contrail-related climate forcing. By introducing harsh hydroprocessing, the use of paraffinic kerosene could be enabled on the majority of flights. Alternatively, adjusting the airport infrastructure to target entire long-range flights with paraffinic kerosene would further increase the mitigation potential of a targeted use concept in the medium-term. In case of very low market shares of paraffinic kerosene, also segments of flights could be targeted. In this case, the efforts due to aircraft modifications for a segment-specific allocation could be alleviated by implementing a flight-specific allocation strategy at scale and using a segment-specific allocation strategy only on newly produced aircraft. Furthermore, a segment-specific allocation strategy might also facilitate targeting of long-range flights. Since this strategy requires rather small amounts of paraffinic kerosene per flight, these might be supplied by refueller trucks to long-range aircraft, while the remaining kerosene for the respective flight is fuelled from a hydrant system.

Contrarily, provided that market shares of renewably sourced kerosene ramp up swiftly towards almost 100 % by 2050, the benefits from additional hydroprocessing or a targeted use concept would be smaller, because the lower aromatics content of renewably sourced kerosene itself would yield about the same effects as hydroprocessed conventional kerosene. In this case, a specification for neat renewably sourced kerosene would still be required. Assuming that such a specification maintains a requirement for minimum aromatics content, it could still be beneficial to consider the approval and use of a strategy to target e.g., each 10^{th} flight by (neat) paraffinic kerosene.

In the medium term, flight route modifications might also provide a further option to mitigate contrail-related climate forcing. Even if neat paraffinic kerosene is used, contrail formation takes place, but the contrail lifetime and optical density is reduced (cf. section 3.1.2.2 [8, 10, 131]). Even if all contrail-relevant flights could be targeted with paraffinic kerosene, route modifications might avoid the formation of the contrails with reduced lifetime and optical density. To which extent this can further mitigate contrail-related climate forcing should be a further field of research.

5.2.3 Long-term

In the long-term, more radical and innovative strategies could unleash further potentials but also require careful consideration and further investigations in order to avoid adverse and unexpected outcomes. It might be valuable to investigate the extent to which the cooling climate impact of flights forming contrails with a negative, i.e., cooling, energy forcing could be maintained. This might be possible by the admixture of specific molecules, such as renewably sourced aromatic compounds or cycloalkanes. However, this option needs to be studied in greater detail regarding the specific influences of such molecules and the validity of estimating the contrail-related climate forcing of individual flights.

Additionally, further fuel options (e.g., alcohols and / or gases), and technologies (e.g., a counter-rotating open rotor engine) might be available. Provided that the mitigation targets of the airline industry will be achieved, aviation's carbon dioxide emissions should be entirely mitigated by then. Other climate forcing, e.g., from contrails are not (yet) included in such mitigation targets, despite their large contribution towards the overall climate impact of aviation. The years to come will tell, if and how far the air transport system's overall climate forcing will be mitigated – by the fuel-related measures discussed here or other, not fuel-related mitigation measures.

6 Appendices

This chapter contains the supplementary information published with the scientific publications included in this thesis. Specifically, this concerns the sections 3.1 “Hydroprocessing of Fossil Fuel-based Aviation Kerosene” (Appendix A), 3.2 “Renewable Fuel Options For Aviation” (Appendix B) and 4.1 “Targeted Use of Paraffinic Kerosene” (Appendix C). Additionally, a list with definitions of relevant terms used in this thesis is provided (Appendix D).

A. Appendix Section 3.1

A.1 Background

For aviation until 2018, the most prominent climate factors based on effective radiative forcing (ERF) are contrails, in particular contrail-cirrus cluster at night, followed by historically accumulated CO_2 emissions and indirect effects of NO_x emissions. Water vapor emissions in the stratosphere, aerosol-radiation interaction, and aerosol-cloud interaction (both by soot and sulfur) have a still relevant but smaller climate impact than indirect effects caused by NO_x emissions [5]. Accordingly, this study focusses on the contrail-climate impact for the following reasons:

- For the reduction of CO_2 emissions in aviation, extensive research exists (e.g., [32, 94, 123, 156]).
- Indirect NO_x effects are primarily influenced by combustion temperatures and thus primarily dependent on engine technology instead of the properties of the hydrocarbon fuel (here: aviation kerosene) in use (e.g., [31, 1185 ff.]).
- All the other remaining effects on global climate recognized and understood so far are either almost one order of magnitude smaller than the contrail effective radiative forcing (ERF). In some cases, they are not yet scientifically well understood; e.g., for aerosol-cloud interactions it is not even clear yet if they have a warming or cooling climate impact [5].

The goal of aviation kerosene processing to reduce soot emissions is to reduce the share of components with a high sooting tendency. This can be achieved by saturation or separation of aromatics. In principle, aromatics can be separated by extractive distillation, where a high-boiling point polar solvent is added to the corresponding fraction [81]. Subsequently, high-polar components such as aromatics bind to the solvent, form high-boiling point molecules, and can thus be removed by distillation. As a high sulfur content characterizes some crude oils and their straight-run kerosene fraction, the solvent needs to resist these contaminations. Presently used solvents do not fulfil this criterion; thus, the development of new solvents would be required [83]. As this development requires time, it appears unlikely that aromatic separation can be used in the short-term. In contrast, hydroprocessing is a common process used for fuel finishing within modern

refineries [39]. Depending on reaction types, hydroprocessing can be distinguished by rather mild processing conditions ("hydrotreatment") or rather harsh processing conditions ("hydrocracking"):

- Mild process conditions are typically around 270 to 340 °C and 15 to 30 bar [39] and involve the removal of contaminants such as sulfur and others and the saturation of unsaturated components, such as alkenes. The saturation of aromatics into cycloalkanes is also included in this process, but not the cracking of C-C single bonds.
- Harsher process conditions are typically considered around 370 to 510 °C and 140 to 170 bar [39] and also involve cracking of C-C single bonds. Thus, cracking of aromatics into acyclic alkanes is possible in principle under hydrocracking process conditions.

A.2 Data and Assumptions

A.2.1 Aviation Kerosene Properties

The composition of chemical compounds contained typically within fossil fuel-based kerosene varies significantly by the specific crude oil from which they are refined[21] [135, 357]. The composition of crude oil in turn varies greatly, typically depending on its respective reservoir. Hence, this variation might in turn yield regional variability in aromatics content and subsequently in the resulting contrail climate impact.

Crude oil is a globally traded commodity. This global trading prevents direct conclusions about aviation kerosene properties from the crude oil used as feedstock. Available data for various aviation kerosenes are summarized in Table A1. The substantial variations of the various hydrocarbon groups typically contained within aviation kerosene are apparent.

Table A1 Average fractions of aviation kerosene components and corresponding ranges (m-% – mass-%; vol-% – volume %; N/A – not available)

Component	Average	Min	Max	Region	Reference
n- and iso-Alkanes	47 m-%	32 m-%	64 m-%	global	[179]

[21] Some kerosene is produced based on coal or natural gas. Compared to the overall kerosene demand, production from these feedstock is negligibly small [211]. Additionally, these kerosene types are not considered here as they show significantly higher lifecycle CO_2 emissions (natural gas 1.14 to 1.17 and coal 2 to 2.4 times higher GHG emissions compared to crude oil) [374]. It appears unlikely that a potentially lower contrail climate impact can counterbalance this effect.

Cycloalkanes	32 m-%	23 m-%	47 m-%	global	[179]
Aromatics	18.3 vol-%	12.7 vol-%	24.6 vol-%	global	[180]
	N/A	5.9 vol-%	25.5 vol-%	Germany	[135]
	N/A	11.2 vol-%	25.0 vol-%	UK	[362]
Sulfur	1 580 ppm	1 ppm	2 960 ppm	global	[180]
	490 ppm	N/A	N/A	global	[179]
	N/A	1 ppm	2 676 ppm[a]	Germany	[135]

[a] whereas the majority of batches are below 1 500 ppm

- Alkanes. The assessed samples average at 47 m-% of n- and iso-alkanes, with a considerable variation among samples (e.g., 32 m-% or 64 m-%). Cycloalkanes average at ca. 32 m-% (some samples indicate 23 m-% or 47 m-%) [179].
- Aromatics. Aromatics average at 18.3 vol-%, again with considerable variation (from 12.7 vol-% to 24.6 vol-%) [180]. Other investigations found a range between 5.9 vol-% to 25.5 vol-% in Germany, while in the UK 11.2 vol-% up to 25 vol-% have been measured [135, 362]. Even though the respective standard ASTM D1655 does not explicitly address a minimum aromatics content, the specification for synthetic aviation kerosene, ASTM D7566, does specify a minimum of 8 vol-% [181, 280]. Some samples of fossil fuel-based aviation kerosene batches in Germany fell below this level. They were produced over two months from one refinery and directly delivered to two airports. For one airport, the refinery was the only and the primary supplier for the other. No problems were observed throughout this period [135]. Naphthalene is a bicyclic aromatic hydrocarbon and a component of aviation kerosene's aromatics. Due to its molecular structure, it is suspected to be particularly relevant for soot formation [15]. Average naphthalene content amounts to ca. 1.9 m-% (1.1 m-% to highest 2.3 m-%) globally [179]. As the naphthalene content of an aviation kerosene sample must only be determined if the aviation kerosene's smoke point is below 25 mm [181], the reported sample size is most likely smaller than the sample size for aromatics content.
- Sulfur content. A mean sulfur content of 1 580 ppm, ranging from 1 to 2 960 ppm, has been stated [180]. Other sources report an average of 490 ppm, while for Germany most samples contain less than 1 500 ppm sulfur, even though the specification limit lies at 3 000 ppm [135, 179, 181]. Presently, maximum permissible sulfur contents for diesel and gasoline are more than two orders of magnitude lower (e.g., 10 ppm in the EU [401]).

To sum up, fossil fuel-based kerosene composition varies largely for the respective batch. Additionally, most airports operate an aviation kerosene storage system to decouple aviation kerosene supply and demand resulting in an extra mixing of various batches [208]. If the aviation kerosene is transported via a pipeline to the respective airport (which is the case for most airports with high aviation kerosene demand, e.g., due to intercontinental flights), aviation kerosene batches mingle even before the airport's storage. Those processes create an averaging tendency, and it can be assumed that the fossil fuel-based kerosene composition for large airports and longer time horizons moves closer to the average values typical for the respective region.

A.2.2 Aviation Kerosene Processing

In present-day refineries, mild hydroprocessing is primarily employed to ensure compliance with sulfur limits of aviation kerosene specifications (Figure A1). In Europe, the maximum permissible sulfur content for road transportation fuels is substantially lower than for aviation kerosene (ca. 0.001 m-% vs. 0.3 m-% [181, 401]). Thus, the process conditions for current refinery aviation kerosene hydroprocessing are rather mild compared to gasoline or diesel. To which extent equipment for processing of road transportation fuels could be utilized for aviation kerosene, would need to be the subject of more specific process (simulation) studies.

Harsh hydroprocessing in turn is primarily employed for cracking vacuum gas oil into lighter compounds, such as gasoline or aviation kerosene in order to increase the yields of such lighter fractions. The aviation kerosene fraction from hydroprocessed vacuum gas oil contains almost no aromatics. Alternatively, straight-run aviation kerosene from atmospheric distillation could also be hydroprocessed under harsh conditions. However, it is questionable to which extent the equipment for vacuum gas oil is usable for straight-run aviation kerosene from atmospheric distillation.

As the equipment for hydroprocessing is a well-developed technology, a short-term implementation of the described processing options appears feasible at scale [74]. Thus, neither substantial investments in aviation kerosene processing technology and infrastructure nor the development of new technologies are considered. Additionally, it is assumed that aviation kerosene processing strategies are introduced globally and simultaneously.

Influences on the production of other fuel types or petrochemicals beyond the scope of this study.

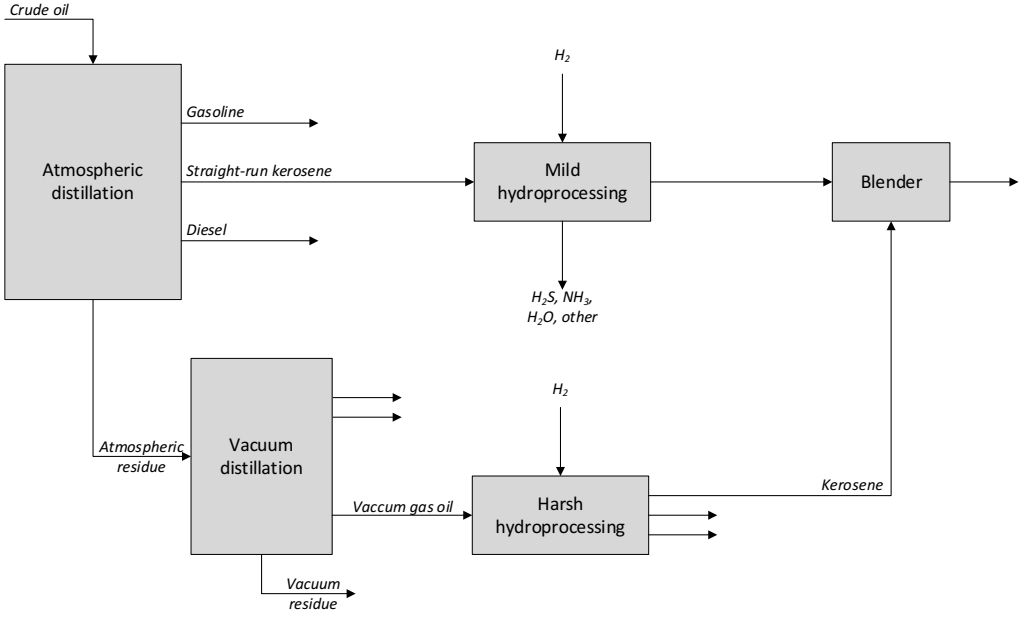


Figure A1 Basic refinery scheme for aviation kerosene production

A.2.3 Contrail Climate Impact

The pycontrails / CoCiP model and the required data have been described extensively elsewhere [9, 10, 164, 177, 185, 186, 193]. Hence, this section discusses only the particularities of the datasets and configurations used here (Figure A2).

Weather data is retrieved from the European Center for Medium-Range Weather Forecast (ECMWF) Reanalysis [192] version 5 for the pressure levels 400, 350, 300, 250, 225, 200, 175 and 150. Meteorological conditions for flights between those pressure levels are interpolated from the two nearest pressure levels [317].

Flight Data are derived from Automatic Dependent Surveillance Broadcast (ADS-B) information from the Opensky historical database [188]. For computational reasons, this study focusses on departing flights of the five largest European airports, by passenger numbers. These are London-Heathrow, Paris Charles De-Gaulle, Amsterdam Schiphol, Frankfurt International and Madrid Barajas airport.

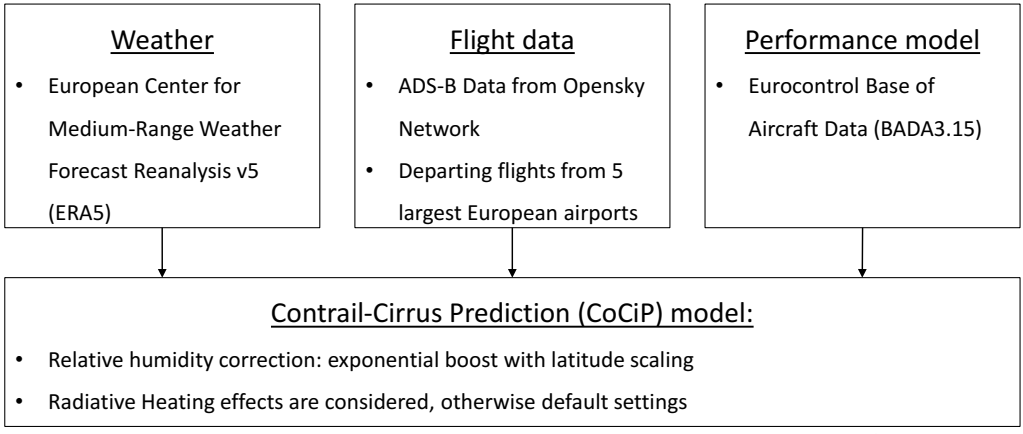


Figure A2 Datasets and configurations used for the Contrail–Cirrus Prediction (CoCiP) Model to estimate the contrail–climate impact

The aircraft performance data used to calculate aviation kerosene consumption and the emissions of each flight are computated using the Eurocontrol Base of Aircraft Data (BADA) [190] version 3.15. It covers 1409 aircraft types, of which 250 aircraft types are directly supported and the remaining aircraft types are matched with a directly supported aircraft type considered to be equivalent [190]. The assignment of engine types to aircraft is based on the Eurocontrol Base of Aircraft Data (BADA) version 3.15.

A.3 Methods

A.3.1 Aviation Kerosene Processing

This study compares three cases against each other: A reference case without additional aviation kerosene processing, a case where all aviation kerosene used in the dataset is hydroprocessed under mild conditions and another case where all aviation kerosene is hydroprocessed under harsh conditions. Both hydroprocessing options are considered to be additional processing steps. The provision of hydrogen for hydroprocessing incurs CO_2 emissions; while their magnitude depends on the respective hydrogen provision pathway.

The process conditions required for aromatics saturation (hydrotreatment) and cracking of aromatics to acyclic alkanes (hydrocracking) both also enable heteroatom removal. For most crude oils, sulfur heteroatoms have the largest share, while other trace elements (e.g., nitrogen or metals)

usually occur at far smaller quantities [39, 402]. Hence, the additional hydrogen requirement is determined by the hydrogen required for aromatics saturation / cracking and sulfur removal.

Hydrogen required for aromatics saturation/cracking is calculated assuming stoichiometric reactions for hydroprocessing. Based on data from the World Fuel Survey [179], a distribution of the aviation kerosene components (alkanes, aromatics, etc.) and their average hydrogen content is assumed. Table A2 shows the corresponding values.

Table A2 Composition of the different aviation kerosene components (HC-ratio – hydrogen-to-carbon ratio; H-content – hydrogen content)

Crude option	Acyclic alkanes	Cycloalkanes	Aromatics	Naphthalene
HC-ratio[a]	*2.168*	*2.000*	*1.347*	*0.800*
H-content[a] [m-%]	15.3 m-%	14.3 m-%	10.1 m-%	6.3 m-%

[a] based on data from [179]

The composition of the aviation kerosene without additional processing is also based on data from the World Fuel Survey [179]. This study includes 57 samples of different Jet A/A-1 fuels, and appears to be the broadest publicly available aviation kerosene properties dataset as of now.

The hydrogen content of each processing case is calculated as weighted average of each component's hydrogen content (Table A3). For hydrotreatment, 50 % of aromatics (incl. naphtalene) assumed to be converted to cycloalkanes and in case of hydrocracking, 80 % of aromatics (incl. naphtalene). This results in an increase in hydrogen content by ca. 0.3 mass percentage points for hydrotreatment and ca. 0.7 mass percentage points for hydrocracking.

Table A3 Resulting composition of the different aviation kerosene options considered here (values are rounded)

Processing case	Acyclic Alkanes [m-%]	Cycloalkanes [m-%]	Aromatics [m-%]	Naphthalene [m-%]	Hydrogen content [m-%]
Reference case[a]	50.0	34.0	15.0	1.0	14.1
Mild hydroprocessing	50.0	42.0	7.5	0.5	14.4
Harsh hydroprocessing	62.8	34.0	3.0	0.2	14.8

[a] based on data from [179]

The amount of molecular hydrogen required for Hydroprocessing $\Delta m_{H,HP}$ is derived by (46):

$$h_2 = \frac{m_{H,2}}{m_{H,2} + m_{C,2}} = \frac{\Delta m_{H,HP} + m_{H,1}}{m_{H,2} + m_{C,2}} \quad (45)$$

With:

$$m_{H,2} = \Delta m_{H,HP} + m_{H,1}$$

$$h_2 = \frac{\Delta m_{H,HP} + m_{H,1}}{\Delta m_{H,HP} + m_{H,1} + m_{C,1}} \Leftrightarrow \Delta m_{H,HP}$$

$$= \frac{(m_{H,1} + m_{C,1})h_2 - m_{H,1}}{1 - h_2}$$

$$\Leftrightarrow \Delta m_{H,HP} = \frac{h_2 m_{total,1} - m_{H,1}}{1 - h_2} \quad (46)$$

h_2 denotes the aviation kerosene's hydrogen mass fraction after processing and $m_{C,i}$ and $m_{H,i}$ denote the carbon and hydrogen mass contained in the aviation kerosene (i=1 before hydroprocessing and i=2 after hydroprocessing). The effect of heteroatoms (e.g., sulfur or nitrogen) is not taken into account. Using the data from Table 3.2, this yields a hydrogen requirement between ~4 $kg_{H2}/t_{Kerosene}$ for mild hydroprocessing and ~8 $kg_{H2}/t_{Kerosene}$ for harsh hydroprocessing. These values match the ranges of other studies [74, 83].

Hydrogen required for sulfur removal $\Delta m_{H,S}$ is determined based on the stoichiometric reaction of all sulfur contained in the feedstock to hydrogen sulphide (H_2S). In (47), $m_{Sulphur}$ denotes the mass of sulfur contained in the aviation kerosene and $M_{Sulphur}$ the molar mass of sulfur and accordingly $M_{Hydrogen}$ refers to the molar mass of hydrogen:

$$\Delta m_{H,S} = \frac{m_{Sulphur}}{M_{Sulphur}} \times 2 \times M_{Hydrogen} \quad (47)$$

The hydrogen sulphide (H_2S) can be further processed to retrieve elemental sulfur [83]. This process step is not considered here. The sum of $\Delta m_{H,HP}$ and $\Delta m_{H,S}$ corresponds to the amount of hydrogen required for hydroprocessing.

The increased hydrogen content of aviation kerosene also affects other properties, than the hydrogen content itself. These are heating value and water emissions, among others. These properties are adopted using a linear relationship between the hydrogen content and heating value / water emissions following the methodology described by Teoh et al. for an increasing aviation kerosene hydrogen content [10].

A.3.2 Contrail Climate Impact

Flight Data from the Opensky database [188] are resampled to a frequency of 1 minute and latitudinal and longitudinal information is filtered to reduce erroneous positional information. Flight sections without ADS-B coverage (e.g., parts of the North Atlantic flight corridor) are estimated using the pycontrails "resample_and_fill" function. It uses a geodesic interpolation for data gaps of longer distances and a linear interpolation for shorter distances. Flights are discarded from the dataset in several cases: (1) when for at least one waypoint altitude, latitude or longitude information is not available or the flight altitude remains below 6000 m or exceeds 13 000 m (6.5 % of the flights loaded from the Opensky Database). (2) Flights are also excluded when their aircraft type is not included in the Eurocontrol Base of Aircraft Data (BADA) performance data (0.2 % of the flights loaded from the Opensky Database). Some flights contain erroneous positional information and are excluded after the Contrail Cirrus Prediction Model (CoCiP) has run (5.6 % of the flights evaluated by CoCiP). The aviation kerosene consumption of the remaining 797 602 flights is used to calculate the amount of aviation kerosene undergoing additional hydroprocessing and the contrail climate impact of these flights is calculated with the Contrail-Cirrus Prediction model (CoCiP).

Aircraft performance model data are used to calculate the emissions of each individual flight by simulating the aircraft performance (e.g., the required thrust for the present flight state at each waypoint, the fuel consumption and together with the engine model the associated emissions). A thorough description of the emissions estimation is included in the pycontrails / CoCiP version 48.1 documentation [185]. Since the thrust setting is a central factor for aircraft emissions and thus also the changes in contrail climate impact by different fuels, an assessment of the simulation results is provided in the following. In order to take into account the effect of an in-

creased aviation kerosene energy content from hydroprocessing, an adjustment factor ($q_{conventional}/q_{processed}$) is used to adjust the thrust specific fuel consumption from the BADA data tables towards the processed kerosene's energy content.

For the assessment of the simulated thrust settings, Figure A3 shows a comparison between the distribution of thrust settings from this study with a previous study [10]. Both studies use flight data from the same year (2019) but different flight routes. While this study covers departing flights from five large, international airports in Europe, the study for comparison focuses on a traffic dataset for the North Atlantic. In general, both distributions show a bi-modal distribution, with one distinct peak at thrust settings around 50 % with a steeper slope at thrust settings below this maximum and a more gradual slope towards thrust settings of 100 %. In this study, the second maximum (around thrust settings of 10 %) is more pronounced than in the comparison study. Simultaneously, the comparison study seems to estimate slightly higher thrust settings compared to the thrust settings estimated here. Both differences can be explained by disparities in the traffic datasets. Most likely, the comparison dataset includes a large share of long-range flights, while this study also includes intra-european connection flights. Thus, the dataset in this study has a larger fraction of descending/decelerating flights with reduced thrust settings which could constitute the more pronounced second maximum at lower thrust settings. The tendency of higher thrust settings in the comparison dataset might be explained by more pronounced traffic patterns (east- or westbound) across the North Atlantic resulting in less airspace congestion and thus fewer speed reduction requirements. In general, however, the difference is not very pronounced and could also be explained by the fact that the comparison study also includes BADA4 aircraft performance data while this study only considers BADA3. In general, both distributions seem to align appropriately.

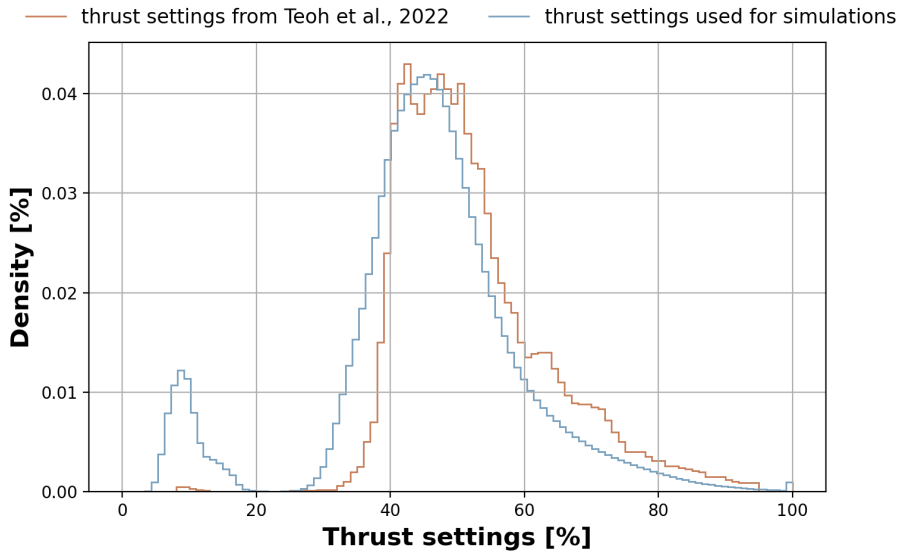


Figure A3 Comparison of thrust settings estimated using ADS–B data from the Opensky Network and the BADA3 aircraft performance data and thrust settings from Teoh et al. [10]

The Contrail Cirrus Prediction (CoCiP) model is applied using the default settings from pycontrails / CoCiP version 48.1 with two exceptions. On the one hand, the humidity data of the ECMWF reanalysis 5 (ERA5) data to in-situ measurements [317] is performed using the "exponential boost with latitude scaling" method [9]. On the other, radiative heating effects, i.e., the influence of radiative heating on the contrail plume and thus contrail lifetime are taken into account [9]. Again, the simulation results are compared to a previous study [10] (Figure A4).

While changes in contrail occurrence, contrail cover and the contrail optical density ($\tau_{contrail}$) are in good agreement between this study and the comparison study, the changes in mean nvPM emissions number (EI_n), energy forcing per contrail distance and the mean contrail age differ by up to 10 %-points. One explanation might be a different susceptibility to fuel changes of the fleets investigated. The comparison study primarily focusses on long-range flights and thus a significantly smaller set of aircraft (and engine) types than this study, which has a higher share of short-haul flights. This larger variation in aircraft and engine types results in a systematic difference between both studies, which might explain the different changes in nvPM emission numbers. As the nvPM emissions number directly affects

the energy forcing per contrail distance and mean contrail age, these parameters are directly affected. Furthermore, the comparison study uses a different method to adjust the humidity information from the ERA5 dataset.

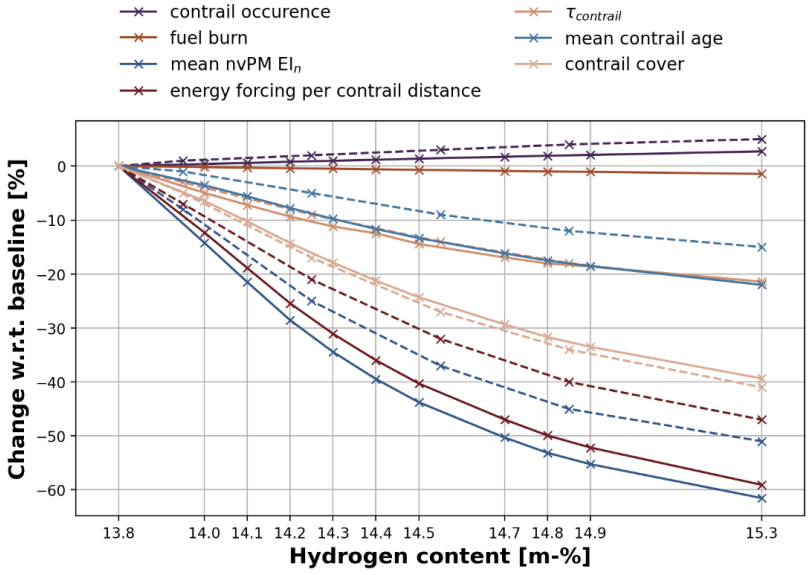


Figure A4 Comparison of simulation results (solid lines) and results by Teoh et al., (2022) [10] (dashed lines)

As the occurrence of ice-supersaturated regions and their degree of supersaturation largely determines the contrail lifetime, the different humidity scaling methods might also contribute to the differences between both studies. For additional information, Figure A4 also shows the fleet's fuel consumption, being anti-proportionate to the increasing fuel energy content from increasing hydroprocessing intensity. This reduction in fuel consumption decreases the required amount of fuel for hydroprocessing but also lowers CO_2 emissions from fuel combustion. For an increase in hydrogen content from 14.1 m-% to 14.9 m-%, the fuel consumption (and thus also the resulting energy forcing) would decrease by less than 1 %, while the energy forcing due to CO_2 emissions from hydroprocessing ($\Delta EF_{hydroprocessing}$) would increase by about 2.5 %.

Contrail efficacy is assumed to be unity in this study. However, various studies suggest that secondary effects such as a reduction in natural cloudiness by contrails or rapid adjustments in atmospheric temperatures substantially lower the climate efficacy of contrails [5, 174, 175, 403]. Such effects are subject to large uncertainties [5, 172] and therefore not subject of

this study. Figure A5 shows the simulation results for contrail efficacies of 1, of 0.31, which is the lowest available estimate [175] and 0.42 [5].

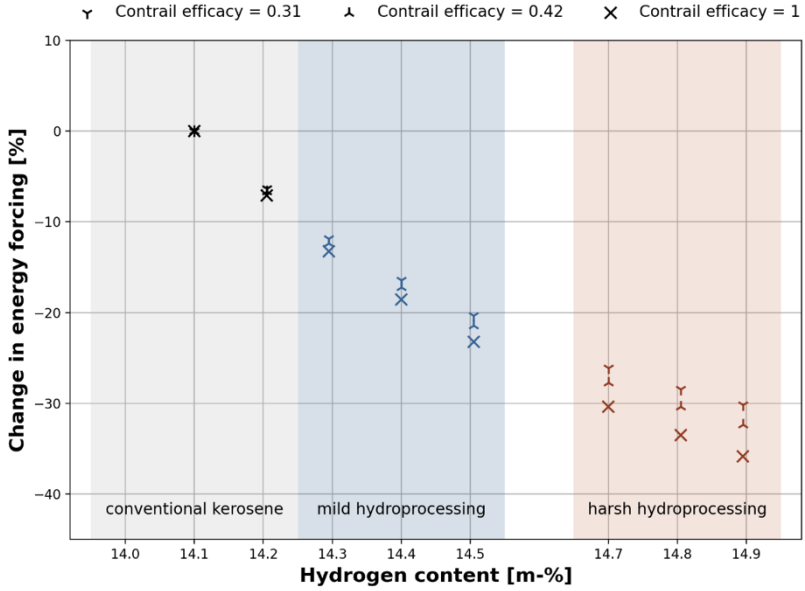


Figure A5 Change in net energy forcing for contrail efficacies 0.31 ( ), 0.42 ( ) ד d λ=1 (× ד ssuming a 50-year time horizon and medium hydrogen provision emissions (m-% mass-percentage)

As depicted above, increasing the hydroprocessing intensity increases the relative climate benefit for all contrail efficacies considered. The climate cost of additional CO_2 emissions from aviation kerosene hydroprocessing ($\Delta EF_{hydroprocessing}$) are substantially lower and thus do not counterbalance the climate benefits of a reduced contrail energy forcing ($\Delta EF_{contrail}$), even for contrail efficacies as low as 0.31. Such low efficacies would only slightly reduce the reduction in net energy forcing by up to 5 %-points. Concluding, while the contrail efficacy is an important factor for the contrail climate impact in absolute terms, the relative mitigation potential of hydroprocessing aviation kerosene remains largely unaffected. This is mainly due to the comparatively low climate cost of hydroprocessing emissions ($\Delta EF_{hydroprocessing}$).

B. Appendix Section 3.2

B.1 Synthetic Kerosene Blends (C_xH_y)

Here, a synthetic kerosene blend is considered as a specification-compliant blend of a fossil and a synthetic kerosene component. Both usually consist of a range of hydrocarbons with a typical chain length of 8 to 16 carbon atoms. The most prominent hydrocarbon types in aviation fuels are n- and iso-alkanes, cycloalkanes and aromatics [137]. Seven conversion and two co-processing options are approved for the provision of synthetic kerosene by ASTM D7566 and ASTM D1655 [87, 92, 94, 102, 123].

- Synthesis gas ("Syngas") is an intermediate suitable to produce several fuel options (e.g., FT-SPK) to be produced based on biogenic and/or non-biogenic renewable feedstock22 [216, 217]. For biogenic feedstock, two elementary pathways exist. The first covers the conversion of biomass by an anaerobic digestion (fermentation) into biogas (mainly CH_4 and CO_2) and the subsequent production of syngas via a reforming process. Second, lignocelluloses-rich biomass can be converted to syngas by a thermochemical gasification and a subsequent gas cleaning and conditioning. For non-biogenic feedstock, syngas can be produced using electricity from renewable energy, water and sustainable CO_2. Water is split into hydrogen and oxygen by electrolysis utilizing "green" electricity. Renewably sourced CO_2 provided from biogenic sources (e.g., biogas or bioethanol production) or from atmospheric CO_2 is converted with hydrogen into a syngas by using a reverse-water-gas-shift reaction. If syngas is produced exclusively based on "green" electricity, these fuels are often referred to as "power-to-liquid" (PtL) fuel [94, 216, 217]. To produce synthetic kerosene, this syngas is fed into a Fischer-Tropsch reactor converting the syngas into a so-called "FT-Crude". This in turn, can be fractionated into synthetic kerosene and other products based on "classical" refinery processes. FT-SPK/A denotes the addition of aromatics, which are considered to be relevant for the sealing of fuel system components (section 3.2.3.3) [204].

[22] A production of syngas based on fossil feedstock (e. g. via coal gasification or methane reforming) is also possible. Due to the fossil origin of the feedstock, this pathway is not included in the present study.

- The “Hydroprocessed Esters and Fatty Acids” (HEFA) pathway or catalytic hydrothermolysis (CH) are suitable conversion processes for lipid feedstock. The first consists of a combination of a hydrogenation, cracking and subsequent isomerization. Hydrogen is used to saturate the ester and/or double bonds of the lipids. The oxygen naturally present in the oil/fat molecule is separated as water. The product is then fractionated. The catalytic hydrothermolysis, in turn, converts the feedstock into alkenes in a water atmosphere under supercritical conditions (high pressure and temperature). The alkenes are subsequently hydrogenated into alkanes and then separated into individual fuel fractions. Compared with HEFA, the process has a lower hydrogen demand but a greater degree of technological complexity [216]. HC-HEFA-SPK refers to a similar conversion pathway, however at present it is only certified for lipids derived from the Botryococcus braunii algae species [204].
- Fermentation is an option to convert sugar into aviation fuel. This is either performed via the Hydroprocessed-Fermented-Sugars to Synthetic Isoparaffins (HFS-SIP) process, where genetically modified yeast microorganisms produce a long-chain hydrocarbon (farnesene) to be further upgraded by separation and hydrogenation to farnesane [89, 94, 216]. Alternatively, for the Alcohol-to-Jet (AtJ) process, sugar or starch is fermented to alcohol, subsequently dehydrated (removal of oxygen from the alcohol molecules in the form of water), oligomerized (formation of long-chain olefins) and hydrogenated. Again, “classic” refinery processes separate the individual hydrocarbon product fractions into, among other products, kerosene [216]. Lignocellulosic biomass can potentially be used for the AtJ-SPK or HFS-SIP via saccharification. However, this technology pathway is still in an early phase [87].
- Co-Processing describes the joint refining of e.g. vegetable oils, animal fats or FT-Crude with fossil crude oil [216]. As these pathways contain a large share of feedstock of fossil origin, they are not considered here.

Currently, the global market share of synthetic kerosene blends is far below 1 %, with the majority being produced via the HEFA process [167]. As they are specifically produced for use as aviation fuels, their major future utilisation would be to gradually replace fossil kerosene.

B.2 Neat Synthetic Kerosene

Due to a (slightly) different chemical composition of neat synthetic kerosene (depending on the specific conversion pathway), compliance with ASTM D1655 requires additional adaptations. Several production pathways do not yield aromatics (e.g., HEFA- or FT-SPK) or show a different distillation curve gradient (e.g., HFS-SIP) [142]. Theoretically, the same production pathways as described for synthetic kerosene blends can be used for neat synthetic kerosene production. To which extent all conversion pathways allow an unblended use has not yet been determined.

As neat synthetic kerosene is not yet certified for aviation use; i.e. it is not allowed to be used for commercial flights. Nevertheless, selected airplane and engine manufacturer are currently pursuing test flights using neat synthetic kerosene [404–407]. Like synthetic kerosene blends, their major use will be as an aviation fuel. Since they allow for a greater reduction of aviation's greenhouse gas emissions and potentially also lower aviation's non-CO_2-related climate forcing [17, 27], from an environmental perspective it would be desirable for them to replace synthetic kerosene blends.

B.3 Methanol (CH_3OH)

Methanol is a colourless, toxic, water-soluble liquid. Together with oxygen (e.g., from air) it forms highly flammable mixtures [223]. Methanol is also produced from syngas (see above) [219]. The origin of methanol (i.e., fossil or renewable) is thus primarily determined by the used syngas (section 3.2.4.1). Presently, global methanol production ranges from 90 to 100 Mt/a (ca. 2 EJ/a). But only less than 1 % of the produced methanol is from renewable sources [46].

Methanol serves as an important bulk chemical for the chemical industry. In some countries (e.g., China), it is also used as a fuel (component) in parts of road transport or as a feedstock for the conversion of other fuel types. Methanol of renewable origin can substitute methanol of fossil origin in its various applications and thus support defossilation. Methanol could play an increasingly important role for mobility applications (e.g., maritime fuel, use in heavy-duty road-transportation). For aviation, methanol could theoretically either be used directly as a fuel or converted to a synthetic kerosene via the Methanol-to-Jet pathway. So far, this pathway is not introduced in the evaluation process for a potential certification by ASTM [204].

B.4 Ethanol (C_2H_5OH)

Ethanol is a colourless, volatile, water-soluble liquid. Like methanol, together with oxygen (e.g., from air) it forms highly flammable mixtures [223]. Presently, the major production pathway for ethanol is an anaerobic fermentation of sugar and starch. Ethanol is basically the only alcohol that is currently produced from renewable feedstock at industrial scale [220, 221]; the global production volume is about 100 Mt/a (ca. 3 EJ/a) [213].

During alcoholic fermentation, sugar is converted by biocatalysts (here: yeasts) into ethanol and carbon dioxide (CO_2). Depending on the used biogenic resource, various pretreatment steps are required to provide a sugar solution. After fermentation has been finished, ethanol is separated and purified. While the use of biomass containing sugar and starch is well-developed, saccharification of lignocellulosic biomass is not yet fully implemented at commercial scale [220, 223, 242, 269].

A provision of ethanol via syngas processing is also technically feasible. But, due to still unsolved technical challenges, this pathway has no importance on the global market yet.

Ethanol has a wide range of applications (e.g., fuel or fuel additive, potable alcohol, bulk chemical for chemical and pharmaceutical applications). Additionally, ethanol of renewable origin serves as a platform chemical within the chemical industry. Also, it can be used as an educt for the Alcohol-to-Jet conversion pathway to produce synthetic kerosene (AtJ-SPK) [87].

B.5 Butanol (C_4H_9OH)

Butanol is a colourless, water-soluble, flammable liquid. It is less volatile than ethanol or methanol [223]. “Green” butanol is produced via the ABE-fermentation realised by bacteria (here: clostridia phylum) or other pathways such as fermentation by genetically engineered biocatalysts or from ethanol via the acetaldehyde pathway. Compared to ethanol production, the conversion efficiency is lower and different products are provided; i.e. there is a need to separate the product spectrum afterwards [220, 222]. Since the synthesis of butanol from fossil fuel based reactants is more cost-effective than ABE-fermentation, most ABE-fermentation plants have been shut down in the past [222]. Annually around 3.7 Mt/a (ca. 0.1 EJ/a) butanol are produced being clearly less compared to methanol or ethanol production [119, 242].

Butanol can be and is used as a bulk chemical within the chemical industry [223]. Additionally, it can be used as a fuel (additive) for road transportation and potentially also for aviation either in direct use or as synthetic kerosene via the AtJ conversion. The use of isobutanol as feedstock for the AtJ-SPK conversion pathway is already certified [204].

B.6 Ammonia (NH_3)

Ammonia is a colourless, water-soluble gas with a pungent smell. The current ammonia production is based on the Haber-Bosch process, which synthesises hydrogen and nitrogen to ammonia. Before that, nitrogen is extracted from ambient air by air separation processes. Currently, hydrogen for such an ammonia production is provided from natural gas via steam methane reforming. This provision pathway could be replaced by hydrogen provided by water electrolysis using "green" electricity [118]. The present global ammonia production amounts to approximately 180 Mt/a (ca. 3.3 EJ/a) [408].

Currently, fertilizer for agriculture is the main market for ammonia. Other consumers are the chemical and the pharmaceutical industry. Beyond replacing the fossil-based ammonia of these industries, ammonia of renewable origin is discussed as an option for energy storage and as a maritime fuel [209, 408–410]

B.7 Methane (CH_4)

Methane is a colour- and odourless gas. It is the main component of natural gas [210]. To produce "green" methane, biomass-based as well as electricity-based supply pathways are possible [210, 220, 226]. During the biomass-based provision, biomass is degraded by anaerobic digestion via various intermediate steps to methane and carbon dioxide. In subsequent gas purification processes, pure biomethane is provided [219]. For the electricity-based pathway a methane synthesis is used. Therefore, syngas (section 3.2.4.1) is converted to methane (CH_4) and water (H_2O). The global methane production amounts to approximately 2,670 Mt/a, of which less than 0.1 % (< 0.2 EJ/a) are produced from renewable sources [210, 226].

Methane resp. natural gas is used today mainly for heat and power generation. Compressed methane serves as a fuel for road transport and liquefied methane as a marine fuel or fuel for heavy duty transportation. Furthermore, it is a feedstock for the provision of hydrogen and methanol – so far

mainly from natural gas. In addition to replacing existing use of methane from natural gas, methane of renewable could also successively replace other fuels in the transport sector.

B.8 Hydrogen (H_2)

Hydrogen is a is a non-toxic, colour- and odourless gas [215]. Most of the global hydrogen production originates from fossil sources based on natural gas and coal. Hydrogen of renewable origin can be produced by water electrolysis. Technically, also biochemical, solar-thermal, and other production pathways are possible being still in an early development stage [215]. If the electricity for the water electrolysis is provided exclusively from sustainable, renewable sources (e.g., from photovoltaic and/or wind power plants), "green" hydrogen can be provided [35, 207, 227]. Annually, about 70 Mt/a of hydrogen are produced worldwide, but only a minor share via electrolysis of water (approximately 0.1 %, ca. 0.01 EJ/a) [244]; the latter does not necessarily exclude the (partial) use of electricity produced from fossil fuel energy.

Hydrogen is a key intermediate product in the chemical industry, presently mainly produced from natural gas via steam methane reforming. It is a base chemical to produce ammonia and methanol, among others. Hydrogen is also used in refinery processes for processing of feedstock and further intermediate products (e.g., desulfurization or hydrocracking). In aerospace applications, hydrogen is used as a rocket fuel [215]. Hydrogen provided by renewable energy is regarded as a central element of a CO_2-neutral energy system [215, 244].

C. Appendix Section 4.1

C.1 Flight Trajectories

C.1.1 Data

Flight Data are derived from Automatic Dependent Surveillance Broadcast (ADS-B) information from the Opensky historical database [188]. Flight trajectories consist of departing flights of the five largest European airports (by passenger numbers). These are London-Heathrow, Paris Charles De-Gaulle, Amsterdam Schiphol, Frankfurt International and Madrid Barajas airport.

C.1.2 Methods

Flight Data from the Opensky database [188] are resampled to a frequency of 1 minute and latitudinal and longitudinal information is filtered to reduce erroneous positional information. Flight sections without ADS-B coverage (e.g., parts of the North Atlantic flight corridor) are estimated using the pycontrails "resample_and_fill" function. It uses a geodesic interpolation for data gaps of longer distances and a linear interpolation for shorter distances. Flights are discarded from the dataset in several cases: (1) when for at least one waypoint altitude, latitude or longitude information is not available or the flight altitude remains below 6 000 m or exceeds 13 000 m (6.5 % of the flights in the 2019 dataset). (2) Flights are also excluded when their aircraft type is not included in the Eurocontrol Base of Aircraft Data (BADA) performance data (0.2 % of the flights in the 2019 dataset). Some flights contain erroneous positional information and are excluded after the Contrail Cirrus Prediction Model (CoCiP) has run (5.6 % of the flights in 2019 evaluated by CoCiP). The aviation kerosene consumption of the remaining flights is used to calculate the amount of paraffinic kerosene available.

Figure C1 shows the daily amount of flights for each day, and the seasonal (in boxes) and annual (at the ordinate) means for the years 2017, 2018 and 2019. A modest seasonal pattern is recognizable. Typically, the summer and autumn months include more flights than winter and spring. A plausible explanation for this behaviour is an increase in leisure air traffic

activity due to the summer holidays. On an annual basis, in 2017 substantially fewer flights (2166 flights per day) were stored in the database compared to 2018 and 2019 (2420 and 2312 flights per day, respectively). This can be explained by an increasing coverage area of the OpenSky receiver network [188], yielding a larger amount of flights to be stored in the database. Additionally, a few short data gaps in the Opensky Database for the year 2018 (e.g., in September 2018) are apparent.

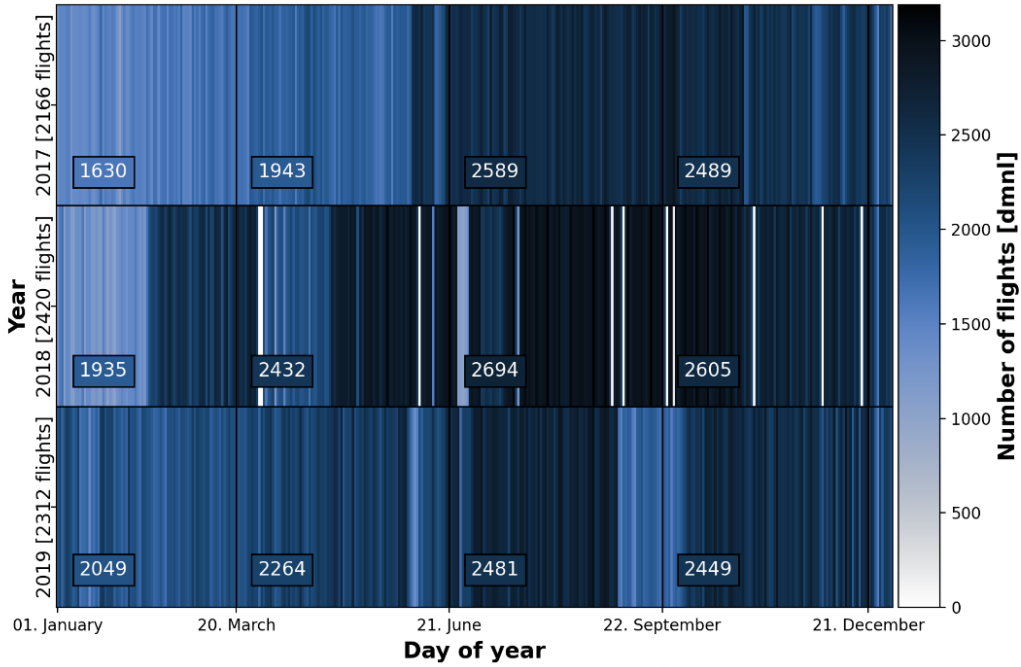


Figure C1 Flights of each day for 2017, 2018 and 2019 (ordinate) (figures in each box show the mean for the corresponding timeframe; means of each year are shown in brackets on the ordinate)

Figure C2 shows the distance traveled per flight for each day, and the seasonal (in boxes) and annual (at the ordinate) means for the years 2017, 2018 and 2019. Again, the distance per flight is higher in summer and autumn than during winter and spring for all three years evaluated. Comparing the different years, the distance travelled per flight seems comparatively constant. Again, the data gaps in the Opensky Database for the year 2018 (e.g., in September 2018) mentioned above are visible.

The mean of 1822 km/flight for the year 2019 is about 17 % higher than the mean distance per flight of 1516 km/flight estimated by Teoh et al. (2024) [317]. This can be explained by this study' focus on large international hubs, which typically have a high share of long-range flights.

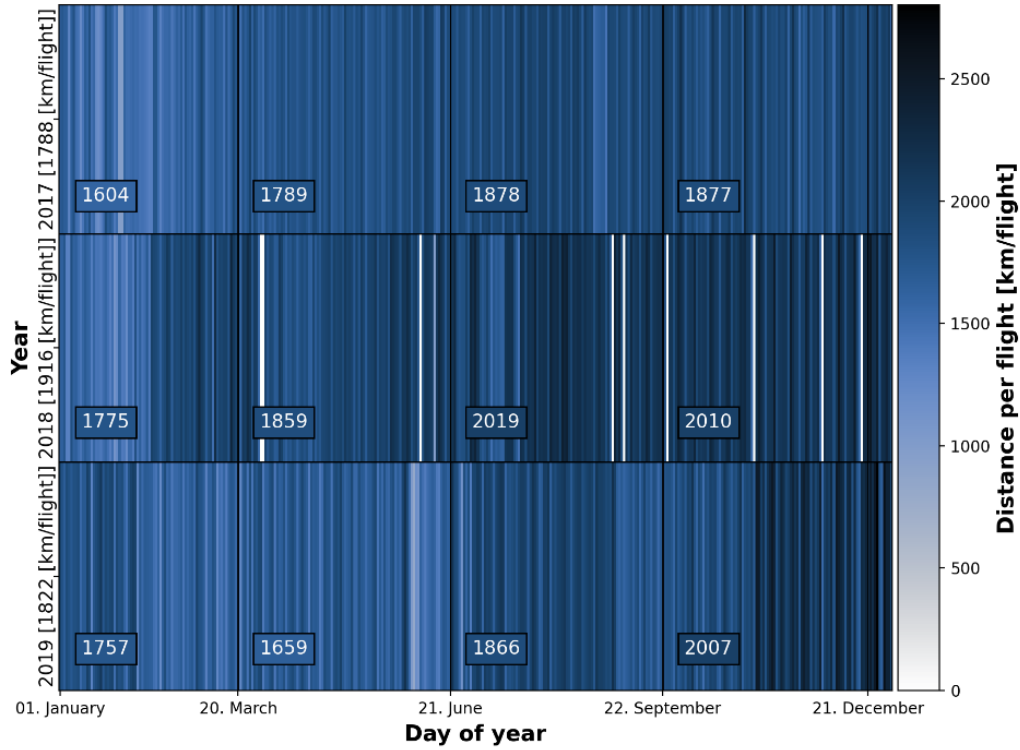


Figure C2 Distance per flight of each day for 2017, 2018 and 2019 (ordinate) (figures in each box show the median for the corresponding timeframe; means of each year are shown in brackets on the ordinate)

C.2 Aircraft Performance

C.2.1 Data

The performance data used to calculate aviation kerosene consumption and emissions of each flight is computated using the Eurocontrol Base of Aircraft Data (BADA) version 3.15 [190]. It covers 1409 aircraft types, of which 250 aircraft types are directly supported and the remaining aircraft types are matched with a directly supported aircraft type considered to be equivalent [190]. The assignment of engine types to aircraft is based on the Eurocontrol Base of Aircraft Data (BADA) version 3.15.

C.2.2 Methods

Data from aircraft performance models are utilized to compute the emissions of individual flights through simulations of parameters such as thrust

requirements at different waypoints, fuel consumption, and emissions associated with the engine model. Detailed information on emission estimation can be found in the documentation for pycontrails/CoCiP version 48.1. To accommodate for the increasing energy content in aviation kerosene with higher hydrogen contents, an adjustment factor ($q_{conventional}/q_{processed}$) is employed to modify the thrust-specific fuel consumption from BADA data tables to align with the energy content of processed kerosene.

Figure C3 shows a comparison between the distribution of thrust settings from this study with a previous study by Teoh et al. [10]. Both studies use flight data from the same year (2019) but different flight routes. While this study covers departing flights from five large, international airports in Europe, the study for comparison focuses on a traffic dataset for the North Atlantic.

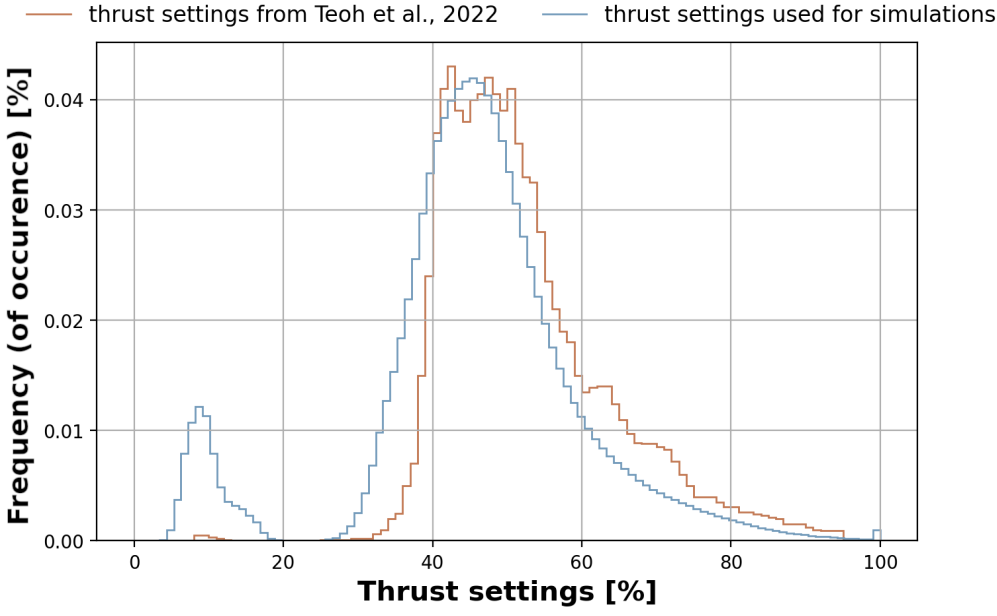


Figure C3 Comparison of thrust settings estimated using ADS–B data from the Opensky Network and the BADA3 aircraft performance data and thrust settings from Teoh et al. [10]

In general, both distributions show a bi-modal distribution, with one distinct peak at thrust settings around 50 % with a steeper slope at thrust settings below this maximum and a more gradual slope towards thrust settings of 100 %. In this study, the second maximum (around thrust settings of 10 %) is more pronounced than in the comparison study. Simultaneously,

the comparison study seems to estimate slightly higher thrust settings compared to the thrust settings estimated here. Both differences can be explained by disparities in the traffic datasets. Most likely, the comparison dataset includes a large share of long-range flights, while this study also includes intra-european connection flights. Thus, the dataset in this study has a larger fraction of descending/decelerating flights with reduced thrust settings which could constitute the more pronounced second maximum at lower thrust settings. The tendency of higher thrust settings in the comparison dataset might be explained by more pronounced traffic patterns (east- or westbound) across the North Atlantic resulting in less airspace congestion and thus fewer speed reduction requirements. In general, however, the difference is not very pronounced and could also be explained by the fact that the comparison study also includes BADA4 aircraft performance data while this study only considers BADA3. In general, both distributions seem to align appropriately.

Figure C4 depicts the calculated fuel use per flight for the simulations by day and as seasonal and annual means. On average, between 4.6 and 5.3 t of aviation kerosene were used per flight. Again, for 2018 and 2019 slightly higher values can be observed for summer and autumn compared to the winter and spring months. Additionally, the estimated fuel consumption in 2018 is considerably higher than in 2019 (on average by about 12 %). This could either be explained by longer flight distances in the 2018 trajectories or a reduced coverage area of the Opensky receivers for the year 2019, causing seemingly shorter flights.

C.3 Meteorological Data

C.3.1 Data

Weather data is retrieved from the European Center for Medium-Range Weather Forecast (ECMWF) Reanalysis version 5 [192] (ERA5) for the pressure levels 400, 350, 300, 250, 225, 200, 175 and 150. Since these data are an ex-post analysis, they are not available for flight planning purposes. For the realization of a targeted paraffinic kerosene use, the use of ex-ante data from a weather forecast would be necessary, which might incur further uncertainties.

C.3.2 Methods

Meteorological conditions for flights between those pressure levels are interpolated from the two nearest pressure levels. The properties and lifetime of the simulated contrails is highly sensitive to relative humidity data [9, 193, 318], but the data are limited in this regard. Relative to radiosonde measurements, the ice-supersaturated regions within the ERA5 data could be overestimated [411], but in-situ measurements suggest an underestimation [412]. Additionally, in-situ measurements suggest generally higher ice supersaturation values than found in the ERA5 data [186, 343, 411, 412]. Teoh et al. developed a correction method to improve consistency between the ERA5 humidity data and in-situ measurements [9]. This method is also applied in this study to adjust the ERA5 humidity data.

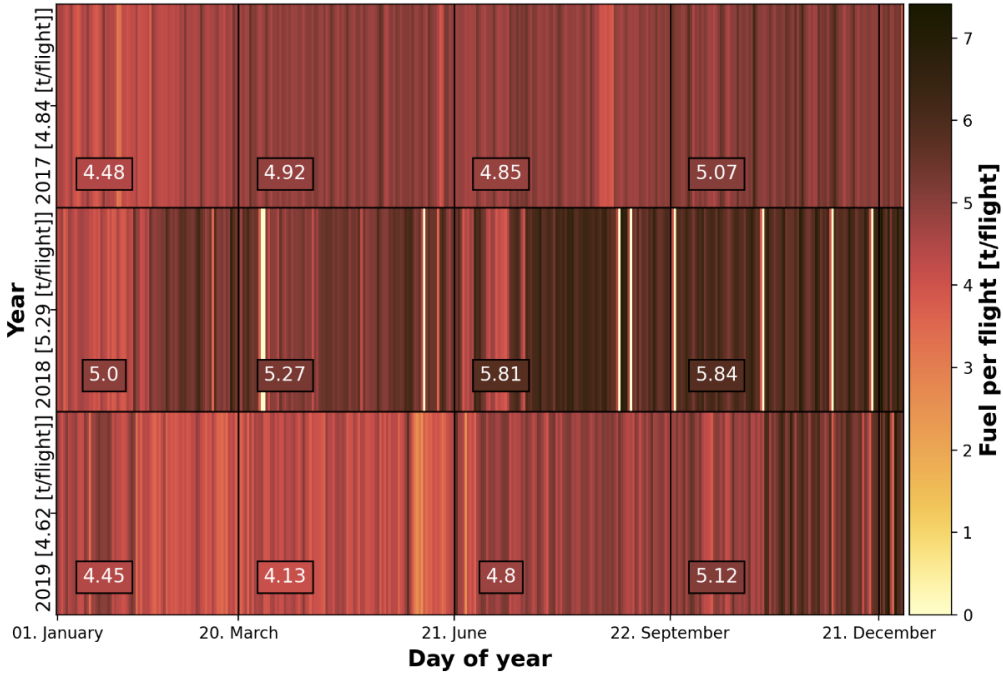


Figure C4 Calculated fuel use per flight for each day for 2017, 2018 and 2019 (ordinate) (figures in each box show the mean for the corresponding timeframe; means of each year are shown in brackets on the ordinate)

D. Terms in this Thesis

Table D1 Description and synonyms of common terms used throughout this thesis

Term specification	Description	Used in Chapter	Synonyms
fuel	any substance which can be used as an energy source in combustion engines	1-9	
alternative f.	a fuel which is atypically used, e.g., the use of ethanol where typically gasoline is used	1, 3, 4.2, 5 6.1, 6.3, 6.4, 7-9	
aviation f.	any substance, which can theoretically be used as an energy source in combustion engines of aircraft, regardless of its compliance with aviation fuel specifications	1-5, 6.1, 6.2, 6.3 8	
alternative jet f.	alternative fuel for aircraft engines (s. above)	6.1, 6.4	
kerosene	a mixture of hydrocarbons comprising cyclic and acyclic molecules of an approximate chain length of eight to 16 carbon atoms	1-9	aviation kerosene
aviation k.	s. kerosene	1-3,4.1, 6.1, 6.2, 6.3	kerosene
alternative k.	kerosene-like alternative aviation fuel, fuel, e.g., renewably sourced kerosene or crude oil-based kerosene with a reduced aromatics content	2, 4.2, 6.3, 7	
conventional k.	typically used kerosene from conventional sources, i.e., crude-oil, natural gas liquid condensates, heavy oil, shale oil and oil sands [181]	1-9	
synthetic k.	kerosene from alternative sources, i.e., coal, natural gas, biomass, fatty esters acids among others [280]	3, 4.2, 4.3 6.2, 6.3, 7	
fossil (fuel-)based k.	kerosene from fossil sources, e.g., crude oil, heavy oil, coal, natural gas	2, 3 4.1, 4.3 5, 6.1, 7-9	
renewably-sourced k.	kerosene from renewable sources of energy, e.g., biomass, hydrogen and carbon dioxide provided by renewably sourced energy	2, 3, 4.3 5, 6.1, 6.2	
biofuels	s. renewably sourced k.	6.3, 6.4	
powerfuels	renewably sourced k. from non-biogenic sources, e.g., hydrogen and carbon dioxide provided by renewably sourced energy	2, 3, 6.3	electro-fuels
electrofuels	s. powerfuels	6.4	power-fuels

low contrail k.	kerosene with an increased hydrogen content (mainly by removing aromatic compounds) to reduce contrail-related climate forcing	4.1, 6.2
paraffinic k.	kerosene containing only alkanes (straight-chain, saturated hydrocarbons)	3, 4.2, 4.3, 5, 6.1, 6.3, 7-9
drop-in k.	kerosene compliant with current fuel specifications, i.e., ASTM D1655 (and ASTM D7566, if applicable)	4.2, 4.3, 5
non drop-in k.	kerosene not compliant with current fuel specifications, i.e., ASTM D1655 and ASTM D7566	4.2, 5

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