Alternative pathways to sustainable aviation fuel from CO2 and H2: an enviro-economic assessment

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Abstract

With air transportation responsible for 2% of the total GHG emissions and 10% of the fuel consumption worldwide, sustainable aviation fuel (SAF) is considered a key enabler to reach net-zero aviation by 2050. In this work, we carry out an enviro-economic comparison between a one-step Fischer-Tropsch process (1sFT) and a methanol-to-jet process (MTJ). 1sFT is based on a novel Mn-Fe-K catalyst promoting direct conversion of CO2 and H2 to liquid hydrocarbons. In MTJ, methanol is produced first, followed by methanol-to-olefin conversion, oligomerization, and hydro-processing. Our analysis considers 1 MJ of liquid fuel as functional unit and the following key performance indicators: levelized cost of production, global warming potential, and monetized end-point environmental impacts. Our results suggest that 1sFT outperforms MTJ by 23-36%, depending on H2 and CO2 costs. 1sFT is also found to be superior to MTJ from an environmental point of view, with up to 33% reduction in GWP and 28% reduction in monetized environmental externalities on a well-to-wake basis.

**Keywords**: SAF, technoeconomic analysis, LCA, Fischer-Tropsch, Methanol-to-Jet

* 1. Introduction

The aviation industry is heavily reliant on fossil resources, and, unlike other transportation modes, it cannot be decarbonised through electrification due to the high energy density required for long distance travel (Becattini et al. 2021). Sustainable aviation fuel (SAF) is defined as a drop-in alternative that can be used in existing aircrafts while meeting certain sustainability criteria, and it is considered a key step towards net-zero aviation. From a regulatory perspective, alternative fuels need to achieve a minimum of 50 % GWP reduction on a life-cycle basis to be classified as SAF in the UK.

Two routes under investigation for producing SAF from CO2 and H2 are Fischer-Tropsch (FT) synthesis and alcohol-to-jet routes with either methanol or ethanol as intermediates. In particular, the methanol-to-jet (MTJ) pathway is attracting significant attention, with major companies such as Honeywell, Topsoe and ExxonMobil announcing the development of proprietary technologies. Recently, Bernardi et al. (2022) compared two FT routes, a one-step FT process (1sFT) based on a novel Mn-Fe-K catalyst (Yao et al., 2020) and a two-step process (2sFT) using a reverse water gas shift reactor to convert CO2 and H2 to syngas first, followed by a conventional FT reactor (Zang et al., 2021). 1sFT was found to outperform 2sFT both from an economic and environmental standpoint, but significant reductions in CO2 and H2 prices as well as policy interventions such as carbon taxation were deemed necessary for the synthetic fuel to be economically competitive with its fossil counterpart. Schmidt et al. (2018) compared MTJ with a two-step FT process in terms of their economics, GHG emissions, water consumption and land use, and concluded that they were performing similarly.

The main objective of this paper is a comparison of the 1sFT process analyzed in Bernardi et al. (2022) with an MTJ process. These two processes are also compared to a fossil-based alternative in terms of economic and environmental performance. The methodology is described in Section 2, followed by results and discussions in Section 3, before concluding the paper in Section 4.

* 1. Methodology

Block flow diagrams of the two processes are shown in Figure 1. Aspen HYSYS v11 is used to simulate the processes at scale, considering a feed of 100 t/h of CO2 either from direct air capture (DAC) or biogenic, and H2 from water electrolysis. Both CO2 and H2 gases are fed at 25 °C and 30 bar, with no significant impurities, and the produced fuel blends are sent to an existing refinery. The NTRL-RK fluid package is used in the methanol synthesis section and the Peng Robinson fluid package everywhere else. Heat integration is performed in Aspen Energy Analyzer.

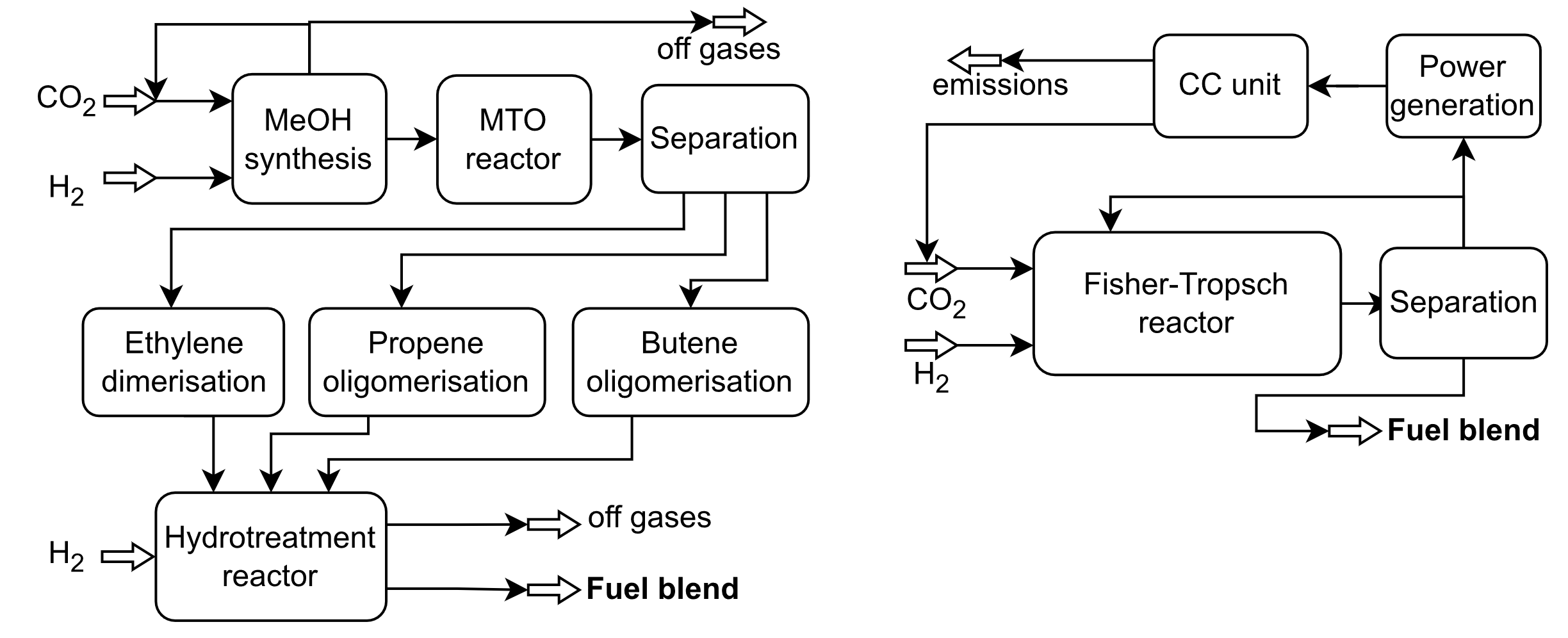
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Figure 1: block flow diagrams of the MTJ (left) and 1sFT (right) processes. The power generation and carbon capture units are used for the off-gases of both processes but only represented in 1sFT.

* + 1. Process simulation and economic analysis

**Feed streams.** We considered two options for CO2 procurement: DAC, and carbon capture from a pulp and paper mill (PPCC). In our baseline scenario, we considered a solid sorbent DAC process, with heat requirements fulfilled by a natural gas steam boiler or coming from a low-grade heat source **(**considered available free of charge), which result in a cost of 430 $/t­CO2 and 281 $/t­CO2, respectively (Sabatino et al 2021). The CO2 captured from the pulp and paper mill is 95% biogenic and has a cost of 75 $/tCO2 in the baseline scenario (Onarheim et al. 2017). The H2 cost is estimated at 4.3 $/kgH2, considering an offshore wind electricity price of 67 $/MWhel, an energy efficiency of 67.5 %LHV, 20 % cost increase to account for electricity intermittency, and 26% added to the total cost to account for capital and operating expenditures other than electricity. An optimistic scenario is also briefly discussed, which considers prices of 1.5 $/kgH2 (Brändle et al.*,* 2021), 150 $/tCO2, DAC, and 50 $/tCO2,biog. All costs throughout the paper are expressed in US$2023 for consistency.

**One-step FT synthesis (1sFT).** The FT reactor operates at 260 °C and 10 bar with conversion and selectivities obtained from Yao et al. (2020). H2 is fed to the process in a H2:CO2 molar ratio of 3:1. The outlet stream enters a sequence of two 3-phase separators operating at 70 °C and 40 °C both under 10 bar. A small (2%) fraction of the gaseous stream coming out of the second separator is burned to produce heat and electricity in a gas and steam cycle, while the rest is recycled to the FT reactor. The other two streams from the 3-phase separators are wastewater and liquid hydrocarbons. The liquid hydrocarbons are mixed, expanded to 1 bar and cooled down to 35 °C. The vapor phase from a flash separator (CO2 and C1–C4 hydrocarbons) is burned to produce additional electricity, while the liquid phase containing the fuel blend product is sent to the refinery. A carbon capture (CC) unit is installed to capture 95%wt of the CO2 in the flue gas, which is recycled back to the FT reactor. The fuel blend contains 16.4%wt gasoline (C5-C7), 76%wt SAF (C8-C16), 4.6%wt diesel (C17-C20), 2.8%wt light hydrocarbons (C1-C4), and traces (<1%wt) amount of wax (C20+).

**Methanol-to-jet process (MTJ).** Methanol is produced from direct CO2 hydrogenation in an isothermal reactor operating at 260 °C and 65 bar, described by the model by Vanden Bussche and Froment (1996). Methanol and water are recovered in two flash separators operating at 50 °C and under 65 bar and 1 bar. The unreacted syngas is recycled back to the methanol reactor except for a 1% purge stream that is burned to produce electricity. A distillation column is used to separate water from the methanol product that is sent to the upgrading section. Methanol is first converted to olefins in a methanol-to-olefins (MTO) reactor, operating at 450 °C and 2 bar. The outlet stream is cooled to 50 °C to remove the water then sent to an adsorption column to remove the CO2 and a distillation train to separate the ethylene, propene and butene co-products. The olefins stream is compressed to 30 bar before entering the first column, where 99%wt pure ethylene is recovered at the top with a condenser temperature of -13 °C. The bottom stream is sent to a second column operating at 20 bar where propylene and butene are separated. Ethylene reacts at 25 °C and 50 bar to produce n-butane, i-butane and hexene. Propene and butene are further upgraded in oligomerization reactors operating at 270 °C and 40 bar, and 350 °C and 10 bar, respectively. Lastly, a hydrotreatment reactor operating at 300 °C and 30 bar and fed with a stochiometric amount of H2 is used to convert the olefins into alkanes. The final liquid fuel blend is obtained in a flash separator operating at 40 °C and 1 bar. As in 1sFT the off gases are used to produce electricity and sent to a CC unit to capture and recycle 95% of the CO2. The liquid fuel blend produced contains 4.5%wt gasoline, 86.2%wt SAF, 2.3%wt diesel, 6.9%wt light hydrocarbons, and no wax.

**Economic analysis.** In 1sFT, the FT reactor yields and selectivities are obtained from Zao et al. (2020), with correlations from Zang et al. (2021) used to estimate the cost. In the methanol upgrading section of MTJ, conversion and selectivities are obtained from Atsonios et al. (2023). The levelized cost of production (LCP) is calculated assuming a 15% interest rate and 20-year plant lifetime. LCP is compared with the fossil fuel cost, which is assumed to be 14 $/GJfuel in the base case, and 23 $/GJfuel in the optimistic best-case scenario considering a carbon tax of 150 $/tCO2 (IEA 2020).

* + 1. Life cycle analysis

The functional unit (FU) for the LCA analysis is chosen as “*1 MJ of liquid fuel blend*” and the assessment is done considering a Well-to-Wake (WtW) perspective, assuming that all the carbon in the fuel blend is released as CO2 during the use phase. System expansion via substitution is adopted to deal with multi-functionality.

**Data collection and life-cycle inventories.** The life-cycle inventories (LCIs) of 1sFT and MTJ are computed from the two process flowsheets (Section 2.1), as summarized in Table 1. The LCIs for DAC, biogenic CO2, and H2 are adapted from Sabatino et al. (2023), Onarheim et al. (2017), and Brändle et al. (2021), respectively. Offshore wind electricity is assumed for H2 production, and credits given for selling any excess electricity are based on the UK production mix.

Table 1: life-cycle inventories of 1sFT and MTJ processes. HPS = high pressure steam, FH = Fired Heater, CW = Cooling water, WW = Wastewater. The FU is 1 MJ of liquid fuel blend.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1sFT** | **MTJ** |  |  | **1sFT** | **MTJ** |  |
| **Inputs** | **Quantity** | | **Units** | **Outputs** | **Quantity** | | **Units** |
| CO2 | 7.03∙10-2 | 7.15∙10-2 | kg | FU | 1.00∙100 | 1.00∙100 | MJ |
| H2 | 1.12∙10-2 | 1.29∙10-2 | kg | Electricity | 1.08∙10-2 | 7.50∙10-4 | kWh |
| HPS | 3.90∙10-2 | 8.63∙10-2 | MJ | CO2 | 5.55∙10-4 | 1.16∙10-3 | kg |
| FH | - | 2.69∙10-3 | MJ | CO | 3.71∙10-4 | 5.69∙10-4 | kg |
| CW | 2.19∙10-4 | 2.88∙10-4 | m3 | WW | 6.29∙10-5 | 7.60∙10-5 | m3 |

**Environmental impact assessment.** The environmental assessment is conducted in SimaPro 9.3, using Ecoinvent 3.9 Cut-Off database for the background process inventories. The business-as-usual (BAU) fossil-based liquid fuel alternative is assumed to be “Petroleum {Europe without Switzerland} | market for petroleum | Cut-off, U”, a liquid fuel with a LHV of 43.4 MJ/kg. The environmental KPIs are GWP100 alongside the monetized endpoint impacts to human health, ecosystem quality and resource scarcity, all computed with the ReCiPe2016 impact assessment methodology (Huijbregts *et al.* 2017) and using the monetization factors from Dong *et al.* (2019) converted to $2023.

* 1. Results and discussion
     1. Midpoint environmental impacts – global warming potential

The left plot of Figure 2 compares the GWPWTW of 1sFT and MTJ for the different carbon sources against BAU, with the error bars representing the uncertainty of the ecoinvent background data. Both alternatives achieve a significant reduction in GWPWtW, with 1sFT outperforming MTJ by 27-33% depending on the CO2­ source. Overall, 1sFT and MTJ reduce GWPWtW by over 70% and 60% compared to BAU, respectively. With DAC, the process credits for using CO2 correspond to the amount of CO2 removed from the atmosphere minus the indirect emissions related to DAC energy requirements; while with PPCC, CO2 procurement is responsible for 25-32% of the total GWPWtW, but the use phase emissions are 95% lower due to the biogenic CO2 content. Overall, the best performance is achieved when DACLGH is used followed by PPCC and DACLT. H2 production contributes 9.4∙10-3 kgCO2-eq/MJfuel, 1sFT and 1.0∙10-2 kgCO2-eq/MJfuel, MtJ of GWPWtW, while indirect emissions related to hot utilities are ~55% lower in 1sFT compared to MTJ. Finally, the direct emissions from both processes are negligible with PPCC and account only for ~2% of GWPWtW with DAC.

* + 1. Endpoint analysis and total cost

The right plot of Figure 2 compares the total cost (TC) of 1sFT and MTJ against BAU. From an economic point of view all the options come significantly more expensive than using fossil fuel. H2 procurement is always the dominant cost, representing 82% and 77% of the LCP in 1sFT and MTJ, respectively, when the cheapest CO2 alternative (PPCC) is used. With DAC, the cost of CO2 makes up 23-36% of the LCP depending on the heat source. It is worth noting that the CapEx of 1sFT is 40% lower compared to MTJ, but since the LCP is mainly determined by the operating costs the LCP1sFT is only 14-20% lower than LCPMTJ depending on the H2 and CO2 prices.

Figure 2: Enviro-economic results for the 1sFT, MTJ and BAU routes, using green H2 and CO2 from carbon capture in a pulp and paper mill (PPCC), low temperature direct air capture (DAC-LT) and DAC using low grade heat (DAC-LGH). Left: Well-to-Wake GWP, square symbols indicate net GWP100; Right: total cost (TC) including environmental externalities.

The monetized externalities cost is always lower than BAU, but burden shifting is occurring between GWP (where SAF is performing better than BAU as previously discussed) and other midpoint environmental impacts including particulate matter formation, human toxicity, land use, and water consumption (where SAF is performing worse). This results in overall damage to human health spanning between 1.10∙10-2 $/MJ and 1.18∙10-2 $/MJ, compared to 1.16∙10-2 for BAU. Burden shifting also affects damage to ecosystem quality, but all the SAF options have a lower overall impact compared to BAU. Looking at the damage to resource availability, DACLT is the least sustainable option with a reduction of only 30-35% compared to BAU. Despite the lower externalities costs all the SAF options have a higher TC than BAU, with the best alternative (1sFTPPCC) having a 48% higher TC, and the worst alternative (MTJDAC-LT) a ~2.3 times higher TC than BAU.

In the optimistic scenario, the LCP of 1sFT decreases to 25.8 $/GJ if CO2,PPCC is used, only slightly higher than the cost of fossil fuels with a CO2 tax of 150 $/t (23 $/GJ), while all the other options remain 42-78% more expensive than BAU. In terms of total cost including externalities, TCBAU is 24-27% higher than TC1sFT and 2-5% higher than TCMTJ.

In terms of fuel blend composition, MTJ produces a higher percentage of SAF and light hydrocarbons, while 1sFT produces a higher percentage of gasoline. A detailed analysis of the effect of fuel composition is beyond the scope of the work, but alternatives to flaring such as a reforming reactor to convert the light hydrocarbons back into syngas to maximize the liquid fuel output could lead to more significant benefits in MTJ, while the fuel blend from 1sFT might require larger intervention at the refinery.

* 1. Conclusions

This paper presented an enviro-economic assessment of two processes for producing liquid hydrocarbons in the jet fuel range from CO2 and H2, an FT-based process and a methanol-mediated process. Green H2 from water electrolysis was considered along with two carbon sources: low temperature DAC, with heat provided by a natural gas boiler or a low-grade burden-free heat source, and biogenic CO2 captured from a pulp and paper mill. A one-step FT process using a novel catalyst was compared tothe MTJ process, assuming that the product blend is sent to an existing refinery. One key finding is that the FT process is superior both in economic and environmental terms to the MTJ process, due to a lower capital cost, lower heating requirements, and higher energy efficiency. Importantly, all the alternatives considered can qualify as SAF in the UK since they achieve 60-80% GWP reduction on a life-cycle basis, with the largest reduction obtained when DAC with low-grade heat is combined with the FT process. Our environmental assessment also quantified endpoint impacts, confirming a better overall environmental performance of the synthetic fuels compared to fossil fuels, with 60% reduction for the FT process in an optimistic scenario. Nevertheless, the proposed low-carbon synthetic fuels are significantly more expensive than fossil fuels, and even if the prices of H2 and CO2 were to decrease, policy interventions such as carbon taxation would likely remain necessary to make SAF competitive. Future work will focus on adding more options for H2 and CO2, including blue hydrogen, alternative DAC processes, biomass gasification and other biogenic carbon sources. Moreover, reforming of the light hydrocarbons and unreacted syngas will be evaluated in order to minimize the CO2 andH2 requirements.

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