Sustainable Aviation Fuels - Design, Production and Climate Impact

789. WE-Heraeus-Seminar

24 May - 27 May 2023

at the Physikzentrum Bad Honnef, Germany

WILHELM UND ELSE
HERAEUS-STIFTUNG

Subject to alterations!

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 789. WE-Heraeus-Seminar:

Power-to-Liquid fuels are essential for reaching the ambitious climate protection targets and to defossilize the energy sector. Especially in the aviation and maritime sector, liquid fuels are essential due to their high energy density. From today's perspective, there are no technological alternatives to the use of sustainable aviation fuels (SAF) to drastically decrease greenhouse-gas (GHG) emissions from aviation, at least for medium- and long-haul flights.
In order to enable a successful application of SAF, existing production routes and catalysts have to be optimized for efficiency and production yield, new integrative plant concepts and novel reactor concepts have to be developed and novel production routes have to be established.
A smart approach to the design and composition of SAF can reduce pollutant emissions, and maximize technical performance. Screening and machine-learning based evaluation of novel fuel candidates can provide valuable insights into their optimization potential.
Besides GHG emissions, the so-called non-CO2-effects are responsible for major part of aviation's climate impact, with their climate impact being a factor of 2 – 3 higher than the climate impact of GHG-emissions; hence, the non-CO2-effects have to be understood and minimized.
The seminar "Sustainable Aviation Fuels – Design, Production and Climate Impact" is to cover the full process chain from feedstock to production and application of sustainable fuels. This highly interdisciplinary approach combines all aspects with a common target of Synthetic Aviation Fuels. Experts in their field present the current status and developments to come. Young researchers will be encouraged to actively participate with poster presentations, Hot Topic talks, and at a panel discussion.

Scientific Organizers:

Dr. Christoph Arndt	German Aerospace Center (DLR), Germany E-mail: christoph.arndt@dlr.de
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Introduction

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Registration:

Martina Albert (WE-Heraeus Foundation)
at the Physikzentrum, reception office
Wednesday (16:00 h – 20:00 h)
and Thursday (08:00 – 12:30 h)

Program

Program

Wednesday, 24 May 2023

16:00 – 20:00	Registration	
From 18:00	*BUFFET SUPPER and informal get-together*	
20:00 – 20:10	Scientific organizers	**Opening and Welcome**
20:10 – 20:40	Denzil Moodley	**Catalysis for Sustainable Aviation Fuels: Fischer-Tropsch pathways**
20:40 – 21:10	Katharina Seeliger	**Airbus' view on 100% SAF**

Thursday, 25 May 2023

08:00	*BREAKFAST*	
09:00 – 10:00	Bert Weckhuysen	**Operando Spectroscopy and Microscopy of CO and CO2 Activation Processes**
10:00 – 11:00	Michael Clayes	**Stability of Fischer-Tropsch catalysts studied in-situ**
11:00 – 11:30	*COFFEE BREAK*	
11:30 – 12:30	Peter Pfeifer	**Production of carbon neutral fuels and upgrading towards kerosene**
12:30 – 12:40	**Conference photo** (in front of the lecture hall)	
12:40	*LUNCH*	

Program

Thursday, 25 May 2023

14:00 – 15:00	Jannick Schmidt	**Climate impacts of different SAF pathways**
15:00 – 16:00	Franziska Müller-Langer	**SAF supply as multiblend jet fuel – insight in a demo project**
16:00 – 16:30	*COFFEE BREAK*	
16:30 – 16:45	Stefan Jorda	**About the Wilhelm and Else Heraeus Foundation**
16:45 – 17:45	**Poster Slam 1** (2 min per Poster)	
17:45 – 18:45	**Poster Session 1**	
18:45	*DINNER*	
19:45	**Round Table Discussion** (Denzil Moodley, Bert Weckhuysen, Joshua Heyne, Franziska Müller-Langer, Katharina Seeliger) Moderation: NN	

Program

Friday, 26 May 2023

08:00	*BREAKFAST*	
09:00 – 10:00	Stephan Schmidt	**Production Pathway for SAF via Methanol**
10:00 – 11:00	Patrick Le Clercq	**Sustainable Aviation Fuels: Composition, Properties, and their Effect on Combustion System Relevant Sub-Processes**
11:00 – 11:30	*COFFEE BREAK*	
11:30 – 12:30	Christiane Voigt	**Effect of SAF on contrails and climate – What do we know and what is unknown?**
12:30	*LUNCH*	
	Hot Topic Talks	
14:00 – 14:20	Aleksandr Fedorov	**Extracting Knowledge from Literature by Data Science for Development of Highly-Selective CO2 Fischer-Tropsch Catalysts**
14:20 – 14:40	Florent Dubray	**Production of Jet-Fuel-Range Olefins via Catalytic Conversion of Pentene and Hexene over Mesoporous Al-SBA-15 Catalyst**
14:40 – 15:00	Stefan Bube & Steffen Voß	**Methanol-to-Kerosene - Technical comparison with competing pathways for biomass- and power-based SAF**

Program

Friday, 26 May 2023

	Hot Topic Talks	
15:00 – 15:20	Alexander Rabl	**Experimental investigation of soot emissions of oxygenated fuel blends in a small aero engine**
15:20 – 15:40	Eric Bach	**Pressure gain combustion for next generation aero engines**
15:40 – 16:00	Moaaz Shehab	**The influence of biomass characteristics and their uncertainties on the production of sustainable aviation fuel**
16:00 – 16:30	*COFFEE BREAK*	
16:30 – 17:30	**Poster Slam 2** (2 min per Poster)	
17:30 – 18:30	**Poster Session 2**	
18:30	*HERAEUS DINNER* *(social event with cold & warm buffet with complimentary drinks)*	

Program

Saturday, 27 May 2023

08:00	*BREAKFAST*	
09:00 – 10:00	Joshua Heyne	**Some sustainable aviation fuel drop-in constraints and non-drop-in opportunities**
10:00 – 11:00	Hai Wang	**On Chemical Properties of SAF: What Chemical Composition is Desirable for Efficient and Low-emission Aviation?**
11:00 – 11:30	*COFFEE BREAK*	
11:30 – 12:30	Scientific organizers	**Final Discusion /** **Concluding remarks and poster awards**
12:30	*LUNCH*	

End of seminar and departure

Posters

Posters 1

Eric Bach	**Pressure gain combustion for next generation aero engines**
Isaac Boxx	**Combustion and emission characteristics of Diethoxymethane and Ethyl acetate at RCCI conditions, measured via two-photon laser-induced fluorescence**
Stefan Bube	**Power-based SAF production – A technical comparison of competing synthesis pathways**
Nils Bullerdiek	**A system analysis of cost-efficient SAF deployment pathways under climate-target consistent conditions**
Steffen Cramer & Christopher Zschiesche	**Sustainable Aviation Fuels from Olefin Oligomerization**
Rebecca Dischl	**Inflight measurements of particle emissions from an Airbus A350-900 using 100% sustainable aviation fuel**
Jan Donndorf	**Development of a minimal-fidelity model of a turbofan engine running on SAFs**
Bogdan Dorneanu	**Towards an innovative process for the production of sustainable aviation fuels from biogenic raw materials**
Florent Dubray	**Production of Jet-Fuel-Range Olefins via Catalytic Conversion of Pentene and Hexene over Mesoporous Al-SBA-15 Catalyst**
Philipp Eiden	**Fluidized bed gasification in a 1 MWth pilot plant for sustainable production of biofuels**

Posters 1

Rabia Elbuga-Ilica	**Operando X-ray absorption spectroscopy as a first step towards a knowledge-based optimization of Fischer-Tropsch catalysts**
Ali Elwalily	**Methanol-to-JetFuel Pilot Plant – SAFari Research Project**
Aleksandr Fedorov	**Extracting Knowledge from Literature by Data Science for Development of Highly-Selective CO_2 Fischer-Tropsch Catalysts**
Nina Gaiser	**Insights into SAF Combustion: Molecular-Beam Mass Spectrometry Experiments at DLR's Institute of Combustion Technology**
Cherie Hsu	**Mixed metal (Mn, Al, Ti) cobalt oxide model systems for optimizing sustainable aviation fuel production via Fischer-Tropsch synthesis**
Catalina E. Jiménez	**Multi-scale holistic approach at the BESSY II synchrotron light source for investigating Fischer-Tropsch catalysts**
Haisol Kim	**Liquid fuel-based FLOX® burner development and spray characterization of various injectors**
Federico Lo Presti	**Reduced order modeling of turbocomponents for future short/medium range civil engines**
Hannes Lüdtke	**Comprehensive two-dimensional gas chromatography for prescreening and optimization of sustainable fuels**

Posters 2

Melis Kirarslan	**Direct activation of CO_2 to liquid fuels in Fischer-Tropsch Synthesis over iron catalyst**
Raphael Märkl	**Contrail ice crystal reductions of large passenger aircraft burning 100% sustainable aviation fuel**
David Metzger	**Efficient additive manufacturing reactor concept for the production of e-fuels: From 500 g of metal powder to 500 g of Fischer-Tropsch product**
Leonard Moser	**CIRCULAIR – Coupling of advanced biofuel production via hydrothermal liquefaction with PtX and green hydrogen**
Gregor Neumann	**Investigating Non-CO2 effects from hydrogen engines: Overview and first impressions of the Blue Condor experiments**
Gunnar Quante	**Techno-economic analysis of a smart use of low-soot aviation fuels – options and cost**
Alexander Rabl	**Experimental investigation of soot emissions of oxygenated fuel blends in a small aero engine**
Lennart Rieger	**Modeling and analysis of the regional production potential of sustainable aviation fuel in Bavaria**
Kai Risthaus	**Photonic synthetic gas production as a feedstock for aviation fuels**
Marius Rohkamp	**Detailed gaseous and particulate emissions of an Allison 250-C20B turboshaft engine**

Posters 2

Andreas Rosenstiel	**Cost Optimal Design of Solar E-Methanol Production Powered by CSP/PV Hybrid Power Plants**
Jonas Schmidt	**In situ measurements of contrail ice crystals of a modern passenger airplane burning sustainable aviation fuels**
Moaaz Shehab	**The influence of biomass characteristics and their uncertainties on the production of sustainable aviation fuel**
Enrico Sireci	**Computational investigation of the Co-support interfaces on γ-Al_2O_3, SiO_2 and TiO_2**
Mahima Santhoshi Sivvarapu	**eXplore: A decentralized modular plant for Fischer Tropsch synthesis and upgrading to eKerosene for field demonstration in H2Mare**
Estefania Vega Purga	**Solar fuel production via thermochemical cycles: Process and receiver-reactor technology**
Ferdinand Vogelgsang	**SynergyFuels – An integrated refinery concept for the production of SAFs**
Steffen Voß	**Processing biogenically produced intermediates to jet fuel - Technical comparison**
Dan Zhao	**Revealing the deactivation mechanisms of Co-based catalysts in Fischer-Tropsch synthesis by operando X-ray absorption spectroscopy**

Abstracts of Lectures

(in alphabetical order)

Some sustainable aviation fuel drop-in constraints and non-drop-in opportunities

J.S. Heyne[1,2], R. Boehm[1]

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Sustainable aviation fuels are currently being pursued as a 'drop-in' solution to lower the carbon intensity of existing aircraft and a 'non-drop-in' solution to minimize the climate impact of aviation transportation with kerosene-type fuels. The chemical and physical properties of aviation turbine fuels define the ability of fuels to be 'drop-in' or fungible in all existing infrastructure, aircraft, and engines. Unfortunately, certain property requirements, such as dielectric constant and o-ring swelling, appear to require aromatic molecules, which are disproportionately responsible for non-volatile particulate matter (nvPM) emissions that can nucleate contrails and persistent cloudiness. Meanwhile, non-drop-in kerosene-type fuels offer the potential to reduce nvPM further while maintaining all the attractive properties of kerosene fuels, such as energy density, safety, etc. Here we will detail some considerations to minimize the non-CO2 impact of aviation with kerosene-type fuels for drop-in applications and introduce competing theories for what a non-drop-in fuel should be.

References

[1] S. Kramer, G. Andac, J. Heyne, J. Ellsworth, P. Herzig, K. Lewis, Frontiers in Energy Research **9**, 782823 (2022)

[2] J. Heyne, B. Rauch, P. Le Clercq, M. Colket, Fuel **290**, 120004 (2021)

[3] S. Kosir, J. Heyne, J. Graham, Fuel **274**, 117832 (2020)

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[6] J. Colborn, J. Heyne, S. Stouffer, T. Hendershott, E. Corporan, Proceedings of the Combustion Institute **38**, 6309-6316 (2021)

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[8] R. Boehm, H. Franchesca, Z. Yang, T. Wanstall, J. Heyne, Frontiers in Energy Research **10**, 1074699 (2022)

[9] S. Kosir, R. Stachler, J. Heyne, F. Hauck, Fuel **281**, 118718 (2020)

[10] R. Boehm, Z. Yang, J.Heyne, Energy & Fuels **36**, 1916-1928 (2022)

Sustainable Aviation Fuels:

Composition, Properties, and their Effect on Combustion System Relevant Sub-Processes

P. Le Clercq[1], P. Oßwald[1], G. Eckel, C. Hall[1], S. Ruoff[1], M. Stöhr[1], T. Mosbach[1], T. Schripp[1], U. Bauder[1], B. Rauch[1], and M. Köhler[1]

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Sustainable aviation fuels (SAFs) are produced from renewable feedstocks, which also respect strong environmental, social, and economic (circular) criteria. More specifically, the production of such fuels follows a strict ecological balance by avoiding depletion of natural resources and by not contributing to climate change. Based on the feedstocks used (bio-based, waste-based, or directly the combustion products H_2O and CO_2 plus renewable energy) and based also on the transformation processes (thermochemical, catalytic, biochemical, and/or electrochemical) SAFs' composition can be close to a chemical copy of conventional crude-oil based Jet A-1/Jet A or hydrocarbons that are not found in conventional jet fuel.

Safety first in aviation! The technical feasibility of alternative aviation fuels, including SAFs had to be demonstrated prior to any utilization and potentially large-scale production. Since the final composition can differ in its total number of species, in its distribution of species within the kerosene cut, and/or in the species' chemical structures (e.g. different isomers) with respect to Jet A-1/Jet A, one understands that the contemplation of utilizing such fuels in commercial aviation first started with the development of a robust approval process. The assessment of SAF candidates is not based on their chemical composition but rather on their properties and their performance with respect to physical and chemical sub-processes, which are key to the overall safety. We investigate sub-processes that are relevant to the combustion system, in particular atomization, evaporation, and pollutant formation. Often, SAFs are premium quality fuels, meaning their use in legacy or modern aircraft engines leads to additional benefits in terms of performance and pollutant emissions reductions.

To understand the impact of fuels on safety, then on engine performance and emissions, and ultimately the environmental impact and climate forcing of aviation, it is important to investigate and fully comprehend the effect of fuel composition on its physical and chemical properties and further on the sub-processes occurring in the combustion system. We give an overview of the chemical analytics, the experiments, the diagnostics and modeling methods, as well as real system in real world measurement campaigns which enabled us to analyze these effects. Finally, the knowledge regarding these effects become the building blocks for proper fuel design.

Catalysis for Sustainable Aviation Fuels: Fischer-Tropsch pathways

D.J. Moodley[1]

[1]*Sasol Research and Technology, Sasolburg, South Africa*

Sasol is a world-leader in the development and application of the Fischer-Tropsch (FT) technology with more than 70 years' experience. Our own facilities and licensed technologies already produce more than 200 000 bbl/day of products. To reach our GHG emission reduction targets and decarbonize our operations we plan to leverage our proprietary technology, know-how and expertise to produce sustainable fuels and chemicals from green hydrogen and sustainable carbon sources, via Biomass/Power-to-Liquids (BPtL) processes [1]. In this regard a new business unit called Sasol ecoFT was established in 2021, to grow new sustainable businesses through licensing, catalysts, technical services and partnerships with initial focus on sustainable aviation fuel (SAF).

Synthetic kerosene can be produced on commercial FT catalysts and have significant benefits in terms of lower NOx and sulphur and aromatics [2], These FT-derived fuels can contribute to reducing the non-CO_2 warming impacts of aviation fuel [3]. The potential of cobalt and iron catalysts for this will be discussed, along with strengths and weaknesses of each catalyst system [4]. Planned future applications to produce SAF from sustainable feedstocks for both systems will be discussed.

We will highlight the CARE-O-SENE consortium work which is funded by the German Federal Ministry of Education and Research (BMBF) and Sasol. Here, we showcase collaborative work to understand, develop & scale-up new cobalt catalysts that are stable at high conversion and that yield high selectivity in slurry phase reactors. The importance of selective catalysts for increased jet-fuel yield will be discussed. Further improvements and developments in sustainable catalyst preparation and process design will be required to achieve our sustainability targets, and these will be elaborated on [4].

References

[1] https://www.sasol.com/our-businesses/sasol-ecoft
[2] R. van der Westhuizen *et al*, Journal of Chromatography A, 1218(28), 4478. 2011.
[3] C. Voigt *et al*, Communications Earth & Environment, 2(1), p.114. 2021.
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SAF supply as multiblend jet fuel – insight in a demo project

F. Mueller-Langer[1] **and N. Doegnitz**[1]

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The need to reduce and prevent emissions in the aviation industry has been addressed by many national and international strategies. In addition to technical and operational measures to reduce emissions, the focus is on substituting conventional fossil-based jet fuel with sustainable aviation fuel (SAF). Many R&D&D projects were undertaken in the past years with different key issues. In order to fulfill the required amounts to be set in the European ReFuelEU Aviation both biobased SAF (like HEFA hydrotreated esters and fatty acids, ATJ alcohol to jet and BTL biomass to liquids via Fischer-Tropsch) and PtL (power-to-liquids or e-fuels) based SAF are required in large amounts. In this context airports are expected to be supplied with JET A-1 containing different proportions of various types of renewable SAF (multiblend jet fuel).

This issue was motivation for the project DEMO-SPK. The primary objective was to investigate and verify the behavior of mixtures of several renewable SAF under realistic conditions within the supply infrastructure of a major airport. The aim was to successfully demonstrate the deployment of the multiblend JET A-1 in the general fuel supply infrastructure, from procurement to aircraft refueling. In addition to analyzing the properties of the jet fuel, the project measured emissions, conducted life cycle analyses, analyzed the sustainability documentation and studied verification and credit allowances for the renewable fuels as part of European emissions trading. [1], [2]

Part of the seminar will be to present highlights and exemplary results of the DEMO-SPK project.

References

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Production of carbon neutral fuels and upgrading towards kerosene

P. Pfeifer and T. Böltken

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The aviation sector faces a large challenge with respect to carbon neutrality. So far offsetting has been used by airlines to virtually reduce their carbon footprint. However, this is not sufficient in the future. Since the energy density of liquid hydrocarbons and the system weight including the storage vessel are superior to other sources of energy, the aviation sector will largely remain on products like kerosene. Another important issue in this discussion is the drop-in ability of carbon neutral alternatives. The safety of airplanes is ensured by fuel standards set by ASTM D7566 "Standard specification for aviation turbine fuels containing synthesized hydrocarbons".

Power-to-Liquid enables the feasibility of a high degree of carbon neutrality in the production of liquid hydrocarbon fuels i.e., above 90% net CO_2 savings along the full production and use cycle [1]. Therefore, CO_2 from atmosphere needs to be used as feedstock and needs to be converted by hydrogen, which itself is produced by renewable electricity. There are many alternative pathways to produce liquid hydrocarbons, nevertheless, Fischer-Tropsch is today the only pathway which allows to blend up to 50% renewable synthetic paraffinic kerosene "SPK" (ASTM D7566-18); the limit today is set by the minimum of 8 % aromatics, which are required as fuel component for the existing fleet. The benefit of the addition of the SPK is the much lower soot formation; this is an extra add-on as less cloud formation contributes to less global warming [2].

INERATEC is involved in many projects to produce synthetic fuels via cobalt-based Fischer-Tropsch synthesis and has therefore developed a process combination of reverse water gas shift and synthesis which is capable to allow load flexibility with intermittent renewable energy input. Such flexibility is required to avoid large hydrogen intermediate storage. The upgrading of the synthetic crude material can be done alongside in refineries but also as standalone process. The latter is followed in several projects such as PowerFuel, Kopernikus PtX and Ref4Fu with partners DLR and KIT. In the present contribution the status of crude synthesis and upgrading development is presented.

References

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Climate impacts of different SAF pathways

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New pathways of advanced fuels for SAF derived from biomass are key components in eliminating fossil and net biogenic CO2 emissions. However, the new pathways come with the risk of severe trade-offs related to indirect land use changes and other indirect effects. Today, these risks are poorly addressed in policy and life cycle assessment (LCA) guidelines and regulations. The production of SAF often involves the use of waste materials and dedicated cultivated biomass as feedstock. Promishing pathways are pyrolysis, gasification, and Fisher-Tropsch, which involve the production of syngas along with biochar. The syngas can then be further processed into SAF. The side-stream of biochar can be used as a stable and long-term carbon storage if applied to land. There are several possible feedstocks for syngas production, including cultivated biomass, agricultural and forestry residues as well as waste materials. If the use of biomass requires additional land, it will cause land use changes – either directly or indirectly. The use of residues or waste materials as SAF feedstock will avoid an alternative use or treatment of the material. The avoided treatment may be associated with net positive or net negative GHG emissions. In case of the latter, the use of the residues will cause net positive GHG emissions. Emissions from land use changes or indirect emissions caused by avoided treatment of residues may (partly) outbalance the gains from the use of SAF. This means that some pathways of SAF production involve undesired indirect effects on GHG emissions, which are crucial to detect to ensure that the intended gains from SAF are actually achieved.

This presentation outlines the possible unintended indirect effects from the acquisition of SAF feedstocks. This includes both net positive and net negative effects. Potential low and high GHG emission feedstocks are identified. Recommendations on how to account for indirect effects are provided as well as it is recommended that the indirect effects are accounted for in SAF certifications and regulations.

Production Pathway for SAF via Methanol

S. Schmidt[1], M. Kuschel[1], J. Engelmann[1]

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Assuming that people will continue to use aircraft in the future, SAF will play an important role in our future way of flying. Driven by the need to reduce CO_2 emissions, this opens up a large area for technological innovation. In SAF's production routes, the methanol route plays an important role. By means of this route, two key aspects resulting from the transformation of the energy system can be combined. On the one hand, SAF can be produced with high quality using this route. On the other hand, the production chain can be made more flexible to a high degree on a regional and performance-related basis.

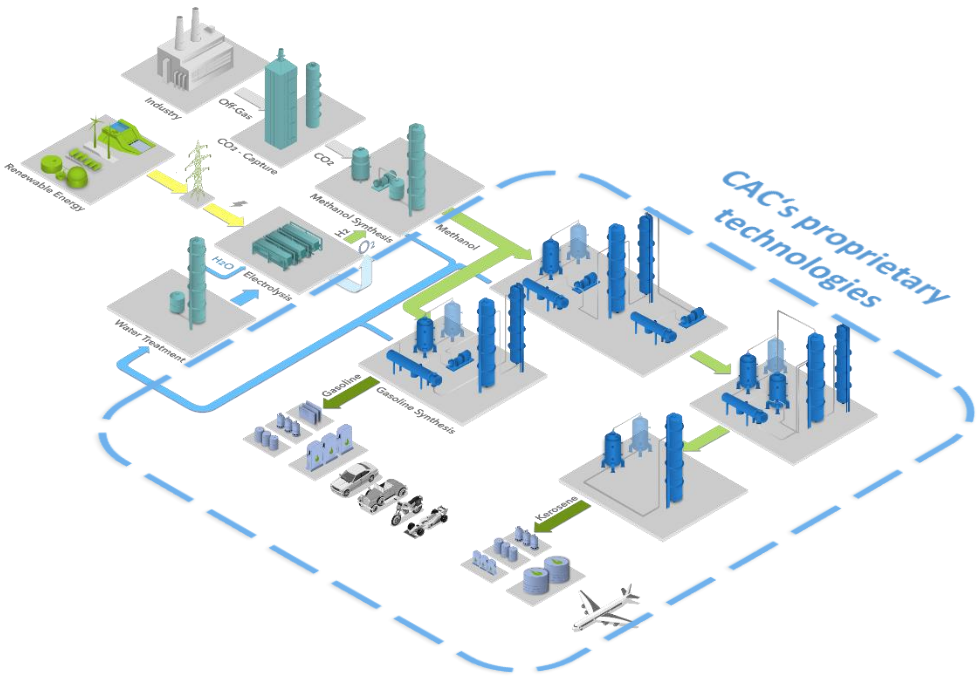

Fig.: PtL methanol pathway

CAC has been doing process development in the field of synthetic fuels for several years. With this presentation, we want to give an overview on the production of synthetic paraffinic kerosene (SPK) via the methanol route. In the methanol route, methanol is produced as an intermediate from CO_2 and H_2. Compared to H_2, methanol can be transported at lower cost. Therefore, methanol is a suitable energy carrier to import renewable energy.

The presentation will give a short overview about the pathway via Methanol to jet fuel as well as about the suitable products and by-products.

Airbus‘ view on 100% SAF

Katharina Seeliger

Airbus

Effect of SAF on contrails and climate – What do we know and what is unknown?

C. Voigt[1,2]

[1] *Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institute of Atmospheric Physics, , Germany*

[2]*Johannes Gutenberg-Universität Mainz, Institute of Atmospheric Physics, Mainz, Germany*

The major share of aviation's climate impact is driven by contrails and aircraft CO_2 emissions. While aircraft CO_2 remains in the atmosphere for about a century, contrails trap energy in the atmosphere over their lifetime of few hours. The reduction of contrails is therefore a fast measure to significantly reduce the climate impact from aviation - contrails are the jokers in the game of cards.

Current research at the Deutsches Zentrum für Luft- und Raumfahrt (DLR) develops strategies to reduce the climate impact from aviation and in particular from contrails by the use of sustainable aviation fuels, modern engine technologies, climate-friendly aircraft routing and contrail avoidance.

Sustainable aviation fuels were investigated by measurements within the project ECLIF1 to 3 and Future Fuels. Aircraft measurements show a significant reduction in particle emissions, when burning low aromatic sustainable aviation fuel (SAF) or synthetic fuel blends. The effects on contrails and climate are investigated. During the Volcan projects with Airbus and French partners, the effects of modern lean burn engine technology on emissions and contrails has been tested in flight and ground campaigns. First results of emission and contrails observations in the rich and the lean burn mode with Jet-A1, hydro-processed Jet and SAF are presented. Strategies to optimize flight routing in order to avoid contrails were developed by DLR and partners. Hourly weather dependent contrail forecasts are tested and evaluated with aircraft and satellite data. Uncertainties in contrail prediction and observation are discussed in detail. Results from these projects are synthesized in order to shape the way for future climate-friendly aviation.

On Chemical Properties of SAF: What Chemical Composition is Desirable for Efficient and Low-emission Aviation?

<u>Hai Wang</u>

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This talk attempts to address two questions. First, what key aviation fuel properties are desirable to maintain predictable combustion chemistry properties and hence safe engine operation? Second, what hydrocarbon components are beneficial to improving engine combustion efficiency and reducing particulate emissions? Key features of the combustion properties of aviation fuels will be overviewed based on a series of Hybrid Chemistry (HyChem) modeling studies of conventional and sustainable aviation fuels (e.g., [1,2]). Challenges and opportunities are discussed in the context of SAF design, utilization, and emission control. Issues concerning reliable modeling of combustion properties will also be discussed.

References

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Operando Spectroscopy and Microscopy of CO and CO2 Activation Processes

Bert Weckhuysen

Utrecht University, Utrecht, The Netherlands

Abstracts of Posters

(in alphabetical order)

Pressure gain combustion for next generation aero engines

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Pressure gain combustion is a promising technology for significantly increasing the efficiency of gas turbine and rocket engines, as the heat addition does not occur along a path of constant pressure, resulting in lower entropy generation [1]. The most practical implementation is through rotating detonation combustors (RDC), in which a supersonic detonation wave propagates continuously around an annular channel for as long as reactants are supplied from the head end. At the aft end, a high-enthalpy exhaust flow exits the combustor and can be used to extract work or provide thrust. Although the process is quasi-steady, considerable oscillations of the flow properties persist at the exit plane with frequencies in the kHz range. Further research work is thus required to successfully integrate an RDC with a gas turbine architecture [2]. Recent experimental results, however, have shown to mitigate the associated risks, advancing the progress of RDCs towards viable commercial products [3]. Stable, reliable, and efficient operation of the detonation combustor is not only dependent on the chamber and injector design, but also on the reactant type. The inherently unsteady detonation wave is driven by a large number of transversally propagating shocks that interact with one another. An important parameter of this system is the detonation cell size, which is heavily influenced by the combination of fuel and oxidizer [4]. Thus, as RDC technology matures and the aviation industry shifts towards the utilization of sustainable aviation fuels, it is of paramount interest to tailor those fuels in a way that is conducive to RDC operation. The present study first introduces the benefits and challenges associated with RDCs, along with a discussion of liquid fuel injection strategies. Afterwards, a short review of detonation structures and cell sizes is given, culminating in a set of important aspects that should be considered in future aviation fuels. Ultimately, this progresses the technology readiness level of RDCs for the next generation of ultra-efficient aero engines.

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Combustion and emission characteristics of Diethoxymethane and Ethyl acetate at RCCI conditions, measured via two-photon laser-induced fluorescence

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Abstract
Reactivity-controlled compression ignition (RCCI) is a promising combustion process that can further optimize the combustion of renewable fuels. By combining the advantages of both compression ignition and spark ignition, RCCI can achieve high efficiency, low emissions, and reduced fuel consumption. The use of RCCI, in combination with renewable fuels, can lead to a more sustainable and environmentally friendly transportation sector. One potential disadvantage of using RCCI is the high amount of CO (carbon monoxide) and UHC (unburned hydrocarbon) emissions that can be produced due to the low-temperature combustion. Bio-hybrid fuels are promising to overcome these emission disadvantages when tailor-made for low-temperature combustion. To analyze possible emission benefits and the formation during the entire combustion process, CO and UHC have to be measured time and spatially-resolved not only at "end-of-pipe" but inside the combustion chamber.

In this study, we apply two-photon laser-induced fluorescence (TPLIF) to detect and quantify CO and UHC formed during the combustion diethoxymethane and ethyl acetate at RCCI conditions in an optically accessible high-pressure combustion chamber. The measured data yield new insight into the formation of CO and UHC during the combustion process at different locations and times.

Key words
Optical Diagnostics, Emission Analysis, RCCI, LIF

Power-based SAF production – A technical comparison of competing synthesis pathways

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Substituting fossil jet fuel with kerosene-type Sustainable Aviation Fuel (SAF) is a crucial instrument for achieving the climate targets of the aviation sector. Presently, the majority of SAF is produced from lipid-based waste and residues, which have an inherently limited feedstock potential. On the contrary, the feedstock potential for jet fuel produced from power-based synthesis gas using Power-to-X (PtX) technologies is at least theoretically unlimited. The most prominent PtX production pathways are the Fischer-Tropsch and the Methanol route.

Against this background, a technical comparison of both SAF pathways via power-derived synthesis gas (Figure 1) is carried out to evaluate the respective routes' advantages and disadvantages and associated opportunities and challenges. For this purpose, the process design of the individual pathways is first determined according to the current state of technology. Based on these process designs, both pathways are modeled using a steady-state flowsheet simulation. The mass and energy flows resulting from the simulation are used to determine process parameters and evaluate the overall process key figures like carbon and energy efficiency. In addition, a sensitivity analysis of selected process parameters is performed to assess the influences of technical uncertainties on the overall plant performance. In conclusion, a qualitative discussion of both paths from a systemic perspective is presented to derive potentials and preferential areas of application. The results show the differences in up- and downstream processing resulting from the fundamentally different chain formation mechanisms determining mainly the achievable kerosene fractions. From a systemic point of view, the use of methanol as intermediate feedstock allows for more flexible supply chains and potential synergies with other sectors demanding methanol (derivatives).

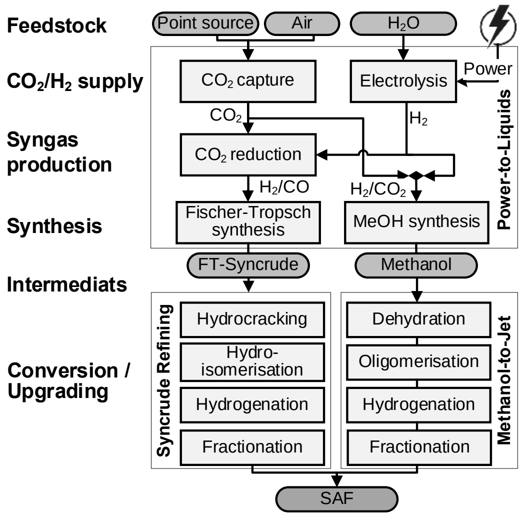

Figure 1: Fischer-Tropsch- and methanol-based SAF production pathways

A system analysis of cost-efficient SAF deployment pathways under climate-target consistent conditions

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A large-scale use of kerosene-type Sustainable Aviation Fuel (SAF(K)) is vital to reduce aviation related climate impacts. Although various SAF(K) options have been tested for more than 15 years, current SAF(K) shares are well below 0.1 % compared to the global aviation fuel consumption. For the production of SAF(K), various feedstock options and conversion technologies exist. Individual options can differ considerably in key attributes (e.g. in terms of usable feedstock options, feedstock availability, feedstock costs, technological maturity). The interaction and effects of such aspects with regard to an overall deployment and scale-up of SAF(K) over the course of time is difficult to estimate, which can hamper an overall cost-efficient SAF(K) usage. Against this background, an optimisation model is developed and applied that allows to analyse cost-efficient SAF(K) deployment pathways under climate-target-compatible conditions for the years 2025 to 2050 on a global level. Within the optimisation model, a defined kerosene demand must be supplied on a yearly basis. This demand can be met by both conventional aviation fuel as well as various SAF(K) options (e.g. HEFA, ATJ, FT-BTL, FT-PTL). The overall fuel use must be compliant with defined CO_2-emissions targets (e.g. maximum yearly CO_2-emissions), while CO_2-offetting can be used up to defined shares. The production of SAF(K) requires corresponding production plants that can be commissioned and decommissioned on a yearly basis under consideration of defined minimum plant duration periods. On a feedstock level, a production of SAF(K) is limited by a defined availability for different feedstock options. The optimisation model is applied in a scenario analysis based framework to derive SAF(K) deployment pathways for various frameworks conditions. Such pathways are assessed, amongst others, with regard to individual SAF(K) volumes, feedstocks demands (e.g. for different biomass options, electricity, hydrogen or carbon dioxide (CO_2)), the number of SAF(K) production plants built, or aviation fuel cost in the course of time.

Sustainable Aviation Fuels from Olefin Oligomerization

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Introduction

The catalytic oligomerization of low olefins originated from the methanol to olefins (MTO) process is a promising pathway to form highly branched hydrocarbons useful as jet fuel. Suitable catalysts for the olefin oligomerization require large surface area and high acidity as provided by zeolites or solid phosphoric acids.[1,2] The olefinic oligomers produced reveal negligible amounts of aromatics and need to be hydrogenated before fractional distillation. For the synthesis of jet fuel components, the olefin oligomerization is the key step within the process chain and therefore the evaluation of the most important reaction parameters as well as type of catalyst is of particular interest.

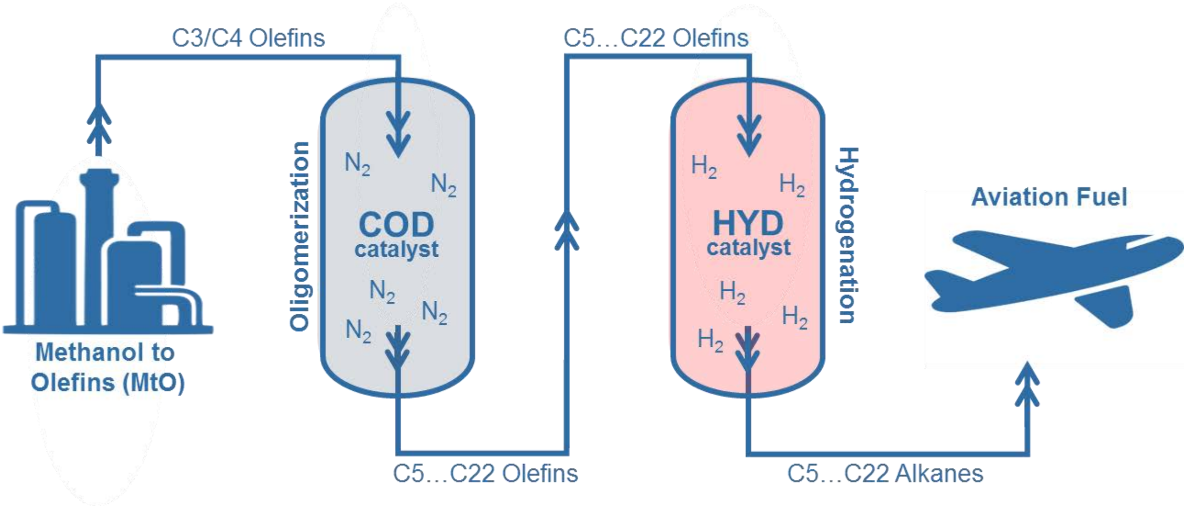

Fig. 1: Process routes for production of aviation fuels from MTO-intermediates.

In this regard, a series of experiments were conducted on the microreactor scale using different types of catalysts such as BEA and Y. After evaluation of the catalysts and clarification of promising setup of operation parameters, some studies on the hydrogenation of the oligomeric product have been performed using a commercial catalyst.

Results and Discussion

In the experimental studies on the olefin oligomerization BEA and Y catalysts have been used while taking MFI as a benchmark. Additionally, important operation parameters such as temperature, pressure and space velocity have been systematically varied to investigate their effect on the respective product distribution. Variation of temperature shows a maximum yield of the jet fuel fraction at moderate temperatures also providing rather stable production rates over prolonged time on stream. By contrast, higher temperatures primarily lead to increased deactivation of the catalysts. The subsequent hydrogenation of the olefinic oligomers has been carried out at very low temperatures, i.e. below 100°C, to avoid potential cracking retaining the maximum yield of jet fuel components. Finally, the properties of the fractionated and hydrogenated product match all requirements of commercially relevant jet fuel.

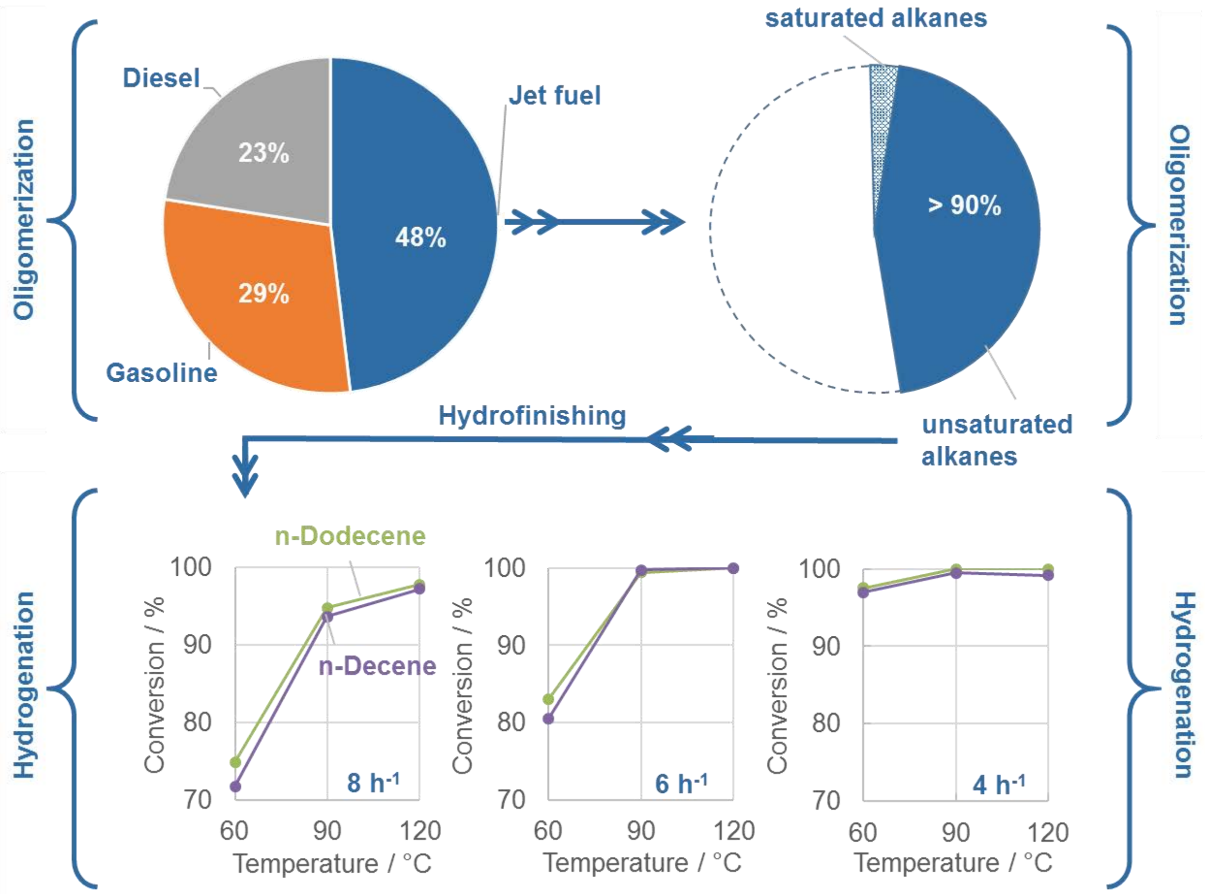

Fig. 2: Product distribution of raw and hydrogenated oligomerisate.

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Inflight measurements of particle emissions from an Airbus A350-900 using 100% sustainable aviation fuel

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With an effective radiative forcing of about 57 mW m^{-2}, contrail cirrus provide the largest individual contribution to the climate impact of aviation [1]. Thereby, particle emissions from aviation at flight altitude are a major facilitator to contrail formation. The use of sustainable aviation fuels (SAF) and modern jet engines may have a positive impact on contrail-induced climate impact by reducing particle emissions.

Within the framework of the ECLIF3 (Emission and Climate Impact of Alternative Fuels) project, in-flight measurements of particulate emissions and trace gases have been performed in a close collaboration between DLR, Airbus, Rolls-Royce and Neste.
In two deployments in 2021 the DLR research aircraft Falcon 20 captured emissions from an Airbus A350-900 aircraft burning 100% HEFA (Hydroprocessed Esters and Fatty Acids) jet fuel and for comparison also conventional Jet A-1 as well as a blend of HEFA and Jet A-1.

Particle measurements in-flight have been probed close to the engine to capture the emissions prior to any significant atmospheric processing. In this way, it was also possible to measure changes in the emissions resulting from the variation of specific engine power settings of the Rolls-Royce Trent XWB-84 engine.
A thorough evaluation of the effects of using different jet fuels and engine power settings on particle emissions will be shown. These results are important for future assessments of strategies to mitigate aviation's climate impact through the use of sustainable fuels in aviation.

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Development of a minimal-fidelity model of a turbofan engine running on SAFs

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To address future application of sustainable aviation fuels (SAF) in a senseful manner the engines of future aircrafts need to be optimized for the new chemical compositions of the SAF and also manage to use different types of SAF based on their availability. This is important to lower the running costs of airplanes and to lower market entry barriers of these fuels to reach climate goals of the aviation sector. The capability of engines to consume more than just one type of SAF will empower competition between them, thus will put power onto more efficient production of SAFs and will result in gaining a competitive advantage for an engine manufacturer.
The goal of this preliminary work is to develop a parametric aero engine model. This model initially derived from the use of conventional fuels, will be used to design a minimal-fidelity design also useable for the application of SAFs in an aero engine. The model will analyse the cycle run with SAF to determine the most efficient thermodynamic operating points for different SAFs in the same engine. From high interest is how the thermodynamic parameters of an engine react to changes of fuel composition and how geometries of engine parts have to change because of this.
The EU project MYTHOS (Medium-range hybrid low-pollution flexi-fuel/hydrogen sustainable engine) focus on the application of SAFs, hydrogen and conventional Jet A to make aviation more sustainable and adjust in a phase where different fuel types will be existing next to each other. In the longer run of the project the model will be part of the basis for CFD simulations of engine parts and by that machine-learning supported data examining by Physical Informed Neural Networks (PINNs).
The poster will present preliminary results of the current work on the development of the parametric aero engine model and the possible SAFs potentially used in the project.

Towards an innovative process for the production of sustainable aviation fuels from biogenic raw materials

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Several thermochemical pathways (e.g., gasification, pyrolysis, hydrothermal carbonization, etc.) are available for the transformation of biomass into various products, including a gaseous stream from which syngas ($CO+H_2$) can be obtained [1]. When combined with further downstream processing such as Fischer-Tropsch synthesis (FTS), this gas can be converted into renewable hydrocarbons, enabling the production of a wide range of high-value added products, including sustainable aviation fuels (SAF) [2].

This contribution introduces an ongoing research project that aims to overcome challenges related to the inefficiencies of the syngas-to-SAF pathway for the development of a new integrated process for the production of environmentally friendly aviation fuels from biogenic raw materials. The end product is expected to meet the requirements for a Jet A1 fuel according to the ASTM D 1655 standard [3].

For the achievement of this objective, industrial and academic partners work together for the development of new advanced catalytic systems to carry out the conversion of biomass-based syngas via FTS and hydrocracking in a single step using an interdisciplinary approach. The hybrid bifunctional catalysts produced are coated on microchannel reactors, and their performance compared with commercial catalysts available on the market.

Subsequently, the reactor modules are manufactured using 3D printing and tested at pilot scale, and the SAF production via the innovative one-step process is integrated with the biomass conversion to syngas, for validation in a relevant industrial environment.

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Production of Jet-Fuel-Range Olefins via Catalytic Conversion of Pentene and Hexene over Mesoporous Al-SBA-15 Catalyst

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In the context of energy transition, a significant portion of anthropic greenhouses gas emissions is related to aviation industry. However, due to specific requirements on aviation fuel properties, there are no commercial applicable alternatives to standard aviation fuel currently available. The design of commercially applicable pathways for the production of renewable aviation fuel is consequently primordial for the successful contribution of aviation industry in reducing human related greenhouse gas emissions. The oligomerization of biomass-based olefins offers potential for the synthesis of sustainable jet-fuels comprised of C_{10}-C_{18} hydrocarbons that are compatible with current infrastructures. However, the control of the oligomerization selectivity remains a challenge. In this contribution, the influence of process parameters comprising temperature, pressure, contact time, and feed composition on the catalytic conversion of a mixture of pentene and hexene over mesoporous Al-SBA-15 catalyst in continuous operations is thoroughly investigated. Kinetic evaluation resulted in the observation that pentene is more reactive than hexene while selectivity to jet-fuel range products exceeding 98% at low to moderate conversion (<50%) was achieved. Increasing the conversion to ca. 90% resulted in a decreased selectivity towards jet-fuel range products at ca. 75%. Notably, the product distribution of the oligomerization reaction is mostly independent of the process conditions under study, implicating that adjusting the conversion level is the primary way to tune oligomerization selectivity over the Al-SBA-15 catalyst. This understanding of the oligomerization process identifies the direction of research devoted on the oligomerization of complex olefin mixtures mimicking the process stream of biomass-based olefin production units, with the goal to achieve and optimize the “biomass to jet-fuel” transformation.

Fluidized bed gasification in a 1 MW_{th} pilot plant for sustainable production of biofuels

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In July 2021, the EU-Commission proposed a regulation to increase the use of sustainable aviation fuel (SAF) on air transport as part of the "REFuelEU Aviation" initiative. This will result in a significant increase in SAF from 2 %-vol. in 2025 to 63 %-vol. in 2050.

An attractive synthesis route for SAF is the gasification of biogenic residues or waste to syngas followed by the conversion of the syngas with a Fischer-Tropsch catalyst to SAF.

The feasibility of this complete synthesis route was already demonstrated in pilot scale at the TU Darmstadt using two different gasifier technologies. The High Temperature Winkler (HTW) gasifier was chosen as it convinces by allowing a wide range of feedstock and by producing a low-tar syngas. The only currently operated HTW gasifier, a 500 kW_{th} pilot reactor, was successfully operated for more than 2.500 hours at the TU Darmstadt.

The second used gasifier technology is the chemical looping gasification (CLG) as it is a promising process for the thermochemical solid to liquid conversion route using lattice oxygen, provided by a solid oxygen carrier material, to deliver a nitrogen free synthesis gas. Also, the CLG was optimized in 3 test campaigns.

The produced syngas was purified in a next step via a novel gas purification concept using a regenerable fatty acid methyl ester wash to dissolve light hydrocarbons followed by an amine scrubber.

Next, alternative input materials as well as bed materials in the gasifier will be investigated.

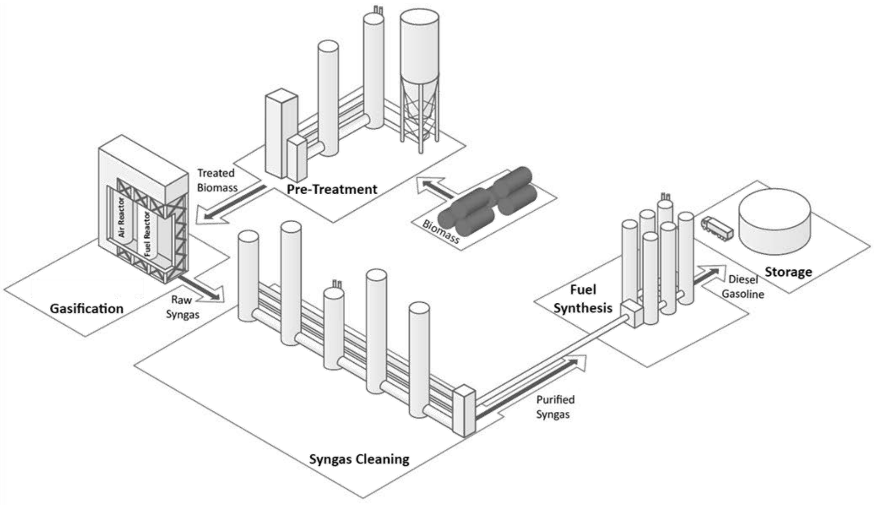

Figure 1: Industrial-scale concept for sustainable aviation fuel production via gasification of biogenic residue.

Operando X-ray absorption spectroscopy as a first step towards a knowledge-based optimization of Fischer-Tropsch catalysts

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Power-to-liquid processes can be considered the key for renewable electricity-based liquid fuel generation. [1,2] For this purpose, H_2 generated *via* water electrolysis and CO_2 provided *via* "carbon capture" are converted together on a suitable catalysts [3] and hydrocarbons, various olefins and methanol can be synthesized *via* Fischer-Tropsch process (FTS)[2]. For catalyst improvement, *in-situ* and *operando* characterization of FTS catalysts is considered essential to derive structure-activity relationships. [4] In this respect, *operando* X-ray absorption spectroscopy (XAS) can be used to observe structural changes of active sites of heterogeneous catalysts at work. The study is of significant importance, mainly in view of growing demand for energy storage using CO_2 as feedstock and renewable electrical energy.[5] For this purposes, a dedicated *operando* reactor system has been recently developed at the CAT-ACT beamline at KIT Light Source [6] that allows an operation close to the industrially relevant FTS conditions [4]. The high-pressure and high-temperature setup was developed in-house [5] and installed at the CAT-ACT beamline.[6] As a pilot study, commercially representative Co-Ni-Re/γ-Al_2O_3-FTS-catalysts were investigated at 250°C and 30 bar for more than 300h. The products were investigated by online µ-GC and offline GC-FID to trace the catalytic activity and selectivity. The study showed that considering the high stability of the catalysts, the main reason of catalyst deactivation is due to macroscopic effects such as pore blocking by reaction products and diffusion limitation. Based on this obtained information, we aim to prepare a model FTS catalyst and further optimize it for improved activity and selectivity. Part of the findings, will support new energy-related initiatives in Germany, like the CARE-O-SENE project [7], a research collaborations focused on the production of sustainable aviation fuel.

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Methanol-to-JetFuel Pilot Plant – SAFari Research Project

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The SAFari project (**S**ustainable **A**viation **F**uels based on **A**dvanced **R**eaction and Process Intensification) is a research initiative aiming to produce sustainable aviation fuel from green methanol in a tailor-made pilot plant with a capacity of about 30 t/a SAF. The project partners, including the Fraunhofer ISE, will develop the pilot plant, which will encompass the entire process chain required to produce SAF. The objective is to obtain full market approval from the American Society for Testing and Materials (ASTM) for methanol-based SAF.

Green methanol, as a feedstock for SAF production, can be produced worldwide in locations with high availability of renewable energy sources. Additionally, it can be transported efficiently as a pure liquid using existing infrastructure. Therefore, the methanol pathway for SAF production offers a great opportunity to generate added value in Germany and other countries.

The project partners are taking an innovative approach in the SAFari project, aiming to reduce hydrogen demand and achieve high overall process efficiency on an industrially relevant scale. This will be accomplished by using innovative reaction technologies throughout the various sub-processes and intelligently integrating heat and mass flows. The objective is to increase SAF yield and reduce production costs, ultimately aiming for a blending rate of up to 100% with methanol-based SAF. Currently, the various ASTM-approved SAFs allow a blending rate of up to 50%.

The SAFari project has the potential to become a disruptive technology that can completely replace the fossil process and significantly reduce the carbon footprint of aviation fuels in an economically viable manner. In the first phase of the project, the focus will be on the Methanol-to-Olefines (MtO) synthesis to produce SAF.

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Extracting Knowledge from Literature by Data Science for Development of Highly-Selective CO_2 Fischer-Tropsch Catalysts

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Recently, there has been a rapid rise in applying machine learning and data science for solving a lot of tasks in the different fields of science, industry, and business. Due to an increase in the number of scientific articles it is becoming attractive to use these methods for literature analysis because it can help in the systematization and evaluation of the pool of data, extract latent knowledge and formulate new ideas. CO_2 hydrogenation to hydrocarbons (CO_2-Fischer-Tropsch (CO_2-FT)) is an actively developing topic in science. This interest is caused by the dramatic rise in emissions of CO_2 resulting in greenhouse effect. The present work is devoted to analyzing the literature of CO_2 hydrogenation catalysts to find relationships between catalyst characteristic and performance as well as its experimental validation [1, 2]. A challenge was to include performance data obtained by different groups which vary in the applied reaction conditions but vary also in the set of performance indicators that are reported. Methodology for analysis of CO_2-FT catalysts was developed [1]. It was found that the key parameters of catalyst selectivity (the chain growth probability and an excess in CH_4 selectivity) only slightly depend on reaction condition and were defined by the catalysts. The obtained knowledge was used for smart screening of highly selective and active CO_2-FT catalysts. Analysis of the approach to equilibrium of the reverse water gas shift reaction indicated the presence of an unexpected direct route of CO_2 hydrogenation to higher hydrocarbons via FT mechanism at least for some catalytic systems. The existence of such reaction pathway was validated by carrying out additional catalytic experiments [2]. Thus, applying modern methods of data science and machine learning allows extracting new knowledge from the literature that could help in preparing new catalytic systems with improved performance and high selectivity to the desired products.

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Insights into SAF Combustion: Molecular-Beam Mass Spectrometry Experiments at DLR's Institute of Combustion Technology

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Sustainable Aviation Fuels (SAFs) are an essential part to reduce the environmental impact of aviation. To fully understand the SAF combustion behavior, complex chemical reactions have to be investigated to understand and mitigate pollutant formations.

Molecular-beam mass spectrometry (MBMS) is a powerful tool that provides real-time insights into the combustion behavior of SAFs, their reaction pathways, and mechanisms. This poster presents an overview of the MBMS-experiments used for the investigation of the combustion behavior of SAFs at DLR's Institute of Combustion Technology. Through our experiments, we aim to identify potential pollutants and their precursors, explore combustion reaction networks, and validate combustion models. Complementary experimental setups are used to provide diverse and conclusive information:

First, an atmospheric flow reactor with fixed boundary conditions allows for controlled and repeatable experiments. The investigated fuel enters the reactor premixed and highly diluted to avert heat release and self-sustaining reactions. The temperature profile (up to 1700K) and residence time are imposed boundary conditions. In-situ samples are taken directly out of the reactor flow and analyzed by a mass spectrometer to determine the mass-to-charge ratio of the present molecules [1].

The second experiment utilizes a high-pressure reactor that can achieve higher pressures than the atmospheric flow reactor, providing insights under more technical operating conditions. The third setup involves a flat-flame burner, which allows for the study of self-sustaining combustion processes at even higher temperatures compared to the flow reactors (~2000K) and the quantification of highly reactive species such as radicals [2].

To achieve a complete investigation and to answer fuel-specific questions, we utilize all experimental setups, in combination with photoionization. It enables the detection of highly reactive species such as radicals as well as isomer separation, which allows studying the effects of different molecular structures on the combustion behavior [3].

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Mixed metal (Mn, Al, Ti) cobalt oxide model systems for optimizing sustainable aviation fuel production via Fischer-Tropsch synthesis

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In the era of energy transition with the goal to lower greenhouse gas emissions and to overcome the impact on climate changes, the Power-to-Liquids (PtL) technology poses as a key potential solution, especially in the hard to abate aviation sector. Sustainable aviation fuel (SAF) may be produced through Fischer-Tropsch (FT) synthesis, the conversion of synthesis gas into long-chain hydrocarbons using cobalt-based FT catalysts. Recently, manganese promotion was demonstrated to efficiently increase the yield of SAF,[1] while modification of metal oxide supports allows for operation at high conversion levels in the FT synthesis.[2] Herein, model catalysts are prepared and characterized to study the isolated roles of support (modification) and manganese promotion regarding catalyst activity, selectivity, and stability during FT synthesis.
The efficiency of FT catalysts largely depends on the physico-chemical properties of the surface of the catalysts. Manganese promotion of cobalt-based FT catalysts may result in Mn^{2+} on the edge of manganese oxide structure, which interacts with adsorbed carbon monoxide species.[3] At a molar Mn:Co ratio of 0.15, the promotional effect of manganese on cobalt-based FT catalysts was amplified.[1] In general, deactivation of cobalt-based FT catalysts via formation of metal-support compounds (MSCs), such as cobalt titanate or aluminate, represents another challenge when operating at high conversation rates.[4,5] In the present study, we investigate the role of promotion on the formation of cobalt titanate or aluminate in cobalt FT model catalysts. Cobalt oxide and mixed cobalt oxide nanoparticles are prepared separately via the surfactant free benzyl alcohol route.[4] Subsequent deposition of these nanoparticles on various support materials yield model catalysts, which are thoroughly characterized to advance the development of efficient FT catalysts for SAF production.

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Multi-scale holistic approach at the BESSY II synchrotron light source for investigating Fischer-Tropsch catalysts

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The CARE-O-SENE project focuses on the optimization and development of knowledge driven Fischer-Tropsch (FT) catalysts to enable highly efficient production of sustainable aviation fuels. Within CARE-O-SENE, a unique, multi-scale combination of complementary imaging and spectroscopic tools for *ex-situ*, *in-system*, *in-situ*, and *operando* analysis of FT catalysts at the BESSY II Synchrotron Light Source is developed and used to guide the project's catalyst optimization. This holistic approach is demonstrated by exemplary results from cobalt-based catalysts characterized *in-system* with soft- and hard- X-ray photoelectron and absorption spectroscopies yielding chemical profile information and how they are affected by redox cycles without exposure to air. Extending this *in-system* approach, a dedicated FT reactor designed for achieving industrial FT conditions (20 bar at up to 500 °C), compatible with the vacuum conditions of the attached thin-film synthesis and spectroscopic soft and hard X-ray analysis is currently being set up. Near-ambient pressure X-ray photoelectron and absorption spectroscopy is further exploited to *in-situ* investigate the catalyst activation and catalyst-promoter interaction for thin-film model FT catalysts. Ultimately, thin-film model catalysts are also studied at reduced pressure conditions in H_2:CO:H_2O gas mixtures at 1 mbar. This multi-scale concept is also applied to imaging techniques, using a commercially relevant FT catalyst characterised by synchrotron tomography and scanning electron microscopy enabling 3D data analysis strategies using machine learning approaches to identify regions of interest for detailed focus ion beam (FIB) tomography. The selected examples showcase how electrons, soft- and hard X-rays probes combined provide insights on all relevant information depth and size scales, ultimately aiming at a complete (locally resolved) picture of the chemical, electronic, and geometric properties of FT catalysts to lay the foundation for deliberate catalyst optimization beyond the current state-of-the-art in terms of activity, selectivity, and stability.

Liquid fuel-based FLOX® burner development and spray characterization of various injectors

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The successful application of high momentum jet-stabilized combustors, based on the FLOX® burner concept, in gas turbines designed for gaseous fuel operation has demonstrated numerous benefits, such as increased fuel and load flexibility, reduced pollutant emissions, and improved resistance to combustion instabilities. Furthermore, with the growing significance of liquid fuels in energy conversion, research efforts have been underway to expand the use of jet-stabilized combustors to liquid fuel operation.

The current study introduces the recent development of FLOX® burners operating with liquid fuels and further focuses on spray characteristics depending on the injector geometry variation using optical diagnostic techniques. Firstly, characteristics of traditionally manufactured injectors and injection concepts were analyzed and compared, including pressure-swirl injectors, wall-impingement atomizers, and jet in crossflow concepts. Results indicated that the combination of a pressure-swirl injector and wall-impingement concept, called air-blast atomization, performs best for the combustor and is highly efficient. A combustion study was then conducted using this injection concept, yielding promising results under various experimental conditions.

Secondly, further investigation of the chosen injection concept is underway through varying injector geometry and employing optical diagnostic techniques. Shadowgraphy at varying magnifications is being used to observe spray behaviors, including spray cone angle and droplet size. Optical patternation is a powerful technique used to investigate droplet distribution on cross-sections that are perpendicular to the spray axis. Furthermore, the Scheimpflug rule was applied to the light source and detector alignment to optimize the focal plane on the cross-sections, and structured illumination was employed to minimize interference from multiple scattering, reducing the occurrence of false signals from droplets in the spray.

Direct activation of CO_2 to liquid fuels in Fischer-Tropsch Synthesis over iron catalyst

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Sustainable aviation fuels (SAF) are gaining popularity as an environmentally friendly alternative to conventional aviation fuels. Power-to-Liquid technology (PtL) has been used to produce SAF for a carbon-neutral mobility. PtL is a concept of producing liquid hydrocarbons based on electricity, water, and CO_2 as resources. H_2 is obtained by water electrolysis which is powered by renewable electricity. CO_2, which is captured from air, reacts with hydrogen to produce liquid hydrocarbons (Figure 1). Liquid hydrocarbons can be used as SAF after upgrading. This concept is important for the aviation sector as it relies on liquid fuels [1,2].

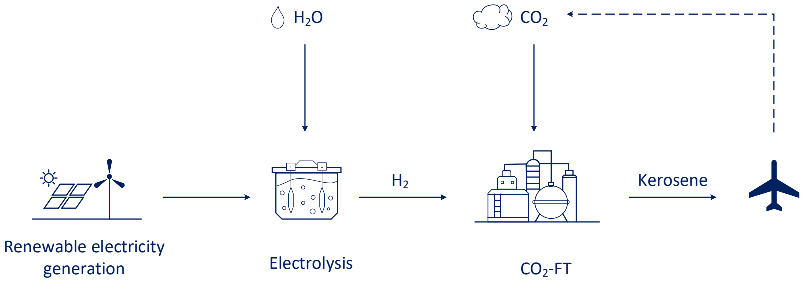

Figure 1. Power-to-Liquid concept [3] with direct hydrogenation of CO_2 in Fischer-Tropsch Synthesis.

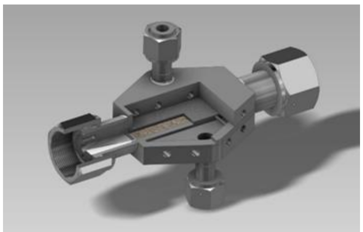

Figure 2. Microstructure reactor.

Liquid hydrocarbons can be produced by direct activation of CO_2 in Fischer-Tropsch synthesis (CO_2-FT). In our study, CO_2-FT takes place in a microstructure reactor which was manufactured and implemented into a new test bench at the Institute for Micro Process Engineering (Figure 2). The improvement of the process is to run Reverse water was shift (RWGS) and Fischer Tropsch (FT) synthesis in one reactor instead of two reactors in series. Iron is chosen as active phase for this catalytic reaction due to its activity for both, RWGS and FT reaction [4]. Catalysts were synthesized by flame spray pyrolysis method, which aims to produce Fe nanoparticles. In scope of this study, it is also aimed to work on under dynamic operation conditions and integrate the reactor into a load-flexible PtL concept.

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Reduced order modeling of turbocomponents for future short/medium range civil engines

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The adoption of Sustainable Air Fuels (SAFs) in aviation engines poses new challenges for the design and evaluation of performance and local pollutant emissions. While scientific research primarily focuses on the combustion section due to the direct influence of fuel substitution, changes in the composition and temperature of the reacting mixture bring about new design challenges for the expansion and compression sections.

To address these, machine learning and data-driven approaches are becoming increasingly significant. Models able to predict how modifications of the operating conditions will affect components and overall performance (inverse problems) are derived making use of data from high fidelity numerical simulations under known conditions.

Proper Orthogonal Decomposition (POD) is a classical data reduction technique able to identify dominant patterns and structures in a dataset. An innovative approach are Physics Informed Neural Networks (PINNs) that incorporate physical principles into a machine-learning infrastructure. The network makes it possible to derive intrinsic parameters and operators characterizing the system. These can be used to construct a data-driven Reduced Order Model of the engine components, to be integrated in a seamless engine prediction system.

The scientific challenges here described are part of the tasks of a new European project (MYTHOS: Medium-range hybrid low-pollution flexi-fuel/hydrogen sustainable engine) whose goal is to develop and demonstrate and innovative and disruptive design methodology for future short/medium range civil engines capable of using a wide range of liquid and gaseous fuels including SAFs and, ultimately, pure hydrogen.

The poster will present preliminary results of the ongoing work on high fidelity simulation of turbocomponents, demonstrating the capabilities of the numerical solver employed and data-reduction techniques, while summarizing the perspective results and goals of the tasks in the project.

Comprehensive two-dimensional gas chromatography for prescreening and optimization of sustainable fuels

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The first step in evaluating new sustainable aviation fuels (SAF) and assessing their climate impact is the investigation of the fuel´s composition. The two-dimensional gas chromatography (GCxGC), is a comprehensive and one of the most commonly used instrumental methodologies for this purpose.[1] It is capable to provide more detailed information for complex sample compositions than, for example, a linear GC. As a result, the GCxGC approach can even achieve the detection of small compositional changes caused by slight adjustments of synthesis parameters, and thus help in the design process of new SAFs as well. Depending on the respective fuel type and synthesis pathways, hundreds of different compounds may need to be separated and identified. This comprehensive data can then be further used to predict fuel properties using in-house prescreening models. Small volume samples can therefore provide quick and affordable feedback on whether novel SAFs might be suitable for practical application before they enter an extensive approval process (e. g. according to the ASTM D4054 standard).[2] However, in order to improve the available models, the identification precision must be improved as well. Currently, detected molecules are frequently assigned based on group types and, to a lesser extent, classified compound-by-compound. Nevertheless, as the carbon number increases, the complexity and possibilities of different isomeric structures grow exponentially. This leads to greater variability of properties which could result in increased model uncertainty and larger deviations between predicted and true fuel properties.[3] Therefore, the investigation into the individual identification of isomers is a crucial issue. This poster will present the current capabilities of GCxGC for fuel analysis while simultaneously emphasizing the improvements that are still needed.

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Contrail ice crystal reductions of large passenger aircraft burning 100% sustainable aviation fuel

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Contrail ice particles form on jet engine particle emissions and significantly contribute to the climate forcing of aviation and can even outweigh the climate impact of aviation's CO_2 emissions on the short time scale. The use of sustainable aviation fuels (SAF) is one proposed pathway to mitigate the climate impact of aviation. In addition to lower effective CO_2 emissions, lower amounts of soot-forming compounds and sulphate compounds are produced. This results in a possible reduction in contrail ice forming on emitted non-volatile particles and thereby a reduction in non-CO_2 climate forcing.

During formation flights conducted in April 2021 in a collaboration between AIRBUS, DLR, ROLLS-ROYCE and NESTE in the course of the ECLIF3 (Emission and Climate Impact of Alternative Fuels) project, 100% HEFA (Hydro-processed Esters and Fatty Acids) and Jet-A-1 as a reference fuel were burned at similar ambient conditions, engine conditions and altitudes by an Airbus A350-900 aircraft powered by Rolls-Royce Trent XWB-84 engines. Chasing the lead aircraft at cruise conditions, the DLR Falcon 20 research aircraft equipped with a comprehensive set of trace gas, aerosol, and ice particle instruments conducted in-situ contrail ice particle measurements of one- to two-minute old contrails. From these measurements we calculate apparent ice crystal emission indices and compare them for the respective fuels at supersaturated ambient conditions to exclude sublimation effects. In addition, particle size distributions of ice crystals are compared for the used fuels in a range of detection-to-emission altitude deltas.

This thorough analysis of contrail ice particle microphysics for the first time allows insights into the effects of burning 100% SAF on contrails, thereby facilitating the evaluation of the potential role of SAF in future climate-friendly aviation.

Efficient additive manufacturing reactor concept for the production of e-fuels: From 500 g of metal powder to 500 g of Fischer-Tropsch product

David Metzger, Prof. Dr.-Ing. Christoph Klahn,
Prof. habil. Dr.-Ing. Roland Dittmeyer

Additive manufacturing (AM), also known as 3D printing, enables us to produce process engineering devices, such as chemical reactors, with highly optimized functions in a matter of hours. The class of highly exothermal, heterogeneously catalyzed reactions of renewable H2 with CO/CO2 is important in terms of the energy transition. Reactors for these so-called Power-to-X (PtX) processes that are suitable for decentralized flexible operation are scarce and difficult to manufacture. A reactor for the production of renewable liquid fuels on the lab scale was additively manufactured and tested for Fischer-Tropsch reaction under industrially relevant conditions. It shows excellent temperature control and high productivity of raw renewable liquid fuels of up to P=3.3 g/h.

Additive manufacturing is suitable for PtX reactors operated under challenging conditions. Manufacturing of one lab-scale Fischer-Tropsch reactor takes approx. a day. It can comprise porous regions, as well as heating and sensing. The reactor concepts can be further improved and scaled up. They should be investigated with simulations and employed for other P2X reactions than Fischer-Tropsch synthesis.

CIRCULAIR – Coupling of advanced biofuel production via hydrothermal liquefaction with PtX

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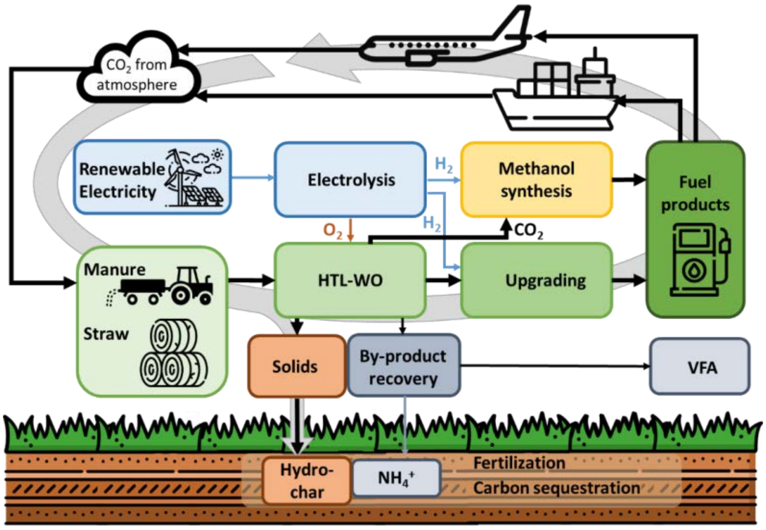
Advanced biofuels can play an important role in deep decarbonization of aviation, while also being cost-effective and drop-in capable. With these characteristics and a large production potential due to a high feedstock flexibility, one of the promising options to convert biomass into an intermediate fuel product, a so-called biocrude, is hydrothermal liquefaction (HTL). This biocrude can further be upgraded into jet fuel and other fuel products. HyFlexFuel [1], an EU Horizon 2020 project, was completed in 2021 and delivered groundbreaking research and innovations in HTL fuel production. Its follow-up project, CIRCULAIR [2], builds on the foundation of HyFlexFuel, and introduces additional improvements. In HyFlexFuel, it was found that hydrogen and HTL heat supply are the two main drivers of the Global Warming Potential of HTL fuel production. Both issues will be addressed in the CIRCULAIR project. HTL heat will be supplied by the exothermic wet oxidation of the HTL process water, which also presents a promising option to deal with the organic species in the process water, which was found to be the key technological bottleneck of HTL fuel production. Wet oxidation results in a gas phase, which can be combined with the HTL gas phase, both mainly consisting of CO_2. After purification, this CO_2 stream can be used in a Power-to-X scheme. This coupling of biofuel production with e-fuel production accelerates the need for green hydrogen supply, which will be investigated in the CIRCULAIR project. This contribution presents the novel approach to advanced biofuels, which promises large potential and introduces interesting challenges from a system analysis point of view.



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Investigating Non-CO2 effects from hydrogen engines: Overview and first impressions of the Blue Condor experiments

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The research on hydrogen as an alternative, CO_2 emission-free fuel is becoming a crucial topic in aviation. The EU's goal of CO_2 reduction in aviation until 2050 requires rapid development of H_2 fuel cells and combustion engines. However, non-CO_2 effects like nitrogen oxide emissions and contrails from these technologies have not been investigated thoroughly due to the lack of measurement data. In the Blue Condor campaign led by Airbus UpNext in cooperation with DLR, AV Experts and the Perlan Team an Arcus Glider equipped with a hydrogen jet engine will be followed by a Grob EGRETT at a distance of 50-500 m to measure emission and contrails at cruise conditions. We assembled a new autonomously working measurement system to determine non-volatile (nvPM) and total particle concentrations, nitrogen oxides (NO and NO_2), water vapor (H_2O), carbon dioxide (CO_2) emissions and characterize contrail ice crystals formed in the exhaust. We will provide an overview of the DLR measurement systems and the rationale behind it. In April 2022, first test flights were performed in Texas at FL 165 with the EGRETT and Perlan's Arcus glider equipped with a conventional kerosene engine (TJ 100). The measurement system was tested measuring inside the exhaust plume and in ambient conditions. We provide first results on aerosol emission indices and comment on the impact of lubricant oil and discuss the significance of the measurements for future larger engines on regional to short range aircraft. The Blue Condor measurements will be the first measurements of contrails from a hydrogen engine and are planned in autumn of 2023 in the northern United States to take advantage of ideal meteorological conditions for contrail formation.

Techno-economic analysis of a smart use of low-soot aviation fuels – options and cost

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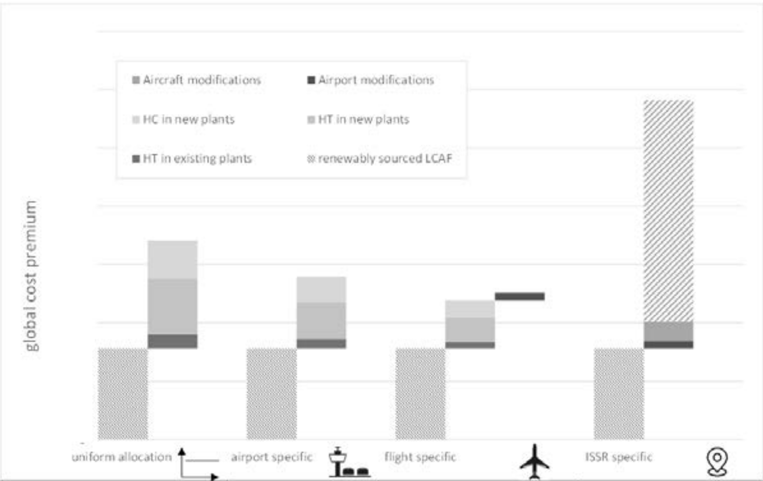
Renewably sourced aviation fuels ("SAF") can reduce GHG emissions by 50 %-90 % on a lifecycle basis. However, the aviation-induced climate impact is only partially caused by GHG emissions, a significant fraction can be attributed to contrail formation and NOx emissions, amongst others. The formation of contrails is substantially influenced by soot formation during combustion. It has been demonstrated that an increased hydrogen content, e.g., by using SAF or hydroprocessed fossil-based kerosene, can reduce soot formation. Studies have shown that between 2 % and 10 % of the flights cause almost 80 % of the contrail energy forcing. However, the market share of renewably sourced aviation fuels is presently far below 1 %, and requirements for hydroprocessing of fossil-based kerosene do not exist.

Against this background, using "low-soot" fuels exclusively where contrails form appears promising. However, this would require dedicated fuel supply chains, e.g., to accommodate two different fuel types at one airport. This study aims to assess the techno-economical feasibility of such concepts. Fuel production costs are derived for varying degrees of hydroprocessing severity and all major SAF production pathways, such as HEFA-SPK, FT-SPK, and AtJ-SPK. Fuel allocation concepts are assessed from a uniform distribution towards a dedicated use on particular flight segments by estimating associated costs and potential durations for their implementation. In comparison with market-ramp-up scenarios for such "low-soot fuels", the mitigation potential of various fuel allocation concepts is discussed. Hereby, this study aims to contribute towards the design of measures to effectively and swiftly reduce the overall climate impact of aviation.



share fossil based LCAF	90%	60%	40%	0%
share renewably sourced LCAF	10%	10%	10%	10%

Experimental investigation of soot emissions of oxygenated fuel blends in a small aero engine

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Recent investigations show that contrails, induced by high-altitude aircraft soot emissions, have a huge adverse environmental impact. At the same time, many studies concentrate on reducing aviation CO_2 footprint, but only a few account for reducing soot emissions in aero engines. In this study, Jet A-1 blends with 5 vol% polyoxymethylene dimethyl ether 3-5 mix (OME3-5) and 5 vol%, as well as 20 vol% Ethanol, are investigated for their impact on performance and soot emissions in an Allison 250-C20B turboshaft engine with the help of a condensation particle counter (CPC).

Besides the beneficial environmental effect of carbon-neutral drop-in fuels regarding the CO2 balance, fuels with no aromatic content but containing oxygen – known as oxygenated fuels – offer the possibility of particle emission reduction already at low blend ratios. OME3-5 is a promising candidate since most of its physical and chemical properties are close to Jet A-1. While the characteristics of Ethanol are further away from jet fuel requirements, small blend ratios are still possible. Ethanol could be delivered to the airline industry for economical prices right away since large production capacities are already available.

The two oxygenates are investigated regarding their suitability as blending fuels for gas turbines. The tests are performed on an Allison 250 C20B engine, which features additional measurement equipment to calculate engine performance parameters. An attached eddy-current brake dissipates the power output of the engine. A MEXA-2100SPCS series particle counter fabricated by Horiba with a measurement resolution down to 10nm is used for the soot emission analysis. The results recorded show a percental soot particle concentration reduction which, in most cases, is significantly larger than the volumetric percentage of the oxygenated fuel within the blend. OME offers the best mean particle concentration reduction effect with a relative reduction three times as high as its volumetric blend-in ratio. This correlation between oxygenated fuel blends and soot emission decrease, already at small blend ratios, makes them suitable for an immediate reduction of the aviation industry's climate impact.

Modeling and analysis of the regional production potential of sustainable aviation fuel in Bavaria

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To combat climate change, completely new challenges are arising for industrial locations in Germany. This is particularly true for the chemical industry and traditional chemical sites such as the Bavarian Chemical Triangle. The goal of the collaborative research project “H2 Reallabor Burghausen / ChemDelta Bavaria” is to transform the Bavarian Chemical Triangle, including its refinery sites.

The H2-Reallabor develops a holistic solution for a transformation strategy regarding the future energy supply and in particular concepts for the transformation of different production paths.

The activities planned by Bauhaus Luftfahrt focus on identifying the potential and integrating sustainable aviation fuels into the Bavarian energy system. The goal here is to evaluate the production potential for Sustainable Aviation Fuel (SAF) in Bavaria, where the integration into the existing refinery infrastructure in Burghausen, which has a pipeline connection to Munich Airport, serves as a reference case.

For this purpose, biogenic feedstock and renewable electricity supply will be assessed, various fuel conversion pathways will be modeled and the factors necessary for site optimization will be analyzed. The results will be incorporated into the development of a roadmap for the sustainable transformation process of the chemical industry in Bavaria and Germany.

Photonic synthetic gas production as a feedstock for aviation fuels

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For the production of carbon-based liquid fuels, synthetic gas (i.e., a mixture of hydrogen and carbon monoxide) is required as a building block. Currently, synthetic gas is predominantly produced by steam reforming or partial oxidation of fossil fuels. However, to become sustainable, the synthetic gas must be produced from biogenic or carbon dioxide captured from the air. This can be achieved for example electrochemically employing steam via co-electrolysis or via the reverse water gas shift reaction using green hydrogen. Nevertheless, such approaches still have a low technology-readiness level. In a future, fossil free energy system, a large fraction of the energy is likely to stem from solar resources. Furthermore, solar power can be used directly to provide heat for the endothermic reverse water gas shift reaction for synthetic gas production. To reduce the required temperature level, efficient catalysts are necessary. Recently developed plasmonic catalysts can absorb a large fraction of the solar spectrum and were demonstrated to have a high selectivity towards carbon monoxide production[1]. Consequently, systems based on this type of catalysts are promising in terms of efficiency and land use. In the EU co-funded project SPOTLIGHT, such a system is currently implemented and analyzed. The system comprises of a transparent flow reactor holding the powdery plasmonic catalyst and a concentrating solar system including a flux guide that illuminates the reactor homogeneously with a flux density of up to 20 kW/m². The concept shows one potential process for the future feedstock of sustainable liquid aviation fuels.

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Detailed gaseous and particulate emissions of an Allison 250-C20B turboshaft engine

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Aviation is known to be one of the most significant contributors to air pollutants. This includes gaseous emissions, like carbon-dioxide (CO2) and nitrogen oxides (NOx), and also particulate matter (PM), especially in the form of soot. The University of the Bundeswehr Munich and Technical University Munich conducted emission measurements on an Allison 250-C20B turboshaft engine operating on Jet A-1 fuel with a focus on gaseous compounds (e.g. ozone precursors) and PM, regarding their number and mass concentration. The different engine loading points were chosen based on the percentage thrust ratios of the International Civil Aviation Organization (ICAO) Landing and Take-Off-Cycle (LTO-Cycle). A standard FTIR/O2/FID system to measure general combustion compounds e.g. CO2, carbon monoxide (CO), unburned hydrocarbons (UHC), and NOx, was used for the gaseous measurements. For the investigation of the volatile organic compounds (VOC), which are known to act as ozone precursors, a gas-chromatograph (GC) was applied. Different measurement methods were used to characterize the PM emissions. For the particle size distribution (PSD), we used two types of electrical mobility analyzers (SMPS and DMS500) and an aerodynamic aerosol classifier (AAC). All measurement systems yielded comparable PSD results, indicating reliable results. The particle measurement methods all show increasing aerosol diameter modes (electrical and aerodynamic) with increased engine loading. The aerosol diameter modes were shifting from 29nm to 65nm. Furthermore, the size and shape of different individual particles were evaluated with a scanning electron microscope (SEM). In addition, a correlation between the injection system and the particle formation was established. Gaseous turboshaft engine emissions show high CO and UHC values in Ground Idle (GI) level. NOx levels were the highest at Take-Off (TO) conditions. Acetylene and ethylene were the most significant contributors to ozone formation. Measurements will be repeated this year with other fuels (including SAF and various blends) with the identical setup and the performance and emissions will be investigated as a function of the fuel properties.

Cost Optimal Design of Solar E-Methanol Production Powered by CSP/PV Hybrid Power Plants

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Global trade of renewable hydrogen derivatives could become a key factor in reducing global greenhouse gas emissions. Methanol, a versatile chemical building block, is one of the most promising hydrogen carriers in this context [1]. If produced with hydrogen and CO_2 from a sustainable source, methanol could be used, for example, to produce sustainable aviation fuel (SAF) through the Methanol-to-Jet fuel process [2]. Due to the enormous potential of solar energy and the availability of unused land, the Earth's sunbelt could become a major producer of green hydrogen and thus an exporter of renewable e-methanol [3]. However, producing hydrogen derivatives such as e-methanol cost-efficiently using solar energy is challenging. Low electricity costs can be achieved by using photovoltaics (PV), but the availability of the electricity source is limited to daytime, and depending on the solar irradiation the supply can fluctuate. To reach more electrolyser full-load hours and to ensure the required minimum electricity demand of the plant, a stand-alone system without grid connection needs some kind of storage solution. Combining PV with concentrated solar power (CSP) and thermal energy storage (TES) seems to be a good way to meet these requirements at sites with high solar irradiation. In the absence of solar radiation, stored thermal energy can be used to generate electricity in a steam cycle, allowing very continuous operation of the electrolyser and the overall plant [4]. These hybrid solar energy systems for synthetic fuel production offer a wide range of operating modes and plant configurations. Therefore, this work introduces an energy system model for e-methanol production powered by CSP/PV hybrid power plants. Based on included techno-economic data, the model is able to determine cost-optimal designs of such solar e-methanol production plants based on a global optimization algorithm. The optimized plant designs are presented and compared to plant configurations without hybridization of CSP and PV.

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In situ measurements of contrail ice crystals of a modern passenger airplane burning sustainable aviation fuels

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One of aviation's major climate impacts is the radiative forcing of contrails and contrail cirrus. It is therefore crucial to investigate the parameters influencing their formation and their microphysics in order to understand aviation's climate impact reduction potential on a short time scale. The use of sustainable aviation fuels (SAF) is currently tested in order to reduce aviation's direct carbon footprint. However, it remains uncertain how these SAFs influence the contrail formation and thus, the main driver of aviation's climate impact.

In this study, number concentrations and particle sizes of contrail ice particles from in-flight measurements originating from the burning of different SAFs with varying aromatic and sulphur content and conventional Jet-A1 are evaluated. Contrail ice microphysical properties were measured with a Cloud and Aerosol Spectrometer (CAS) instrument mounted to the DLR Falcon research aircraft, chasing a modern Airbus A321neo aircraft during the VOLCAN campaign. The flights were performed at cruising conditions with ice supersaturated ambient atmosphere to generate comparable datasets.

From the measured data, apparent ice crystal emission indices (AEI) are calculated. The SAF's are then compared to the conventional Jet-A1 regarding their contrail properties in light of the fuels' sulphur content, aromatic compound and overall chemical composition. The findings aim to contribute to a deeper understanding of SAF's impact on aviation's non-CO_2 effects which is a key component on the way towards a sustainable future aviation.

The influence of biomass characteristics and their uncertainties on the production of sustainable aviation fuel

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Sustainable aviation fuel (SAF) is crucial for the decarbonization of the aviation industry. There are different pathways to produce SAF with properties similar to those of conventional jet fuel. A comparative study between the different pathways was performed to determine the optimum route for SAF production through biomass. Gasification of biomass was opted as an optimum route where the biomass is gasified to produce a syngas which is then upgraded to produce SAF. In this study, a model was created to assess the impact of using various biomass sources on SAF yield. Additionally, how the measurement uncertainty of the biomass characteristics affects the efficiency of the process. The outcome from the simulation will be presented in the poster.

Computational investigation of the Co-support interfaces on γ-Al_2O_3, SiO_2 and TiO_2

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Despite its history spans over almost a century, the Fischer-Tropsch process has recently gained renewed interest from the scientific community in light of its potential to speed-up the energy transition. In fact, by converting syngas into a wide variety of hydrocarbon products, this technology makes it possible to produce fundamental chemical commodities from renewable feedstocks.

Supported cobalt catalysts are particularly suitable for the Fischer-Tropsch synthesis as they showcase high activity under mild process conditions, with operating temperatures usually not exceeding 493 K. The interactions between Co and the support prominently affect the performance of the catalyst, as they largely control Co dispersion and reducibility [1]. Nonetheless, due to the complexity of these systems, it is often arduous to univocally resolve the nature of the metal-support interactions based solely on experimental observations, and, as a result, a consensus on the phenomena governing the formation of the Co-support interfaces is largely missing.

In this work, DFT calculations at the GGA+U level of theory were employed to gain molecular understanding of the conformation of the interfaces between Co and three of the most widely employed supports, namely γ-Al_2O_3, SiO_2 and TiO_2. It was found that, while TiO_2 displays reasonable chemical affinity with metallic cobalt, for SiO_2 and especially γ-Al_2O_3 the existence of an intermediate oxidic layer that glues together Co^0 and the support must be postulated to explain the adhesion between the two materials. On alumina, this intermediate layer can form readily and ensures strong adhesion of Co^0 everywhere on the support, promoting high cobalt dispersion. On SiO_2, the formation of the oxidic glue is less favored and is expected to strongly depend on the synthesis procedure; additionally, strong adhesion is only possible on specific anchoring sites with low concentration of surface silanols such as defects.

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eXplore: A decentralized modular plant for Fischer Tropsch synthesis and upgrading to eKerosene for field demonstration in H2Mare

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From the past few decades, the greenhouse gas emissions has been a key issue facing by our planet as it results in severe climate changes and human activities are largely responsible for it. Simultaneously, human beings play a vital role in maintaining the ecological balance to attain the *Sustainable development*. Since the last 40 years, CO2 emissions per year doubled from 16 Gt in 1973 to 32 Gt in 2012 [1], leading to increase in the CO2 concentration in the atmosphere from 280 ppm to 400 ppm. The transport sector being globally responsible for about 23% of anthropogenic CO2 emissions, the entire dependency on carbon intensive fossil fuels is considered as the central issue. To address this, the transition towards renewable fuels, Power-to-Liquid technologies offer a promising path, complementing the electrification of vehicles. Several mobility sectors such as aviation and maritime transportation call for high energy density, which rules out the use of batteries. Therefore, the synthesis of liquid fuels from CO2 extracted from the atmosphere via Direct Air Capture and H2 from renewables, i.e., water electrolysis, is a concept, which is increasingly coming into focus. It consists of two steps, syngas production via reverse water-gas shift (RWGS) and synfuel production by Fischer-Tropsch synthesis.

In this context, this transition needs a massive change of technologies and infrastructures for energy supply and industrial production. Along with the conventional technologies for large-scale plants, intensified technologies for decentralized plants are considered as they enable decentralized applications such as remote or offshore solutions. One of such modular plants is the eXplore container plant. It is a compact transportable offshore research platform for electrically generated, low emission synthetic fuels at Energy Lab 2.0 in KIT. With the aim of enabling load-flexible PtX plants, modular microstructured reactors were developed at the Institute for Micro Process Engineering (KIT IMVT) over the past 5 years for both Fischer-Tropsch synthesis and methanation from lab-scale devices to prototypes for demonstration. The presentation highlights the overview of the development status and the perspectives of compact decentralized PtL processes based on Fischer-Tropsch synthesis.

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Solar fuel production via thermochemical cycles: Process and receiver-reactor technology

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Solar fuels such as hydrogen, syngas and drop-in fuels pose a sustainable alternative to fossil fuels and represent a promising pathway for achieving deep-decarbonization not only in the transport sector but also in the industry and energy sectors. To produce these renewable energy carriers, solar thermochemical processes are favoured due to their high theoretical efficiency potential and lack of intermediate electricity generation. Of special interest are two-step thermochemical cycles based on metal oxide redox pair systems, which utilize concentrated solar irradiation, water and/or carbon dioxide to produce hydrogen, carbon monoxide or syngas. The syngas produced can be subsequently processed using the already established Fischer-Tropsch synthesis to produce drop-in fuels, such as kerosene. To obtain a carbon neutral solar fuel, the CO_2 feedstock can originate from direct air capture.

The conference poster will introduce the concept of solar thermochemical fuel production with a focus on kerosene. Initially the current state-of-the-art reactor technology, which has been demonstrated in the SUN-to-LIQUID project in 2019, will be reviewed including remarks on operating conditions and experimental results [1]. Next, the novel R2Mx receiver-reactor concept, which promises a significantly higher solar-to-fuel energy efficiency potential, will be introduced [2]. Insights into the laboratory scale proof-of-concept, which is currently under development at the DLR, and other projects aiming to scale-up the technology will be given.

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SynergyFuels – An integrated refinery concept for the production of SAFs

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The Paris Climate Agreement led to an increase in renewable energy production and the European Union's Green Deal aims to achieve climate neutrality by 2050. A significant aspect of the Green Deal is the substitution of fossil-based energy carriers for mobility and transportation. One important strategy for the defossilization of the transportation sector is the utilization of CO_2 and other bio-based carbon feedstocks. Recently, a research project started that focuses on the utilization of different renewable resources for the production of synthetic fuels. 'SynergyFuels' combines processes for producing alcohols as platform chemicals and their consecutive conversion to synthetic fuels and fuel additives in an integrated refinery concept.

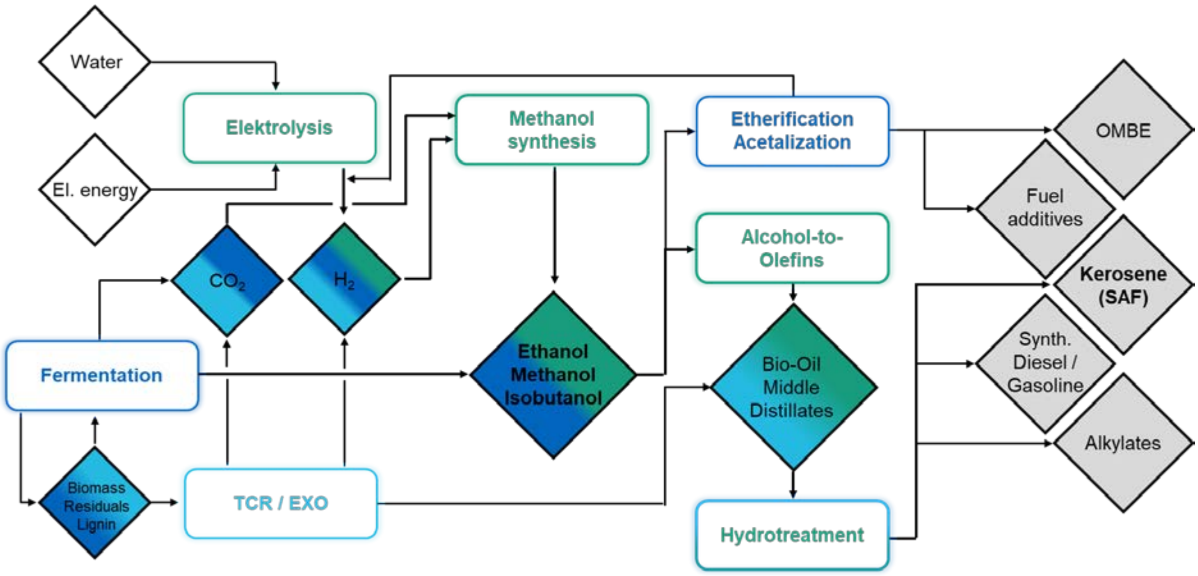

Figure 1: SynergyFuels concept of an integrated refinery. The key intermediates are alcohols obtained by CO_2 hydrogenation or fermentation processes. These alcohols are converted catalytically to olefins and subsequently are oligomerized to fuel pre-cursors.

This work aims to develop processes to produce synthetic aviation fuels by converting alcohol intermediates into light olefins through etherification, consecutive reactions, and dehydration. One way to produce light olefins like ethylene and propylene is by converting CO_2-derived CH_3OH through hydrogenation. Another method involves dehydrating C_2H_5OH or a mixture of methanol and ethanol. The light olefins are then converted into middle distillate range olefins and hydrogenated into fuel products. The goal is to scale up from small lab to pilot scale and establish a refinery process.

'SynergyFuels' is funded by Bundesministerium für Digitales und Verkehr

Processing biogenically produced intermediates to jet fuel – Technical comparison

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Sustainable aviation fuels (SAF) can already be produced today from various biogenic and non-biogenic feedstocks by biochemical or thermochemical processes or a combination of these. In contrast to non-biogenic fuels, biogenically produced fuels and energy carriers are already being produced today in large quantities and used as an energy source. In addition to hydrogenated ester and fatty acid (HEFA)-based SAF, these include biogas and bioethanol, which are used today in particular in heat generation, electricity generation or road transport. In addition, there are other biogenically produced intermediates, such as 2,3-butanediol, which can be used to produce an SAF.

Against this background, a comparison of different SAF production routes based on the current industrially available products biogas and bioethanol, as well as a possible production of 2,3-butanediol to SAF with technical key figures will be evaluated against each other. The goal is to focus on processes with a maximization of the carbon yield without considering CO_2 reduction with hydrogen and thus a combined biological and non-biological process. Thus, the installation of large amounts of renewable power generation is not required explicitly for SAF production and a potentially faster availability of larger SAF quantities could be achieved. To achieve this goal, the first processes are designed on the basis of a detailed literature research and evaluated with regard to their carbon efficiency. In the process route based on biogas as feedstock, carbon activation must first be achieved by reformation. The resulting synthesis gas can be further processed via the methanol or the Fischer-Tropsch pathway. Since the methanol intermediate is already available on an industrial scale - albeit from fossil sources - the methanol process route is considered, since this results in an independence of the various process steps. The alcohol-to-jet process designs and concepts are then analyzed for the ethanol and for the intermediate product methanol process route.

The project received EU funding from the European Climate, Infrastructure and Environment Executive Agency (CINEA) under the Grant Nº 101084336. The CINEA receives support from the European Union's Horizon Europe research and innovation programme

Funded by the European Union

Revealing the deactivation mechanisms of Co-based catalysts in Fischer-Tropsch synthesis by *operando* X-ray absorption spectroscopy

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Supported Co-based catalysts have been well studied in the past decades and now are widely used in the large-scale Fischer-Tropsch synthesis (FTS), in particular for sustainable aviation fuels (SAF) production[1-3]. The Co-based catalysts, however, suffer from deactivation under harsh reaction conditions and the deactivation mechanisms are up to now still unclear due to the difficulties in monitoring structural changes of active sites under real reaction conditions. X-ray absorption spectroscopy (XAS) is a powerful technique to get insights into the oxidation states and local structures of active sites as it can be applied for the measurements at high temperatures and pressures through a reasonable design of *in-situ* reaction cells. For this purposes, a dedicated *operando* reactor system has been recently developed at the CAT-ACT beamline at KIT Light Source[4] that allows an operation close to the industrially relevant FTS conditions[5].

The recent studies in revealing the deactivation mechanisms of Co-based catalysts using XAS can be summarized as following: the catalyst deactivates as the number of catalytically active sites decreases under the low temperature syngas flow due to different processes under different time scales. Many pioneers have reported[6-8] that (i) sintering of Co nanoparticles (NPs); (ii) solid state reaction of Co NPs and supports; (iii) coke or wax depositions and (iv) oxidation of Co NPs during long-term tests are the main reasons for the catalyst deactivation. For instance, through a careful evaluation of X-ray absorption near edge spectra and Fourier transformed extended X-ray absorption fine structure data on commercially representative Co-Ni-Re/γ-Al_2O_3-FTS-catalysts, the coordination number(CN) of Co-Co was found to be increased, hinting to the fast sintering, and $CoAl_2O_4$ and CoC_2 phase were formed during long-term FTS operation tests[4]. The catalytically active sites, i.e., metallic Co sites, could also be oxidized to CoO_x in the presence of water, which is irreversible in FTs. These processes need to be studied in detail on commercially relevant catalysts and on model structures and will support new energy-related initiatives in Germany, like the CARE-O-SENE project[9], a research collaboration focused on the production of SAFs.

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