



HAL
open science

From CO₂ and H₂ to Sustainable Aviation Fuel – TAKE-OFF

Peter Moser, Knut Stahl, Sandra Schmidt, Georgiana Stan, Lawien Zubeir, Mark van der Veek, Jan-Willem Könemann, Andrei Khodakov, Mathieu Sauthier, Nicolas Merle, et al.

► **To cite this version:**

Peter Moser, Knut Stahl, Sandra Schmidt, Georgiana Stan, Lawien Zubeir, et al.. From CO₂ and H₂ to Sustainable Aviation Fuel – TAKE-OFF. 17th Greenhouse Gas Control Technologies Conference (GHGT-17), Oct 2024, Calgary, Canada. <10.2139/ssrn.5016154>. <hal-05578955>

HAL Id: hal-05578955

<https://lilloa.hal.science/hal-05578955v1>

Submitted on 3 Apr 2026

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Distributed under a Creative Commons CC BY-NC-ND 4.0 - Attribution - Non-commercial use - No Derivative Works - International License



17th International Conference on Greenhouse Gas Control Technologies, GHGT-17

20th -24th October 2024 Calgary, Canada

From CO₂ and H₂ to sustainable aviation fuel - TAKE-OFF

Peter Moser^{a,*}, Knut Stahl^a, Sandra Schmidt^a, Georgiana Stan^b, Lawien Zubeir^b, Mark van der Veek^b, Jan-Willem Könemann^b, Andrei Khodakov^c, Mathieu Sauthier^c, Nicolas Merle^c, Vitaly Ordonsky^c, Massimo Corda^c, Samy Aissiou^c, Isah Abdulrahman^c, Morten Birkved^d, Benyamin Khoshnevisan^d, Hadis Marami^d, Tanja Weirich^e, Dzenan Causevic^e, Hiroyuki Arai^f, Tomoyuki Ishikawa^f, Eva van Mastbergen^g, Dusita de Hoop^g, Ntarinai Konosidou^h, Malte Döntgen^h, Max Mallyⁱ, Antonio La Mantia^j, Lara Tottolo^j

^aRWE Power AG, Altenessener Strasse 32, Essen, Germany

^bTNO, Leeghwaterstraat 44, Delft, The Netherlands

^cUnité de catalyse et chimie du solide (UMR 8181 CNRS, Ecole Centrale de Lille, Cité scientifique CS 20048, Villeneuve d'Ascq Cedex, France

^dUniversity of Southern Denmark, The Faculty of Engineering, Campusvej 55, Odense M, Denmark

^eMitsubishi Power Europe GmbH, Schifferstraße 80, Duisburg, Germany

^fAsahi Kasei Europe GmbH, Fringsstrasse 17, Düsseldorf, Germany

^gSkyNRG, Paradijsplein 1, Amsterdam, The Netherlands

^hRWTH Aachen University, Chair of Thermodynamics of Mobile Energy Conversion Systems, and High Pressure Gas Dynamics, Forckenbeckstraße 4, Aachen, Germany

ⁱFEV Europe GmbH, Neuenhofstraße 181, Aachen, Germany

^jCO₂ Value Europe, Ave. de Tervueren 188A, Brussels, Belgium

Abstract

Sustainable aviation fuel (SAF) is technological, economical, and – in terms of the time demand for implementation – temporal, essential for the aviation industry to meet the net zero GHG target. As a “drop-in” fuel SAF allows to use the existing aircraft fleet and fuel infrastructure. When produced from renewable feedstocks SAF can offer a lower carbon footprint than fossil-based aviation fuels through their entire life cycle. Additionally, it is substituting fossil-based kerosene, including its upstream production chain – oil extraction, and refining processes. The climate effect is maximised when a renewable power-based *e*-Fuel is produced from green power, green hydrogen, and green CO₂. Launched in 2021, the EU project TAKE-OFF (Production of synthetic renewable aviation fuel from CO₂ and H₂) has demonstrated and evaluated all parts of the thermo-chemical Power-to-SAF production chain with pilot plant testing, laboratory work, technical, economic, and environmental analysis. The TAKE-OFF route consists of capturing CO₂ from industrial flue gas or air, which reacts with hydrogen produced by electrolysis to create directly light olefins, or indirectly via the intermediates methanol and dimethyl ether. The light olefins are subsequently chemically upgraded into SAF with innovative catalysts to target a higher energy efficiency and a better carbon conversion rate for jet fuel product than the current benchmark, i.e. the Fischer-Tropsch process. The physical, chemical, and combustion properties of the produced SAF samples have been studied in detail to evaluate the readiness of TAKE-OFF products for use in aviation.

Keywords: SAF, CCU, closed carbon cycle, CESAR1, alkaline electrolysis, LCA, TEEA, methanol, DME, olefins, Fischer-Tropsch, aviation

* Corresponding author. E-mail address: peter.moser@rwe.com

Nomenclature

CFD	Computational Fluid Dynamics
DME	dimethyl ether, CH_3OCH_3
DTO	Dimethyl ether-to-Olefine
FT	Fischer-Tropsch
GHG	Green House Gas
HEFA	Hydrotreated Esters and Fatty Acids
HVO	Hydrotreated Vegetable Oils
LASA	low acidity silica-alumina
MeOH	methanol, CH_3OH
MTO	Methanol-to-Olefins
RFNBO	Renewable Fuels of Non-Biological Origin
rWGS	reverse Water Gas Shift
SAF	Sustainable Aviation Fuel
SAPO	silicoaluminophosphate zeolite
SOMC	surface organometallic chemistry
WHSV	Weight hourly space velocity
ZSM-5	Zeolite Socony Mobil-5, aluminosilicate zeolite belonging to the pentasil family of zeolites

1. Introduction

To achieve a world with net zero GHG emissions, societies, economic systems, and all sectors must contribute. Aviation is a growing industry in Europe, for which it is essential to drastically reduce overall CO_2 and other greenhouse gas emissions. In the EU in 2021, direct emissions from aviation accounted for 13.4% of the GHG emissions of the transport sector [1], see Fig 1 (left). There are only a limited number of options available for sustainable climate-friendly aviation, as solutions such as hydrogen, electric propulsion using batteries and wind/solar energy, or lower (C_1 - C_8) hydrocarbon fuels do not provide the right energy density and other physical/chemical properties to fly airplanes. According to the European legislation for the introduction of a quota for Sustainable Aviation Fuel (SAF), the demand for SAF in the EU and UK together is expected to increase to 50 Mt by 2050 [2], see Fig. 2 (right). The quota for SAF will increase to 70% by 2050 and starts with 2% of total aviation fuel in 2025. The projected demand for SAF in Europe is very high [2], see Figure 1. This is driven by regulatory developments such as ReFuelEU, Aviation in the EU, the UK mandate, but also voluntary uptake in the US supported by incentives.

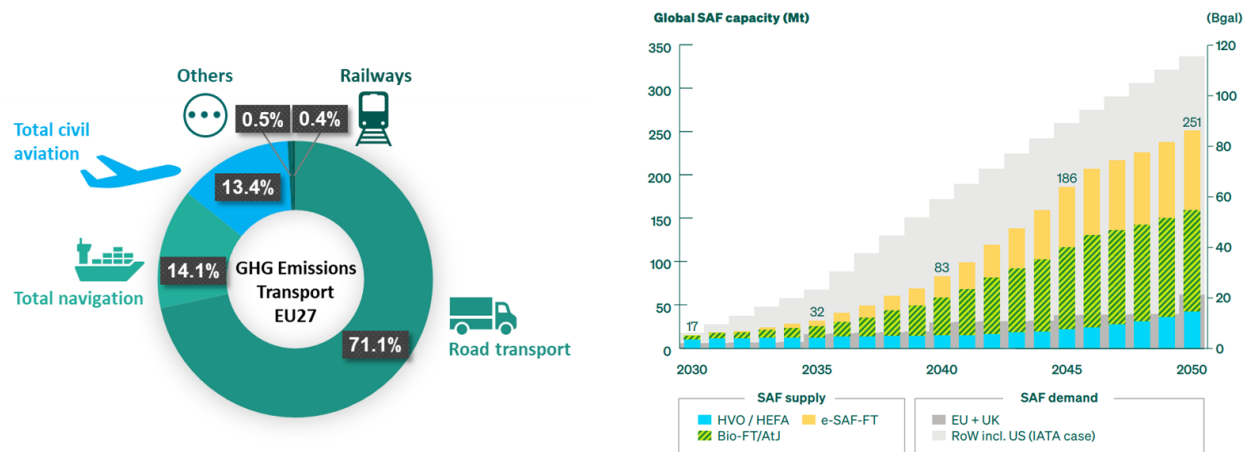


Fig. 1. Left – Civil aviation was responsible for 13.4% of the total GHG emissions of the EU27 in 2021 [1]. Right – Expected global SAF capacity ramp up until 2050 based on rapid technology deployment and feedstock constraints [2].

SAF is today mainly produced from used cooking oil and animal fats, commonly referred to as Hydrotreated Esters and Fatty Acids (HEFA) or Hydrotreated Vegetable Oils (HVO). However, due to a cap on the amount of waste oil permitted for the production of HVO/HEFA and the limited availability of this feedstock as source for SAF, the work on alternative pathways such as alcohol-to-jet, gasification plus Fischer-Tropsch, and power-to-liquid (*e*-fuels) has strongly ramped-up. The quota for synthetic SAF, which means SAF based on Renewable Fuels of Non-Biological Origin (RFNBO), will increase to 35% by 2050 and starts with 0.7% in 2030 in the EU [3,4].

One of the existing and certified routes towards SAF is the production of synthesis gas from CO₂ and renewable H₂ by a reverse water gas shift (rWGS) followed by Fischer-Tropsch (FT) synthesis and hydro-cracking of the FT crude product. The FT route is the benchmark for the evaluation of the performance of the direct and indirect routes investigated in TAKE-OFF. The state-of-the-art Fischer-Tropsch process creates a wide range of carbon products from C₂ to C₃₀₊, typically providing an overall selectivity towards the desired jet fuel C₈-C₁₆ fraction in the range of 45%. In the future it is expected that optimized FT synthesis with a higher SAF selectivity might achieve 60-70% SAF. Noteworthy, when the FT synthesis is operated with renewable H₂ and biogenic CO₂, also the side products diesel, gasoline, and gaseous fractions of light hydrocarbons from the hydro-cracking are sustainable fuels and feedstock. However, due to the progressive transformation of the transport sector by direct electrification and indirect electrification by *e*-fuels like methanol, demand and value of the FT-based side-products might shrink. This implies that the share of the most valuable SAF product should be maximized.

The European project TAKE-OFF (Horizon 2020, project no. 101006799) has developed and demonstrated next-generation technology for the production of SAF from green H₂ and preferably biogenic CO₂ or CO₂ from direct air capture [5]. The synthesized SAF was characterized regarding physical and emission properties and an integrated assessment (technical, economic and environmental analysis) was carried out for the technology pathways.

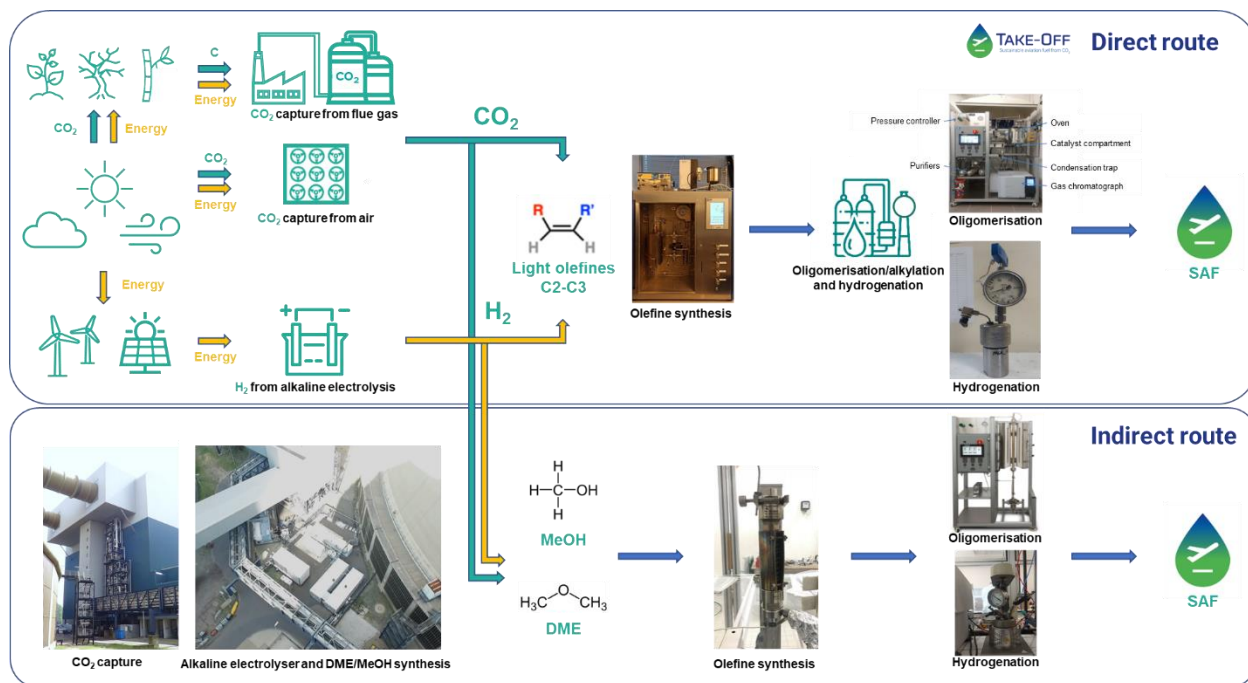


Fig. 2. Investigated synthesis routes in TAKE-OFF: Production of sustainable aviation fuel (SAF) by oligomerisation of light olefins, which are produced from hydrogen and captured CO₂ (direct route) or from the intermediates methanol (MeOH) or dimethyl ether (DME) (indirect route).

TAKE-OFF has investigated two technology chains which consist of two main steps, namely the direct conversion of CO₂ and H₂ to light olefins and the conversion of the olefins to jet fuel (direct route). In the second, alternative route, the olefins are synthesized via a more established intermediate process step from methanol (MeOH) and

dimethyl ether (DME) (indirect route), see Fig. 2. Both routes allow to reduce the formation of the side product methane which is formed in the Fischer-Tropsch synthesis. Additionally, the fraction of the hydrocarbons of the right size for SAF (C₈-C₁₆) can be increased, since the very broad size distribution of the Fischer-Tropsch products (Anderson-Schulz-Flory distribution) does not occur. In both TAKE-OFF routes the intermediate product methanol is formed which is transformed into olefins. Today the Methanol-to-Olefins (MTO) process is the only industrialized technology for the production of light olefins from non-oil feedstocks [6].

Direct route: In TAKE-OFF the optimized oxide/zeolite-based bifunctional catalysts ZnZrO_x/SAPO-34 was used for the direct conversion of CO₂ and H₂ into light olefins with improved selectivity towards light olefins (ethylene and propylene) and minimization of methane formation. The bifunctional catalyst combines the MeOH synthesis function (of the metal oxides ZnZrO_x) and the methanol-to-olefins function (of the zeolite SAPO-34). To further improve the carbon efficiency, the option to recycle the co-produced CO was investigated and process parameters were varied. For the selective oligomerisation of ethylene and propylene to the C₈-C₁₆ hydrocarbon mix of the jet fuel and a high branching content in the aliphatic structure of the oligomers (which is important related to the freezing point of the fuel), a catalyst with an activity higher than the current state-of-the-art heterogeneous systems was needed. The developed catalyst especially had to overcome the drawback of homogeneous zircon-based pre-catalysts activated with methylaluminoxane which just marginally incorporate higher olefins such as propylene and prevent the use of a feed containing oxygenated contaminants due to the highly sensitive metals. Therefore, a nickel-based catalyst was selected as starting point for the oligomerization of light olefins (Ni²⁺ supported on ion-exchanged low acidity silica-alumina (Ni²⁺/LASA)). This particular catalyst was tested due to its ease of preparation and stability. In [7] it was shown that the total conversion of ethylene and a high (91%) conversion of propylene was possible with nickel catalysts obtained by ion-exchange on silica-alumina at a pressure of 35 bar, at around 120 °C, but even lower system pressure is possible which is beneficial to incorporate higher amounts of propylene into the hydrocarbon chains, and subsequently to increase the amount of branched products. To optimise the performance of the supported nickel catalysts (isolation of nickel sites, coordination number, oxidation states) well-defined, single-site nickel catalysts were synthesised by surface organometallic chemistry (SOMC) grafting organometallic fragments by reaction of a selected organometallic precursor with residual hydroxyl groups of an oxide surface such as silica, alumina or silica-alumina. Finally, the oligomers are hydrogenated and distilled to the product SAF.

Indirect route: CO₂ conversion to light olefins via the intermediate product MeOH can be performed in two different ways. The more conventional approach is a two-step process in which at first the CO₂ conversion to MeOH is performed in a reactor, using a catalyst like the commercial CuOZnO-Al₂O₃ one [8], and then the MTO reaction is performed in a second reactor, using as catalysts zeolites, e.g. SAPO-34 and ZSM-5. In TAKE-OFF an already existing demonstrator for the one-step synthesis of dimethyl ether (DME) from captured CO₂ and H₂ based on a bifunctional catalyst (a metal oxide like CuO or ZnO catalyses the MeOH formation and an acidic support such as Al₂O₃ or ZrO₂ increases the formation of DME from methanol) [9]. MeOH and DME can be transformed into olefins using an MTO catalyst. The following process steps are the same as for the direct route and after oligomerization, hydrotreatment and distillation the product SAF is gained.

The two pathways not only differ on the layout of the setup (number of reactors), but also on the reaction conditions. The optimal conditions of the indirect route for both MeOH synthesis (200-300 °C, 20-50 bar) and MTO (400-500 °C, 1 bar) means lower temperature and high pressure compared with the requirements of the direct route which affects the production cost of SAF.

The use of SAF produced via the direct and indirect routes studied in the TAKE-OFF project, does not only reduce CO₂ emissions, but also the release of the air pollutant SO_x. It is free of aromatic compounds and has some potential to reduce NO_x and soot emissions to the atmosphere due to a significantly lower aromatic content and the lack of sulphur components. To validate this, soot measurements of the expected components of the SAF by the established ASTM D1322 Method for measuring the sooting behavior of aviation fuel and fuel components were carried out. Regarding the investigation of NO_x emissions of potential SAF components, a combination of experiments at a Rapid Compression Machine and CFD simulations were used.

Following a holistic approach, life cycle assessments (LCA) and technical and economic assessments (TEA), as two pillars of sustainability, have been used to verify that the SAF production via the TAKE-OFF pathways is sustainable. The assessments involved the development of various scenarios to analyse both short-term and long-term viability. Furthermore, the sustainability of the TAKE-OFF routes has been compared to that of the FT route. Utilizing

shared socio-economic pathways of the TAKE-OFF routes and FT concepts enhanced the comprehensiveness of the sustainability assessment, considering future changes, policy implications, and broader socio-economic aspects. A well-defined framework was established in TAKE-OFF for the LCA and TEEA to enable a fair and reasonable comparison among the scenarios. The investigated pathways in TAKE-OFF comprise a wide range of the Technology Readiness Levels of the individual process steps, from SAF synthesis in laboratory-scale along the direct route, up to capturing CO₂ for the direct and indirect routes by an amine-based CO₂ capture pilot plant, which has achieved 115,000 operating hours since commissioning at a power plant in 2009. The framework takes this into consideration and encompasses several key components, including the definition of assessment methods for both environmental impact assessment and economic feasibility. It also involves the description of scenarios and their corresponding supply chains, the modeling approaches utilized, the inventory data collected for modeling purposes, and the final decision-making approaches. Where possible and reasonable for a fair comparison, data from the testing facilities and reactor set-ups of smaller scale in the laboratory and of the larger pilot plants at the industrial site were used in the models.

2. Methods and materials

2.1. Investigation of the direct route from H₂ and CO₂ to olefines to SAF

The catalytic tests were realized both in a high throughput unit (HTP, Flowrence, Avantium, Fig. 3) and in a laboratory fixed bed microreactor. The catalytic performance was measured at 375°C, and 20 or 30 bar at different WHSV values. Ethylene hydrogenation tests were realized in the laboratory setup at 375°C and 20 bar. The catalyst characterization details are available in [10].



Fig. 3. Flowrence catalytic unit in the RealCat high-throughput experimentation platform in Lille.

2.1.1. Reactor test oligomerisation of olefins

The two-step process of conversion of light olefins into higher olefins fit for a jet-fuel relies on a nickel heterogenous catalyst, specifically designed for the TAKE-OFF project, as well as a commercial acidic resin, see Figure 4. The principle is to use the catalytic properties of nickel to perform the oligomerization of ethylene or propylene at low temperature and high flow-rate. The light oligomers obtained can then be upgraded smoothly into jet-fuel range olefins over a commercial polymeric resin, which can be recycled. To this two-step process the step of hydrogenation of the olefins into saturated hydrocarbons is added.

Catalytic reactions were carried out at 120 °C in a continuous flow pressurized reactor manufactured by Parr Instrument Company, USA. Light olefins are injected at a pressure of 30 bar using digital mass-flow controllers and a high-pressure pump in the case of liquid propylene. The olefin mixture obtained from nickel-catalyzed

oligomerization is put into contact with a commercial acidic resin for upgrading into jet fuel-range olefins at the same temperature.

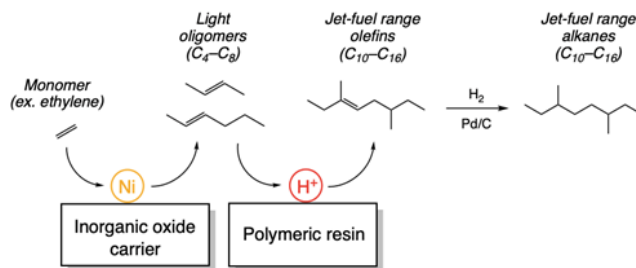


Fig. 4. Two-step process for the oligomerization of olefins to jet fuel.

2.2. Investigation of the indirect route from H₂ and CO₂ to MeOH/DME to olefins to SAF

The synthesis facility of Mitsubishi Power that was used in the TAKE-OFF project as part of the indirect route produced DME and MeOH from CO₂ and H₂. CO₂ was supplied from RWE's amine-based capture pilot plant and H₂ was provided by Asahi Kasei's Aqualyzer, an alkaline electrolyser prototype. All facilities were installed and operated at RWE's Innovation Center at Niederaussem, Germany, see Figure 5. The amine-based post-combustion carbon capture pilot plant provides CO₂ from the flue gas of a 1,000 MW lignite-fired power plant (Unit K at Niederaussem, flue gas content of CO₂ ca. 15 vol.-%, O₂ 5 vol.-%) and is – as well as the electrolyser and the synthesis unit – operated 24/7 by RWE's R&D team.



Fig. 5. left and middle - CO₂ capture pilot plant and synthesis plant at RWE's Innovation Center at Niederaussem, Germany. right - arrangement of the components needed for the CO₂ supply (compression, liquefaction and storage tank) and H₂, (electrolyser) and synthesis plant with process gas compressor and storage site for the intermediates of the indirect route, methanol (MeOH) or dimethyl ether (DME).

2.2.1. CO₂ capture, compression and liquefaction

Since April 2019 the CO₂ capture pilot plant has been operated almost continuously with the non-proprietary aqueous solvent CESAR1, a blend of 3.0 M (~26.74 wt.-%) 2-amino-2-methylpropan-1-ol (AMP) and 1.5 M (~12.92 wt.-%) piperazine (PZ). With 3.0 GJ/t CO₂ at a CO₂ capture rate between 90 and 95% CESAR1 has a significantly lower specific energy demand for the regeneration of the solvent than aqueous 30 wt.-% monoethanolamine (MEA, 3.5 GJ/t CO₂). In the pilot plant, an electric steam generator is used for solvent regeneration, which could eventually be powered by renewables for a smaller CO₂ footprint of the overall process, see Figure 6. CESAR1 is also more stable against oxidative degradation than MEA, lowering the solvent losses due to emissions and ageing (specific solvent consumption 0.45 kg/t CO₂). The compressed and liquified CO₂, which is used in the MeOH/DME synthesis, has food quality and needs no further purification (>99.98% (v/v) dry, sum of O₂/Ar content: <0.016% (v/v), SO₂ <1 ppmv and NH₃ <2.5 ppmv). The storage capacity of the tank for liquified CO₂ is 18 t (pressure 16.5 bar (a)–17.5 bar(a), temperature: minus 26.5 °C), which allows continued operation of the synthesis unit even in cases where the power plant is not in operation and no flue gas is available.



Fig. 6. Process diagram of the amine-based capture-pilot plant at Niederaussem.

2.2.2. H₂ production with alkaline electrolysis

Asahi Kasei's Aqualyzer is an alkaline electrolysis prototype that could be operated efficiently between 1.0 kA/m² to 10.0 kA/m² and produced up to 22 kg H₂/d. At a current density of 4.0 kA/m² a DC power consumption of less than 4.15 kWh/Nm³ H₂ could be achieved, see Figure 7. The purity of the produced hydrogen was >99.97% and was sufficient for the synthesis without further treatment. At rated operation the hydrogen was supplied at a pressure of 10 bar (g). The prototype provided valuable performance data and operational experience for the full-scale electrolyser product of Asahi Kasei, a 10 MW alkaline electrolyser currently under development in Japan.

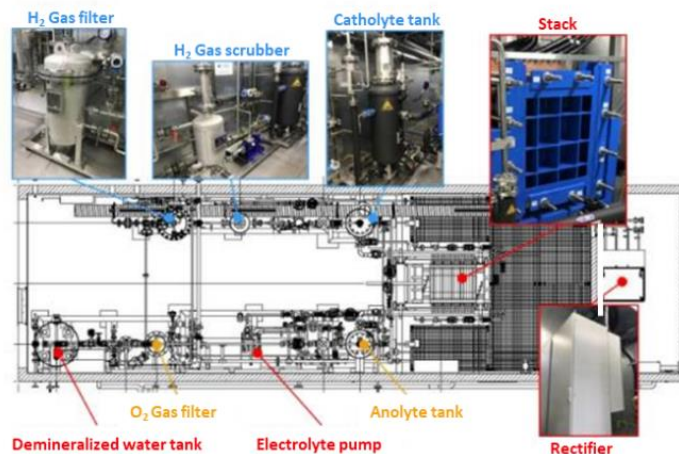


Fig. 7. Set-up of the advanced alkaline electrolysis from Asahi Kasei for the supply of the synthesis with H₂.

2.2.3. DME/MeOH synthesis unit

The MeOH/DME synthesis testing facility from Mitsubishi Power Europe comprised a CO₂ conditioning unit, where liquid CO₂ from the storage tank was heated to ca. 10 °C and then depressurized to ca. 11 bar(a) and passed on for mixing with the hydrogen from the electrolysis. The mixture of the reactants CO₂ and H₂ are first compressed, mixed with recycled process gas, and heated up to the required reaction temperature via a gas-gas heat exchanger and an electric heater. Two separate synthesis lines (MeOH and DME lines which cannot be operated in parallel) are installed, each with a capacity of 50% of the feed gas stream. While the MeOH synthesis uses a copper-based catalyst which is coated on ceramic tubes, for the bifunctional catalysis of DME from CO₂ and H₂ a monolithic catalyst in a reactor is used. After methanol synthesis in the reactor, the gas mixture is cooled down so that a large proportion of

the raw methanol and water are separated in a first separator. In case of the DME synthesis, after the first separator the pressure of the process gas is further increased and due to a sharp drop in temperature using a cryostat, the DME is liquefied and separated in a second separator, see Figure 8.

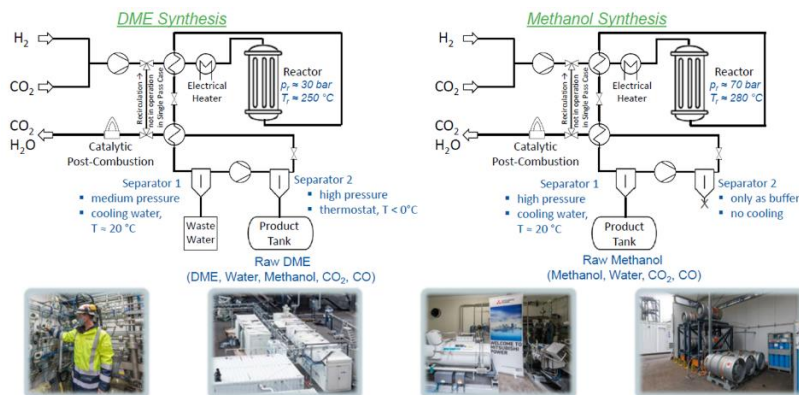
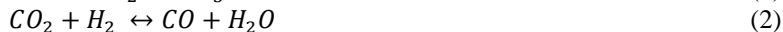


Fig. 8. Process diagrams for the DME synthesis (left) and the MeOH synthesis (right) of the TAKE-OFF testing facility.

This raw DME contains by-products of the synthesis and unconverted reactants, in particular CO₂. The gas phase from the second separator is recirculated to return the unreacted reactants and the intermediate product CO back into the synthesis. Only a small part of this gas is fed to a flameless purge-gas treatment system which consists of three catalytic burners to prevent the accumulation of non-usable by-products in the cycle. The new catalyst for the methanol synthesis and the coating of the monoliths in the reactor were provided by MPW.

2.3. Process optimization – SIENNA reactor tests

The production of MeOH and DME is limited in single pass conversion by their thermodynamic equilibrium. Multiple strategies for overcoming this limitation have been reported in open literature, such as membrane reactors, addition of sorption materials to the catalyst bed and local condensation of the by-product water. These concepts fall under the category *separation enhanced reactions*. By in-situ removal of the by-product water, the reactions are boosted towards the product side, leading effectively to a higher concentration of methanol and/or dimethyl ether according to the reactions listed below.



At TNO, the SIENNA reactor concept is developed where the steam is removed from the catalyst bed through a membrane and condensed on a cooling element in the middle of the reactor, see Figure 9. This concept has the potential of continuous water removal using a single reactor (unlike the reactors with sorption materials) and a driving force induced by condensation of steam on the cold surface (contrasting membrane reactors with utilizing sweep gas). However, a potential drawback is the lowering of the reactor temperature in the catalyst bed.

The effect of the in-situ water separation reactor on the methanol production under various experimental conditions using captured CO₂ delivered by RWE was investigated. Initially, reference experiments were carried out, operating the reactor without the cooling element to ensure that the equilibrium for methanol synthesis is reached. Subsequently, experiments were run with the cold finger set at 50 °C and an average increase in MeOH production of ~40wt% was achieved. Thereby confirming the effectiveness of the SIENNA concept.

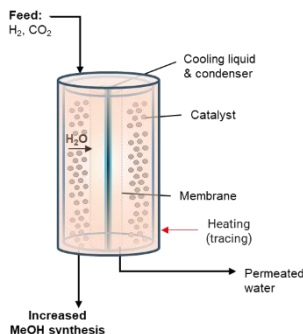


Fig. 9. A schematic representation of the SIENNA reactor.

2.4. Characterisation of SAF samples

The Take-Off test program focused on performance quality and purity related to SAF samples from the different process routes, such as:

- Hydrocarbon composition (classes and carbon number distribution) to identify comparability with conventional jet fuel and other SAFs,
- Distillation profile to indicate combustion properties,
- Key performance indicators such as freeze point, flash point, density, viscosity,
- measurement of sooting tendency and flame speed of different fuel components,
- Identification of non-hydrocarbon impurities and contaminations that may result from the production process, catalysts used or equipment set-up.

2.4.1. Emission evaluation

To assess the impact of the fuel composition on the emission characteristics during operation in a jet engine, two methods have been used. On the one hand, measurements of the threshold soot index (TSI) have been conducted in a standardized measurement device (smoke point tester according to ASTM D1322 [11]). On the other hand, burning velocities are measured in a spark ignited rapid compression machine (RCM). To do the latter, a completely novel approach has been developed. To evaluate the impact of the fuel composition on the nitrous oxide (NO) emissions 3D CFD simulations with reaction chemistry are conducted.

Analysis of TAKE-OFF product samples revealed that the fuel is mainly composed of mildly branched alkanes. Thus, the measurement campaign with the smoke point tester and the RCM focused on molecules with a similar structure. Measurement results are depicted in Fig 10. The TSI of the SAF samples and their individual components was less than 50 % of the TSI value of conventional aviation fuel (Jet A-1). Due to the targeted physical properties of the SAF sample, the targeted components are long-chained, branched alkanes. Long-chained components, molecule branching, and aromatic components can lead to higher sooting tendencies. The results do not indicate a clear dependency of the TSI value on molecule length. The significantly lower sooting tendency of the SAF samples is partly attributed to the lack of aromatic components. Measurements of burning velocities in the RCM revealed little influence of the molecule structure on the burning velocity. Large and strongly branched hydrocarbons burn more slowly, yielding less NO emissions at the same conditions, yet do not allow for more lean conditions.

To evaluate the TSI of different TAKE-OFF product samples the group contribution method (GCM) has been calibrated with the measurement data of the different molecules [12]. Within the GCM, a molecule is separated into different functional groups. The contribution of each group to the TSI is then fitted by means of a least square error. Prediction for TAKE-OFF product have been made based on the calibrated model, which estimated the TSI to be around 25 % of Jet A1. Measurement results of two TAKE-OFF samples revealed a TSI around 55 % of Jet A1. The scarce database and the simplification of the fuel composition which have been made during the prediction are the source of the misalignment. Nevertheless, the method shows high potential to be extended in future projects when the database of fuel components species can be extended. With measurements, it is confirmed that the TAKE-OFF product reduces the soot emissions significantly (mainly due to the lack of cyclic components).

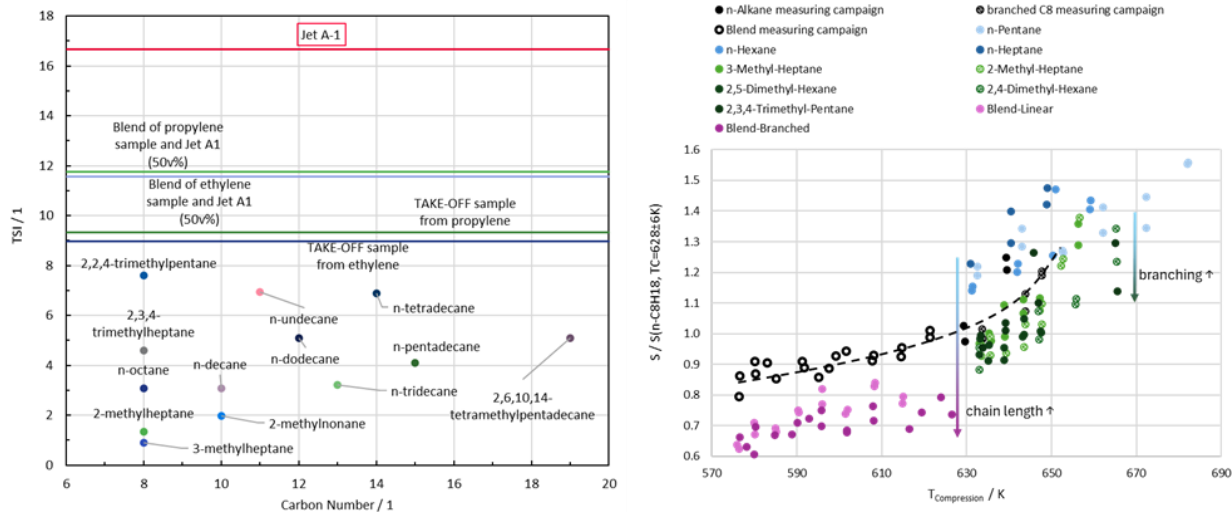


Fig. 10.: Measured TSI values for TAKE-OFF components and TAKE-OFF samples compared to Jet A1 (left), measured burning velocities of TAKE-OFF components in RCM at $p = 10$ bar and relative air-to-fuel ratio of 1.2 (normalized to burning velocity of *n*-Octane at 628 K).

The measurement data of the burning velocities revealed only smaller differences between the burning velocities of the investigated hydrocarbons. To assess the influence of the burning velocity on the NO emissions, 3D numerical simulations of the RCM have been conducted. NO chemistry was evaluated with the Zeldovich mechanism. Even with different combustion velocity, the NO production is mainly dependent on the pressure in the vessel. Almost no difference in NO emissions is observed in the simulation. Thus, it is concluded that the NO emissions of the TAKE-OFF fuel do not differ from conventional jet fuel.

2.4.2. SAF evaluation

Jet fuel quality plays an essential role in the safety of aviation and is regulated by jet fuel standards. ASTM D1655 Standard Specification for Aviation Turbine Fuels is seen as a global standard for fossil-based jet fuel, covering conventional Jet A/A-1 fuels used in all commercial turbine aircraft and engines in operation today. For all other non-petroleum jet fuel containing synthesized hydrocarbons, such as from bio-based feedstocks, the fuel must be certified under ASTM D7566 Standard Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons. Currently, a total of 8 synthesized jet fuel production pathways are certified under ASTM D7566 and every new production pathway must be qualified to enter the standard. The qualification process is governed by ASTM D4054 Standard Practice for Evaluation of New Aviation Turbine Fuels and Fuel Additives. During the qualification process, the fuel must demonstrate performance and composition resemblance to conventional jet fuel and other approved pathways. The TAKE-OFF process is unlike other approved production pathways and will require ASTM approval.

To evaluate the performance and suitability of TAKE-OFF fuel as jet fuel, key jet fuel properties are tested using ASTM methods to demonstrate compliance with relevant ASTM D7566 specifications and show that the fuel can meet other critical properties inherent to jet fuel performance. These key jet fuel properties include, but are not limited to:

Fluidity – The fuel must be able to flow freely through the aircraft's fuel system throughout all altitudes. Viscosity and freezing points are physical properties that characterize fuel fluidity. ASTM D7566 requires a maximum viscosity of 8 mm³/s at -20°C and a minimum freezing point of -40°C for Jet A and -47°C for Jet A-1.

Volatility – Vaporization characteristics impact fuel combustion and are characterized by properties such as flash point, distillation curve, and density. ASTM D7566 requires a minimum flash point of 38°C. The distillation curve and density of neat SAF must be consistent with conventional and approved jet fuels.

Stability – It is imperative to ensure that the fuel properties remain unchanged through time and exposure to different conditions. Jet fuel thermal oxidative test (JFTOT) is an important stability parameter, and it is one of

the most stringent SAF requirements. Stable fuels often display high purity with negligible amounts of alkenes, heteroatomic such as oxygenates, and trace metals. ASTM D7566 requires SAF to pass the JFTOT test at 325°C and the presence of trace metals to be less than 0.1 mg/kg per metal.

Taking into consideration the production process and the available sample volume, a test program is designed to provide maximum insights into the fuel quality.

2.5. Sustainability Assessment of e-SAF-Direct Pathway

Two pillars of sustainability – environmental and economic – is employed in this project to compare multiple scenarios for sustainable aviation fuel (e-SAF) production using CO₂ and H₂ as feedstocks through the direct route within the TAKE-OFF framework. The assessment encompasses both the techno-economic analysis and life cycle assessment (LCA) to evaluate the short-, mid-, and long-term viability. The results are benchmarked against the Fischer-Tropsch (FT) pathway using syngas feed and conventional fossil-based alternatives. Subsequent sections delve into a detailed discussion of the methods used in this evaluation.

2.5.1. Life Cycle Assessment (LCA)

By employing LCA, the environmental impacts associated with e-SAF production and its use, including resource consumption, greenhouse gas emissions, air and water pollution, and other relevant factors, can be accurately accounted and quantified. Such analysis provides a more holistic understanding of the environmental performance of e-SAF and aids in the identification of potential areas for improvement and optimization. However, it is necessary to adopt the most appropriate type of LCA and correctly implement the stages of LCA. The selection of the LCA methodology in the TAKE-OFF project was informed by the decision-making context, system scale, time frame and duration, approach, projection methods, as well as future societal and climate policy scenarios. Figure 11 illustrates the flowchart used to select the most appropriate LCA type within the TAKE-OFF context. The green pathway in this chart justifies the use of a prospective consequential LCA. Our methodology has been established taking into account the well-recognized LCA guidelines such as ISO 14040 [13] and the International Reference Life Cycle Data System (ILCD) handbook [14] as well as a comprehensive literature review of state-of-the-art studies. During the goal and scope definition phase, it is crucial to determine whether the LCA study is intended for decision support or accounting purposes. Europe is projected to see a substantial rise in e-SAF demand, reaching 20 Mt by 2040 and 40 Mt by 2050, with the Power-to-Liquid (PtL) pathway expected to play a major role in meeting this demand [15]. Furthermore, the findings of this LCA aim to support informed decision-making by highlighting the potential environmental benefits of adopting these alternative pathways across short-, mid-, and long-term scenarios. Therefore, the results of this LCA are intended to be used to support informed decision-making. The changes resulting from these decisions in the background and all interconnected foreground systems, influenced by market mechanisms, can manifest at both micro (non-structural) and macro (structural) levels [14]. Accordingly, consequential LCA is used to capture the wider impacts from e-SAF production within TAKE-OFF context. This approach employs system expansion to effectively manage issues related to multifunctionality [14].

Projections over time are integrated into LCA to evaluate the performance of technologies in light of anticipated future societal conditions. Prospective LCA facilitates a comprehensive assessment of design and evaluation uncertainties related to background data across different time frames (i.e., future scenarios), making it applicable to both emerging and established technologies [16, 17]. Within this framework, background data are adjusted according to predicted technical and socioeconomic advancements, employing predictive scenarios [18]. We incorporate Shared Socioeconomic Pathways (SSPs) provided by the Intergovernmental Panel on Climate Change (IPCC) into our environmental assessment to navigate uncertainties in background systems. By examining optimistic (SSP1 - green growth [19]), middle-of-the-road (SSP2) [20, 21], and pessimistic (SSP5 - fossil-fueled development [22]) trends, we can quantify the environmental performance of macro level e-SAF production under various socioeconomic changes. Each pathway is associated with specific climate policy scenarios: base scenarios (no significant changes in emissions policies), RCP2.6 (consistent with the Paris Agreement for limiting warming to 2°C [23]), and RCP1.9 (targeting a

more ambitious 1.5°C warming limit [23]). These projections provide a framework for assessing the short-, mid-, and long-term environmental impacts of e-SAF production under a variety of future conditions.

Accordingly, the environmental impacts are assessed for 2030, 2040, and 2050 implementing the prospective consequential approach based on SSP1, SSP2, and SSP5 under three climate scenarios (base scenario, RCP2.6, and RCP1.9). The Premise tool is used to model SSP-aligned background systems for the production of energy, materials, and chemicals up to 2050 [24]. The aim is to determine whether the TAKE-OFF direct pathway can serve as an environmentally sustainable alternative to FT for synthetic aviation fuel production. The system boundary for this assessment extends from cradle (or well) to the synthetic aviation fuel factory gate. Due to limitation on access to combustion data, the use phase has been excluded from the assessment in the TAKE-OFF project. All inventory data and environmental impacts are scaled and expressed based on a reference flow of 1 kg of jet fuel produced. Within this boundary, key factors such as CO₂ source selection (fossil-based or biogenic), water electrolysis (WEL) technology (alkaline or solid oxide water electrolyser), and carbon capture techniques (direct air capture, amine-based chemical absorption, or oxyfuel) are considered. The project comprehensively evaluates 324 scenarios for the TAKE-OFF direct pathway and 324 for the FT pathway across climate change impact category, accounting for the different SSPs, RCPs, and time frames.

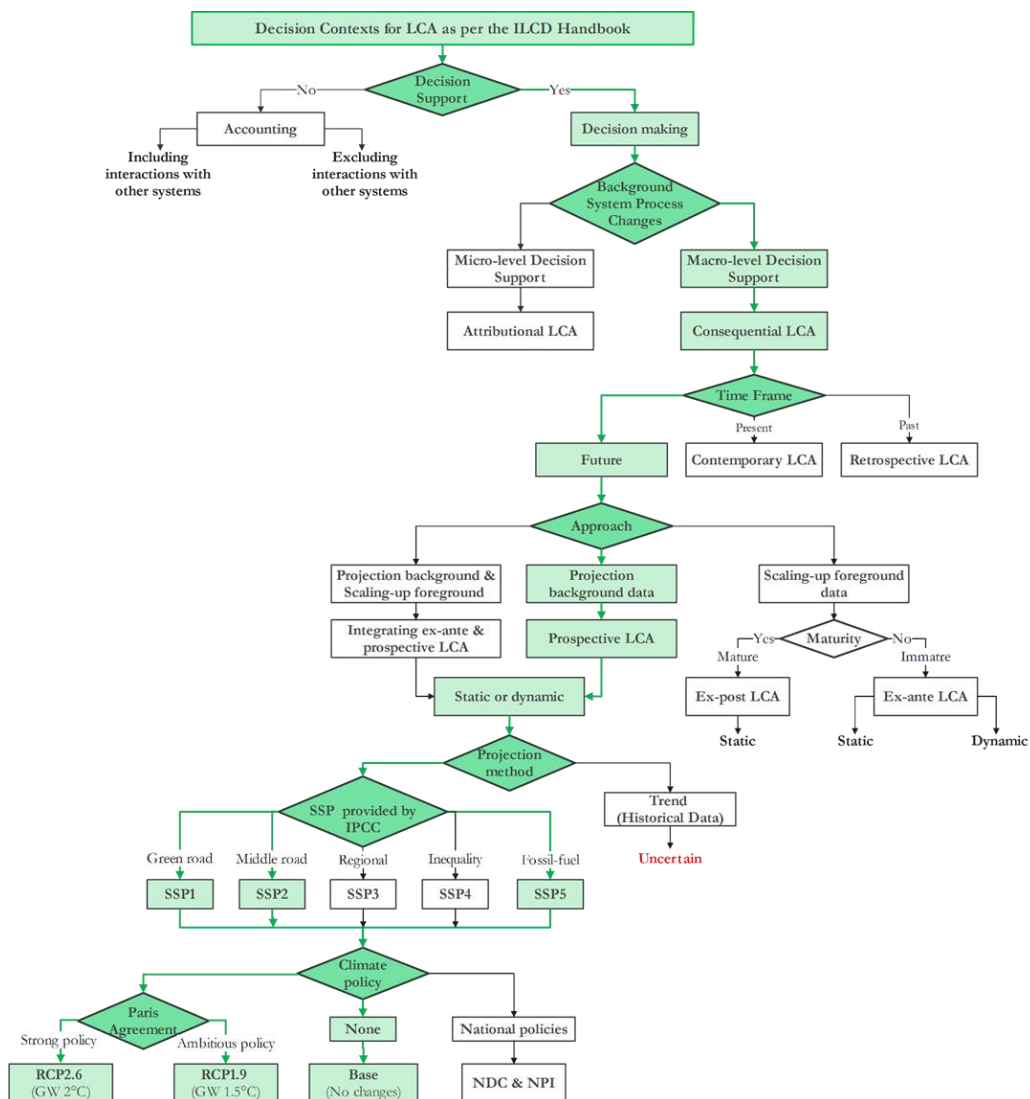


Fig. 11. A framework for decision contexts in selecting the appropriate LCA methodology for the TAKE-OFF project.

2.5.2. Techno-economic analysis framework and tool

Techno-Economic Analysis (TEA) is an integrated approach that combines technical evaluation with economic analysis to assess the economic feasibility of a technology. It plays a key role in understanding both the technical performance and financial viability of an industrial process, product, or service, and is critical for informed decision-making. TEA consists of two primary stages.

The TEA for the TAKE-OFF project begins with the process design and simulation stage, executed by TNO using Aspen Plus software. In this stage, the entire system is modeled to provide essential data on plant capacity, major components, energy consumption, material usage, efficiencies, selectivity, mass and energy balance, as well as plant configuration and layout. This simulation allows for a detailed understanding of the technical aspects of the process. The second stage focuses on the economic analysis, which examines the financial viability of the technology. Building on data from the process simulation, this analysis provides an in-depth evaluation of the Levelized Cost of Sustainable Aviation Fuel (LCOSAF) across multiple scenarios. The economic analysis addresses critical financial factors, including utility costs, raw material expenses, equipment costs, loan interest, inflation, equity structure, salvage value, construction period, discounted cash flow, return on investment (ROI), payback period (PBP), internal rate of return (IRR), and sensitivity analyses.

To streamline this process, a specialized TEA tool has been developed at University of Southern Denmark (SDU), designed to calculate the LCOSAF for multiple scenarios. This Excel-based tool is organized into several tabs, each covering different aspects of the analysis – capital expenditures (CAPEX), operating expenses (OPEX), depreciation, income, and overall economic analysis. The tool incorporates data from extensive literature reviews, focusing on essential cost components such as utilities and material prices, ensuring a comprehensive and reliable economic assessment. The TEA tool calculates the LCOSAF for three distinct time frames – 2030, 2040, and 2050 – while also exploring various scenarios that include fluctuations in CO₂ costs and the Levelized Cost of Hydrogen (LCOH₂).

In this project, the levelized costs of H₂ and CO₂, crucial feedstocks for e-SAF production, were determined using data from extensive literature review and technical reports. Both the FT and TAKE-OFF direct pathways rely on the same feedstocks, which significantly impact the overall cost efficiency of e-SAF production pathways. Rather than using fixed point estimates, we adopted cost ranges to reflect the evolving market for H₂ and CO₂ production. For the levelized cost of CO₂ (LCOCO₂), we assumed that CO₂ would be sourced from plants using various carbon capture (CC) technologies, with projections provided for 2030, 2040, and 2050. Accordingly, the LCOCO₂ is estimated to range between 38 and 221 €/ton, depending on the year and technology used. Among the CC technologies, oxyfuel emerged as the most cost-effective option, while DAC was the most expensive. To estimate the LCOH₂, we based our analysis on literature that thoroughly examines all cost determinants related to hydrogen production via electrolysis. Considering different water electrolysis methods, renewable energy sources, and configurations for connecting electrolyzers to renewable generators, the median LCOH₂ price in Europe is projected to range from 5.32 to 12.89 €/kg, varying by year [25-28]. After collecting the relevant data, the levelized costs of H₂ and CO₂ were integrated into the developed TEA tool.

3. Results and discussion

3.1. Direct route from H₂ and CO₂ to olefins

Methanol-mediated CO₂ selective hydrogenation to light olefins (LO) over bi-functional catalysts comprising metal oxide and zeolite components represents a promising approach to sustainable chemical production. However, achieving a high LO yield in a single pass remains a major challenge, as it requires simultaneously maintaining high LO selectivity and high CO₂ conversion.

The team of CNRS meticulously investigated the critical balance between selectivity and conversion over metal oxide-zeolite bifunctional catalysts. Through comprehensive analysis, the specific roles of each catalyst component were elucidated, offering new insights into this complex process. The team synthesized and evaluated a series of catalytic systems, incorporating oxides of Zn, In, Mn, Cr, and Ga, along with various SAPO-34 zeolites, across different CO₂ conversion levels.

The findings revealed that LO selectivity within the hydrocarbon fraction was primarily governed by the zeolite component, and declines as the hydrocarbon yield increases. In contrast, the metal-oxide component played a pivotal role in driving CO₂ conversion and determining the overall hydrocarbon and CO selectivities. Notably, the morphology and acidity of the SAPO-34 zeolites emerged as key factors dictating CO-free LO selectivity during CO₂ hydrogenation.

By unraveling these intricate relationships, we provided a deeper understanding of how to optimize catalyst design, paving the way for more efficient and selective processes in the hydrogenation of CO₂ to light olefins, see Figure 12.

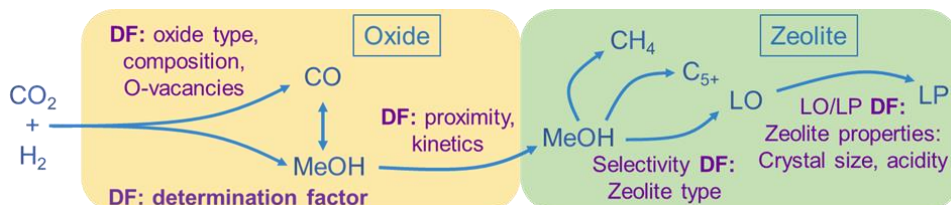


Fig. 12. Illustration of the tandem process reaction for CO₂ hydrogenation to light olefins: roles of oxide and SAPO-34 components in the methanol-mediated CO₂ hydrogenation performance.

3.2. Indirect route from H₂ and CO₂ to olefins

3.3. Oligomerization of light olefins

The low reactivity of light olefins, especially ethylene, with acidic catalysts necessitates the use of high reaction temperatures (>300 °C), which inevitably leads to rapid deactivation, primarily due to coke formation. The use of metal-based catalysts, such as the well-documented nickel catalyst, mainly results in dimerization and trimerization. However, when these two families of catalysts are combined, they provide an efficient approach to producing jet fuel range olefins. In fact, nickel-promoted dimerization yields substituted olefins that can more easily react with acidic catalysts at low temperature to form stable carbocation intermediates upon protonation.

After using conventional nickel-based catalysts, we employed state-of-the-art nickel catalysts prepared via the SOMC (Surface Organometallic Chemistry) methodology. This technique allows for the formation of well-defined single-site nickel centers, thereby maximizing the number of active sites with a controlled coordination sphere. By adjusting the acidity of the silica-alumina support, we achieved activity as high as 20 g·g_{cat}⁻¹·h⁻¹. Notably, the use of high pressure with the ethylene/propylene mixture leads to a liquid phase, which allows better control of the temperature rise during the exothermic reaction, thereby enabling the reaction to be carried out without the need for solvents.

Treating the liquefied product in a batch reactor enabled the upgrading of C₄-C₁₂ oligomers into jet fuel range C₈-C₁₆ hydrocarbons, as shown in Figure 13. Furthermore, remaining light products can be recycled to react with acidic resin.

In addition, due to the formation of highly branched paraffins, most of the C₁₈ oligomers fall within the jet fuel boiling range, unlike the linear C₁₈ compounds produced via Fischer-Tropsch synthesis. The branched nature of the produced oligomers is also advantageous for lowering the freezing point.

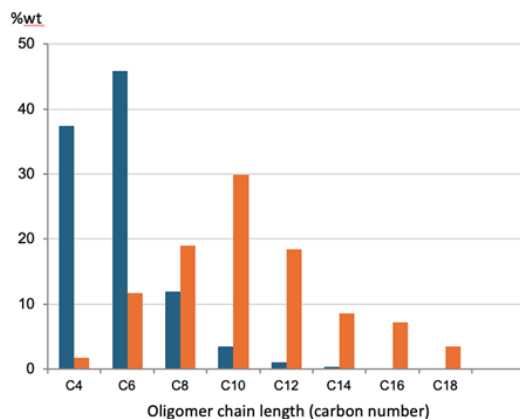


Fig. 13. Distribution of oligomers for the product of oligomerization in flow (blue), and the distribution after treatment over an acidic resin (orange).

The testing of the final fuel samples is ongoing, however, analysis of the preliminary samples has shown that the fuel has the potential to be a suitable fuel. The preliminary samples displayed a freezing point of less than -60°C , meeting freezing point specifications and indicating that the fuel is sufficiently isomerized. Nevertheless, results from the final test program are needed to validate the fuel's suitability as jet fuel.

3.3. Environmental and Techno-economic Assessment of e-SAF

The results presented in this section represent our preliminary findings and are anticipated to improve as the assessment is refined with more detailed simulation data and enhanced modeling approaches. The LCA and TEA results have been used as feedback to TAKE-OFF consortium to investigate potential for future improvements. The early LCA outcomes provide strong evidence that both the TAKE-OFF direct and FT pathways for e-SAF production yield significantly lower environmental impacts compared to fossil-based alternatives ($0.88 \text{ kg CO}_2\text{-eq/kg e-SAF}$) across all time frames. However, it is noteworthy that the climate impact of the TAKE-OFF direct pathway is, on average, about twice as high as that of the FT pathway. Despite both routes leading to negative climate impacts, the FT pathway demonstrates relatively better performance in terms of reducing climate impact due to its higher carbon-to-kerosene conversion efficiency and overall energy efficiency.

For the TAKE-OFF direct pathway, the major contributors to environmental impacts include electricity and heat consumption in key unit processes such as recycling, oligomerization, and distillation, alongside emissions from combined heat and power generation and purge flows – waste gases primarily composed of CO_2 and CO released during recycling processes – significantly impact the overall environmental footprint.

Our preliminary analysis of the impact of alkaline water electrolyser (AWEL) and solid oxide water electrolyser (SOWEL) technologies on e-SAF production reveals that AWEL consistently exhibits higher environmental impacts compared to SOWEL technology. On average, across the TAKE-OFF direct pathway, scenarios employing SOWEL demonstrated a 4-6% lower climate impact compared to AWEL, depending on the time frame. This difference is primarily attributed to the higher energy consumption of AWEL. Supporting this, Zhao et al. compared the environmental performance of various water electrolyser technologies and confirmed that AWEL results in higher climate impacts than SOWEL [29]. Thus, despite the substantial energy demands of both technologies, SOWEL's lower electricity consumption translates into comparatively better environmental performance.

Influence of carbon capture technologies (MEA-based, DAC, and Oxyfuel) on the environmental performance of e-SAF production over time was also assessed. The early analysis shows that scenarios utilizing Oxyfuel technology consistently resulted in the lowest environmental impacts, whereas DAC technology showed the highest impacts. On average, across the TAKE-OFF direct pathway, oxyfuel technology reduced climate impacts by 3-6% compared to

MEA-based capture technology and by 17-18% compared to DAC, depending on the time frame. The higher impacts associated with DAC can be attributed to its significant energy requirements, needing approximately 4.7 MJ of heat and 0.7 kWh of electricity per kg of CO₂ captured.

In the technical assessment, the carbon-to-kerosene efficiency of a pathway reflects the proportion of carbon inputs effectively converted into the desired product. The TAKE-OFF direct pathway demonstrates a carbon efficiency of around 50%, indicating that nearly half of the carbon fed into the system is transformed into e-kerosene, the primary product.

From an economic perspective, short-, mid-, and long-term TEA was conducted for both the TAKE-OFF direct and FT pathways, compared to fossil-based kerosene (visualized in Figure 14). This figure shows the relative costs of all pathways, with the Levelized Cost of e-SAF (LCOSAF) for the TAKE-OFF direct pathway set at 100% for each of the three timeframes: 2030, 2040, and 2050. The FT pathway demonstrates a relative cost ranging from 67% to 69% of the LCOSAF in the TAKE-OFF direct pathway, indicating its consistent cost-effectiveness. Additionally, the LCOSAF from the TAKE-OFF direct pathway is expected to be 6.4 times higher than fossil-based jet fuel in 2030, decreasing to 4.3 times higher by 2050. A detailed cost analysis highlights that hydrogen prices and electricity costs are the dominant factors in determining the LCOSAF for both pathways. The lowest LCOSAF for both the TAKE-OFF direct and FT pathways is expected by 2050, assuming the use of CO₂ captured via oxyfuel technology and hydrogen produced from electrolyzers powered by renewable curtailed electricity.

The results align with other research on the economic viability of e-SAF production. For example, Saad et al. reported e-SAF production costs ranging from 7.86 to 9.77 €/kg when integrating heat recovery into the process [30]. Similarly, Fernanda et al. found that e-SAF production via the FT pathway remains economically uncompetitive with fossil jet fuel, at a cost of 5.16 €/kg, even under more optimistic assumptions for CO₂ and H₂ prices (4.38 €/kg for CO₂ and 3.87 €/kg for H₂) [31].

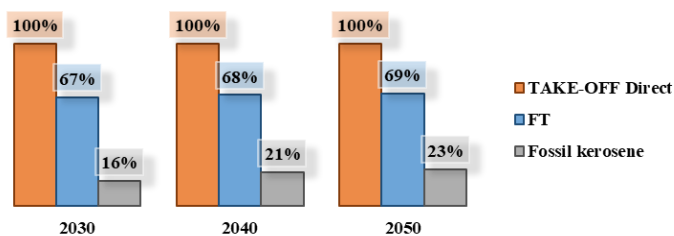


Fig. 14. Levelized Cost of e-SAF from Fischer-Tropsch (FT) and TAKE-OFF direct routes compared to Fossil kerosene (2030, 2040, 2050).

In our ongoing efforts to improve the environmental and economic profile of the TAKE-OFF pathway, several advancements are being made. These include improving process efficiencies, optimizing catalyst performance, fine-tuning reactor conditions, and stabilizing conversion rates to ensure more reliable and robust operations. Additionally, increasing overall system productivity is crucial to improving both carbon-to-kerosene efficiency and the energy profile. Cost reduction is also a priority, with strategies being explored through economies of scale, supply chain optimization, and the implementation of advanced process control systems. Together, these refinements aim to make the TAKE-OFF routes a more competitive alternative to other Power-to-Liquid routes, such as the FT pathway, across short-, mid-, and long-term scenarios.

4. Conclusion and outlook

The preliminary LCA results show that both the TAKE-OFF direct and FT pathways for e-SAF production yield significantly lower environmental impacts compared to fossil-based alternatives. The analysis of the TAKE-OFF product samples revealed that the fuel is mainly composed of mildly branched alkanes and lacks cyclic components which means a significant reduction of soot emissions.

Although the analyses of the results of the development and testing of the TAKE-OFF routes is still in progress, we can already conclude that there is no evidence that the direct synthesis route from H₂ and CO₂ to e-SAF is

economically favorable compared with the Fischer-Tropsch route. The identified options for process optimisation based on the developed new catalysts, advanced control of the synthesis reactions and an intensified use of purge flows have the potential to reduce the price gap to some degree and to increase the carbon efficiency of the direct route. The work on the indirect route via MeOH/DME is ongoing. Nevertheless, e-SAF synthesized by the investigated routes has a significantly lower environmental impact compared to the fossil alternatives.

The EU has accelerated actions to boost the uptake of synthetic aviation fuels in airplanes. The ReFuelEU Aviation legislation mandates minimum quotas for sustainable aviation fuels and subquotas for synthetic aviation fuels, sets penalties for fuels suppliers (most of it) and aircraft operators (part of it) if they don't comply with the targets of the EU's Emissions Trading System (ETS) Aviation. The phase out of free allowances for aviation (-25% in 2024, -50% in 2025 and -100% from 2026, from 2027, airlines will need to pay their ETS fees in full) is accompanied by support to innovation (5 million ETS allowances collected to the European Innovation Fund), support of the transition to sustainable aviation fuels (20 million ETS allowances foreseen for 2024 to 2030) which narrows the price gap between SAF/e-SAF and fossil kerosene.

A clear business case for synthetic aviation fuels depends strongly on the regulative framework. It needs a continuous and systematic supportive long-term policy and financial incentives to move away from fossil fuels in aviation. In the end society, businesses and consumers will decide if they accept the costs of synthetic aviation fuels to gain the benefits of climate protection.

Acknowledgement

The TAKE-OFF project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101006799.

Literature

- [1] EEA Transport and Environment report 2021.
- [2] SkyNRG. SUSTAINABLE AVIATION FUEL MARKET OUTLOOK. June 2024 Update.
- [3] Directive (EU) 2023/2405 on ensuring a level playing field for sustainable air transport (ReFuelEU Aviation).
- [4] Directive (EU) 2018/2001 on the promotion of the use of energy from renewable sources.
- [5] <https://takeoff-project.eu>.
- [6] Chernyak SA, Corda M, Dath JP, Ordonsky VV, Khodakov, AY. Light olefin synthesis from a diversity of renewable and fossil feedstocks: state-of-the-art and outlook. *Chem Soc Rev* 2022;51:7994–8044. <https://doi.org/10.1039/D1CS01036K>
- [7] Heveling J, Nicolaides CP, Scurrell MS. Catalysts and conditions for the highly efficient, selective and stable heterogeneous oligomerisation of ethylene. *Applied Catalysis A* 1998;173,1:1-9. [https://doi.org/10.1016/S0926-860X\(98\)00147-1](https://doi.org/10.1016/S0926-860X(98)00147-1)
- [8] Zhong J, Yang X, Wu Z, Liang B, Huang Y, Zhanga T. State of the art and perspectives in heterogeneous catalysis of CO₂ hydrogenation to methanol. *Chem Soc Rev* 2020;49:1385–1413 (2020). <https://doi.org/10.1039/C9CS00614A>
- [9] Moser P, Wiechers G, Schmidt S, Stahl K, Kuhr Ch, Schroer K, Schemme S, Heberle A, Kakihira H, Arai H, Peters R, Weiske S, Zapp P, Troy S, Lehrheuer B, Neumann M, Honeckere Ch, Glück S, Pieterse JP, Goetheer E. ALIGN-CCUS: Production of dimethyl ether from CO₂ and its use as energy carrier - Results from the CCU demonstration plant. Proceedings of the 15th Greenhouse Gas Control Technologies Conference 2021, <https://ssrn.com/abstract=3812172> or <http://dx.doi.org/10.2139/ssrn.3812172>
- [10] Chernyak SA, Corda M, Marinova M, Safonova OV, Kondratenko VA, Kondratenko EV, Kolyagin YG, Cheng K, Ordonsky VV, Khodakov AY. Decisive Influence of SAPO-34 Zeolite on Light Olefin Selectivity in Methanol-Meditated CO₂ Hydrogenation over Metal Oxide-Zeolite Catalysts. *ACS Catal* 2023;13,22:14627-14638. <https://doi.org/10.1021/acscatal.3c03759>
- [11] ASTM D1322-08. Standard Test Method for Smoke Point of Kerosine and Aviation Turbine Fuel. American Society for Testing and Materials (ASTM), West Conshohocken, PA, 1997
- [12] Graziano B, Ottenwälder T, Manderfeld D, Pischinger St, Grünfeld G. Advanced Methodology for the Detection of Smoke Point Heights in Hydrocarbon Flames. *Energy & Fuels* 2018;32(3) :3908-3919. <https://doi.org/10.1021/acs.energyfuels.7b03584>
- [13] ISO, I., 14044: 2006/AMD 2: 2020—Environmental Management—Life Cycle Assessment—Requirements and Guidelines—Amendment 2. International Organization for Standardization: Geneva, Switzerland, 2020.
- [14] WOLF, MA, et al. International Reference Life Cycle Data System (ILCD) Handbook-general guide for life cycle assessment-detailed guidance. 2010.
- [15] SkyNRG, A market outlook on sustainable aviation fuel. May 2022.
- [16] Arvidsson R, et al. Environmental assessment of emerging technologies: recommendations for prospective LCA. *Journal of Industrial Ecology* 2018;22(6):1286-1294.
- [17] Thonemann N, Schulte A, Maga D. How to conduct prospective life cycle assessment for emerging technologies? A systematic review and methodological guidance. *Sustainability* 2020;12(3):1192.

- [18] de Souza NRD, et al. Integrating ex-ante and prospective life-cycle assessment for advancing the environmental impact analysis of emerging bio-based technologies. *Sustainable Production and Consumption*. 2023;43:319-332.
- [19] Van Vuuren DP, et al. Energy, land-use and greenhouse gas emissions trajectories under a green growth paradigm. *Global environmental change* 2017;42:237-250.
- [20] Fricko O, et al. The marker quantification of the Shared Socioeconomic Pathway 2: A middle-of-the-road scenario for the 21st century. *Global Environmental Change* 2017;42:251-267.
- [21] Fujimori S, et al. SSP3: AIM implementation of shared socioeconomic pathways. *Global Environmental Change* 2017;42:268-283.
- [22] Kriegler E, et al. Fossil-fueled development (SSP5): An energy and resource intensive scenario for the 21st century. *Global environmental change* 2017;42:297-315.
- [23] Rogelj J, et al. Scenarios towards limiting global mean temperature increase below 1.5 C. *Nature climate change* 2018;8(4):325-332.
- [24] Sacchi R, et al. PProspective EnvironMental Impact asSEment (premise): A streamlined approach to producing databases for prospective life cycle assessment using integrated assessment models. *Renewable and Sustainable Energy Reviews* 2022;160:112311.
- [25] Christensen A. Assessment of hydrogen production costs from electrolysis: United States and Europe. *International council on clean transportation* 2020;1(1):1-64.
- [26] IEA, *Global Hydrogen Review*. International Energy Agency, 2023.
- [27] Nami H., et al. Techno-economic analysis of current and emerging electrolysis technologies for green hydrogen production. *Energy Conversion and Management* 2022;269:116162.
- [28] Zhou, Y, Searle S, Pavlenko N. Current and future cost of e-kerosene in the United States and Europe. I: *International council on clean transportation Working paper* 2022;14.
- [29] Zhao G, et al. Life cycle assessment of H₂O electrolysis technologies. *International Journal of Hydrogen Energy* 2020;45(43):23765-23781.
- [30] Saad DM., et al. Life Cycle Economic and Environmental Assessment of Producing Synthetic Jet Fuel Using CO₂/Biomass Feedstocks. *Environmental Science & Technology* 2024.
- [31] Rojas-Michaga MF, et al. Sustainable aviation fuel (SAF) production through power-to-liquid (PtL): A combined techno-economic and life cycle assessment. *Energy Conversion and Management* 2023;292:117427.