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# Techno-economic Assessment of Sustainable Aviation Fuel Production via $H_2/CO_2$-Based Methanol Pathway

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## ABSTRACT

To achieve long-term greenhouse gas neutrality in aviation, replacing fossil aviation fuels with Sustainable Aviation Fuels (SAF) from renewable sources is essential. A SAF production process from renewable hydrogen and carbon dioxide, was designed using Aveva Process Simulation, followed by comprehensive economical assessments. The designed process leads to an annual production of 37kt of SAF, with 97% of the molecules featuring a carbon chain length between 8 and 16. This output indicates a robust and targeted production capability. With an in-depth optimization of the methanol reactor, it was found that the profitability of the plant aligns with other SAF studies, demonstrating a Minimum Selling Price of Product of $2.46/kg after Heat Integration. In terms of economic profitability, the production of SAF using the methanol pathway appears to be an alternative to other SAF production pathways such as Fischer-Tropsch process but resides dependent on the evolution of $H_2$ production technologies, novel SAF production processes and environmental regulations. Despite this, the price remains higher than the current cost of fossil jet fuels, posing a competitive challenge.

**Keywords**: Alternative Fuels, Modelling and Simulations, Methanol, Technoeconomic Analysis

## INTRODUCTION

To limit global warming to 1.5°C, the Paris Agreement of 2015 established goals for reducing greenhouse gas emissions [1]. The transportation sector is a major contributor to emissions, and the aviation field is no exception, accounting for 2.5% of global emissions [2]. By 2025, SAF production will be predominant through the Hydrotreated Esters and Fatty Acids (HEFA) pathway, which will account for 99% of production (42.1 Mt). The HEFA process can reduce greenhouse gas emissions by up to 85% compared to fossil jet fuels, whereas Power-To-Liquid processes have the capability to achieve a 100% reduction [3]. One Power-To-Liquid pathway involves using renewable hydrogen and carbon dioxide to produce methanol, which can then be converted into SAF using the ExxonMobil process [4]. Although SAF production from $H_2$ and $CO_2$ is still under development, it is necessary to evaluate the economic potential of this process. This study explores the process design, optimization and economic viability of the production of SAF from $H_2$ and $CO_2$.

## MATERIAL AND METHODS

### Process Design

The production of SAF from $H_2$ and $CO_2$ consists of 4 main steps: methanol is first formed based on equation 1. Secondly it is turned into dimethyl ether and further to olefins through the Methanol-To-Olefins (MTO) process (equations 2 and 3). Olefins are then converted into longer olefins in the Mobil-Olefins-to-Gasoline-and-Distillate (MOGD) process (equation 4) and finally converted to paraffins through hydrogenation (equation 5).

$$CO_2 + 3\,H_2 \leftrightarrow CH_3OH + H_2O \quad (1)$$

$$2\,CH_3OH \leftrightarrow CH_3OCH_3 + H_2O \quad (2)$$

$$n\,CH_3OCH_3 \leftrightarrow 2\,(CH_2)_n + n\,H_2O \quad (3)$$

$$2\,(CH_2)_n \leftrightarrow C_{2n}H_{4n} \quad (4)$$

$$C_{2n}H_{4n} + H_2 \leftrightarrow C_{2n}H_{4n+2} \quad (5)$$

The process is modelled using the equation-based software Aveva Process Simulation 2024 (APS). The sizing of equipments is based on basic Chemical Engineering Principles and APS modelling assumptions. The process is designed with the following objectives: 37kt/year of kerosene with a purity of 91.3% of C8-C16 Hydrocarbons. The choice of quantity is based on the average value of kerosene from existing and future SAF production projects [5,6]. The purity is based on the percentage of non-desired products from the High Biofuel Blends in Aviation Final Report [7]. Additionally, Liquefied Petroleum Gas (LPG), gasoline and diesel are co-products of the process. Furthermore, Heat Integration (HI) was performed on the major hot and cold streams of the process with a heat duty higher than 200kJ/s.

## Sensitivity analysis

While the process of SAF production and its reactions are studied in the literature, the impact of key design parameters is often neglected, especially for the methanol formation reactor in a SAF production process. An in-depth sensitivity analysis was performed on the methanol reactor to optimize the conversion of reactants. Sensitivity analysis was performed on the temperature, pressure, and reactor design (diameter, length, number of tubes).

## Economical Assessment

The economical assessment was performed on the process for different scenarios. A Matlab script of a Discouted Cash Flow Rate (DCFR) model for Monte-Carlo simulations is used based on 7 input parameters: price of reactants ($H_2$ and $CO_2$), price of Kerosene Fixed Capital Cost (FCI), Working Capital (WC), Operational Cost (OPEX) and Income Tax Rate. The plant is located in Denmark with a lifetime of 20 years.

## Input parameters

### Fixed Capital Investment

The Fixed Capital Investment (FCI) includes the purchase of equipments and their installation. The price of a single piece of equipment is taken from APS 2024 and based on the Chemical Engineering Plant Cost Index (CEPCI) of 2022 (816.0) [8]. This library uses a factorial method considering the Lang factors for the cost of purchase and installation of equipments. The fixed capital cost is calculated using the following formula:

$$C_f = f_L * C_e \quad (6)$$

Where $f_L$ is the Lang factor and $C_e$ is the total delivery cost of all the major equipment items.

The Lang factor is already implemented in Aveva and set to $f_L$=*5.93* for the total capital investment which is the recommended value from Aveva for a fluids processing plant. The total capital cost is equal to the sum of the FCI and the working capital calculated directly from APS. This investment in cost is divided over the first two years.

### Operational Cost (OPEX)

The cost of operations includes the heating and cooling of the streams, the electricity furnished to the process and the cost of raw material and catalyst (assumed to be replaced every 2 years). The cooling of streams is assumed to be done with water or glycol while the heating is assumed to be from steam (low pressure at 160°C, medium pressure at 184°C and high pressure at 254° C) [9]. These costs include the operating costs to generate the utility and the price of the circulated cooling or heating system. Moreover, based on the Danish grid, the cost of electricity is taken as 0.095$/kWh [10]. Operational cost also includes the price of raw material. Finally, the economic assessment needs to take the price of products into account. The perturbation and distribution of reactant and kerosene prices are based on a list of current literature values. The lower, average and upper values are presented in Table 1.

**Table 1:** Lower, average and upper values used for the uncertainty analysis [11-13]

| Parameter | Lower value | Average value | Upper value |
|---|---|---|---|
| $H_2$ price ($/kg) | 1.27 | 3.00 | 10.13 |
| $CO_2$ price ($/kg) | 0.06 | 0.10 | 1.27 |
| Kerosene price ($/kg) | 0.86 | 3.25 | 6.06 |

## Output parameters

Five outputs parameters are studied with their uncertainty:

- The Return of Investment (ROI) is taken as the average of the annual net profit calculation divided by the total investment capital.
- The Payback Period (PBP) is obtained by dividing the FCI by the average of annual operating cash flow.
- The Net Present Value (NPV) is equal to the sum of present worth of annual cash flow of each year of the plant life.
- The Discounted Cash Flow Rate (DCFR) is the iterated discount rate corresponding to a NPV

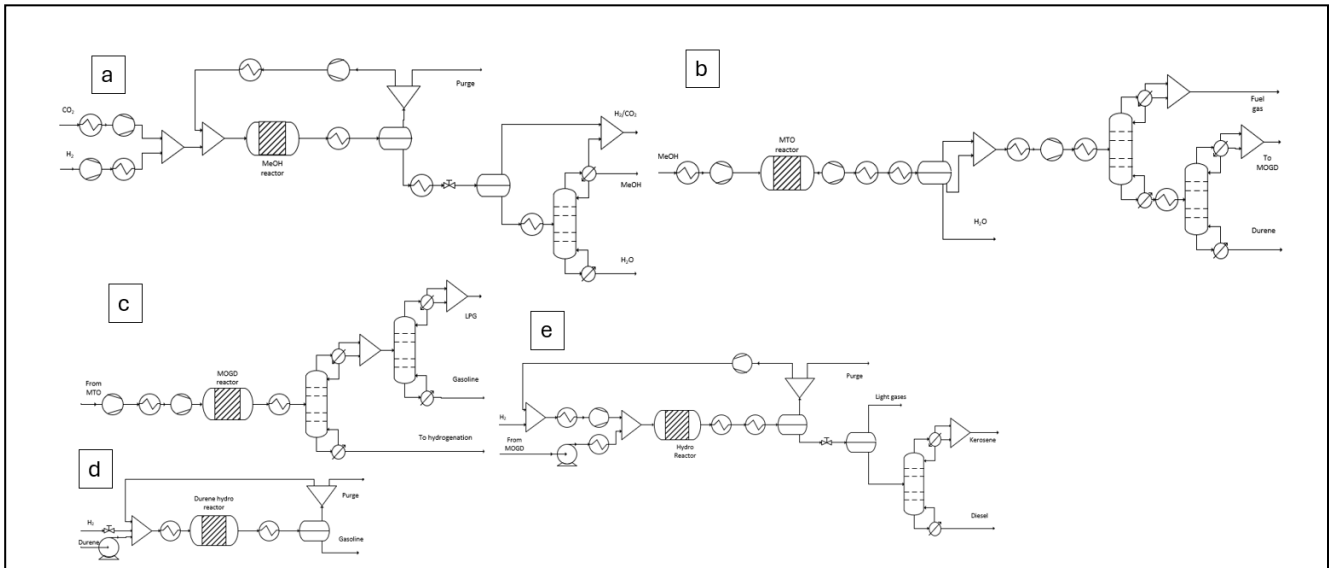


**Figure 1:** Complete process of the production of kerosene from $H_2$ and $CO_2$: Formation of methanol (a), Methanol-To-Olefins (b), Mobil-Olefins-To-Gasoline-and-Distillate (c), Durene Hydrogenation (d), Olefins Hydrogenation (e)

equal to zero.

- The Minimum Selling Price of Product (MSEP) is the price of SAF corresponding to an NPV equal to zero.

The Monte-Carlo simulations are done with 500 iterations and returns the average and standard deviation of each value. The perturbations and distributions for the Monte-Carlo Analysis are presented in table 2. For reactant and product prices, a lognormal distribution has been chosen to fit with the range of prices found in literature [11-13]. Additionally a Latin Hypercube Sampling function is applied to the input parameters to represent their distribution within the minimum and maximum values.

**Table 2:** Perturbation and distribution of inputs parameters for uncertainty and sensitivity analysis of the economical assessment

| Parameter | Perturbation (%) | | Distribution |
|---|---|---|---|
| FCI | -30 | +30 | Normal |
| WC | -20 | +50 | Uniform |
| $H_2$ price | -60 | +230 | Lognormal |
| $CO_2$ price | -40 | +1170 | Lognormal |
| Kerosene price | -70 | +90 | Lognormal |
| OPEX | -30 | +30 | Normal |

# RESULTS AND DISCUSSION

## Final process

The final process is presented in figure 1. In a boiling-water reactor, $H_2$ and $CO_2$ are first converted into methanol and water which are then separated in a distillation column. A kinetic model based on Froment et al. work is implemented [14] over a $Cu/ZnO/Al_2O_3$ catalyst. The second part from methanol to SAF is based on the conversion models from Ruokonen's work [11]. Four reactors are implemented using the zeolite catalyst HZSM-5: the conversion of methanol to olefins (b), the formation of higher olefins (c), the hydrogenation of durene to form a part of the gasoline (d) and the hydrogenation of olefins to form kerosene and diesel (e). Additionally, the ratio kerosene/reactants is based on Ruokonen's work [11] for a production of 37kt of kerosene for 66kt of $H_2$.

## Sensitivity Analysis

### Comparison with experiment

A Sensitivity Analysis was performed on the methanol formation reactor. First the kinetic model needs to be validated with experimental data. The $CO_2$ hydrogenation (equation 8) and Reverse Water Gas Shift (equation 9) are considered to model the methanol formation:

$$CO_2 + 3\,H_2 \leftrightarrow CH_3OH + H_2O \quad (8)$$

$$CO_2 + H_2 \leftrightarrow CO + H_2O \quad (9)$$

As the kinetic model from Froment et al. fits with the experimental data, the model implemented in Aveva Process Simulation is compared with the model implemented by Froment et al. [14]. This comparison is performed for a laboratory scale plug flow reactor with a feed composed of 4 mol% of CO, 82 mol% of $H_2$, 3 mol% of $CO_2$ and 11 mol% inert. The results are presented in Table 3.

The implementation on Aveva fits with the referenced model and therefore with the experimental data. The applied model can be the subject of further studies.

**Table 3:** Comparison of the component fraction at the outlet of the methanol reactor for the model implemented in APS and the model implemented by Froment et al. [14]

| Component | APS model | Froment et al. model |
|---|---|---|
| CO | 0.030 | 0.030 |
| $CO_2$ | 0.021 | 0.021 |
| $H_2$ | 0.801 | 0.801 |
| $CH_3OH$ | 0.023 | 0.023 |
| $H_2O$ | 0.011 | 0.011 |

## Key-design parameters

The key-design parameters of the methanol formation reactor are studied to optimize the carbon conversion to methanol. The initial design is based on the Luyben et al. model of the methanol formation [15]. The methanol formation reaction being exothermic, the reactor is modelled as tubular with an external utility to cool down the fluid. The diameter of the tubes is set as D=0.03675 m, the smallest diameter available, to maximize the heat exchange, with a heat transfer coefficient of 244 $kcalh^{-1}m^{-2}K^{-1}$ [15]. The volume is calculated from the Gas Hourly Space Velocity used in the literature GHSV=3.348 $kg/kg_{cat}/h$ [15]. Hence, for a number of tubes $N_t$=4000, the length of the reactor is L=4 m with a feed of 66kt/year of $H_2$ and 480 kt/year of $CO_2$. Moreover, the pressure drop inside the reactor is assumed to be equal to 1 bar.

The evolution of carbon conversion with the pressure inside the reactor is plotted figure 2. The carbon conversion is defined as the following:

$$conv = \frac{n_{in}(CO_2) - n_{out}(CO_2)}{n_{in}(CO_2)} \quad (10)$$

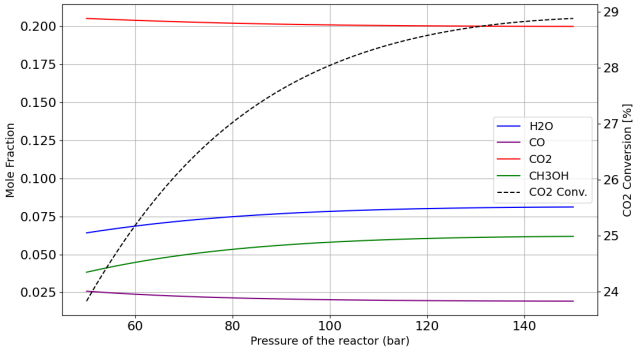


**Figure 2.** Evolution of the gas composition and the carbon conversion at the outlet of the methanol reactor with the inlet pressure at fixed temperature ($T_{feed}$=423.15K)

The carbon conversion increases with the pressure of the reactor. However, the conversion stabilizes after 150 bar. Hence, P=110bar is chosen to optimize the conversion while lowering the operational cost.

Additionally, the evolution of the carbon conversion is studied figure 3 with the variation of temperature. The carbon conversion increases with the temperature of the reactor until 540K before decreasing due to the main reaction of $CO_2$ hydrogenation being exothermic and the competitive reaction (Reverse Water Gas Shift) being endothermic.

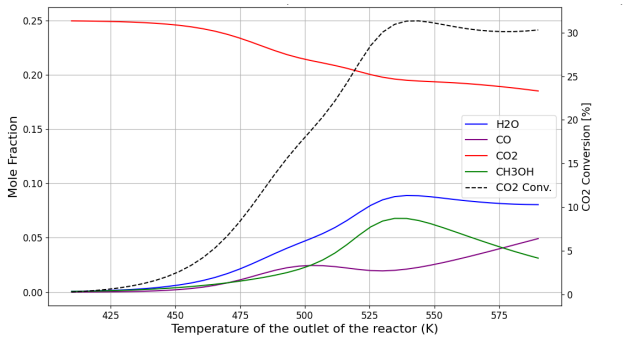


**Figure 3.** Evolution of the gas composition and the carbon conversion at the outlet of the methanol reactor with the outlet temperature (P=110bar, $T_{feed}$=423.15K)

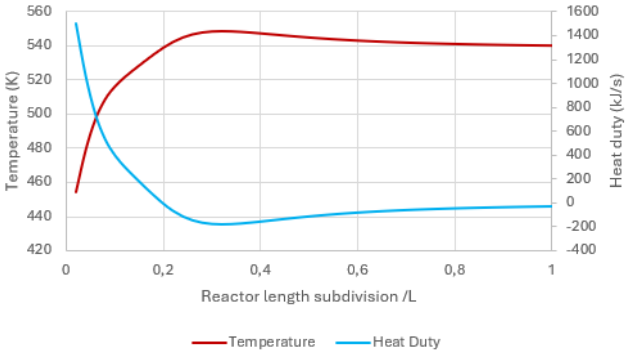


**Figure 4.** Evolution of the temperature and heat transfer duty inside the methanol formation reactor ($Duty_{tot}$=1465 kJ/s)

**Table 4:** Key-design parameters of the methanol formation reactor

| Parameter | Value |
|---|---|
| Pressure (bara) | 110 |
| $T_{out}$(K) | 540 |
| Number of tubes | 4000 |
| Diameter of the tubes (m) | 0.03675 |
| Length of the tubes (m) | 4 |
| Volume ($m^3$) | 17 |
| Catalyst | Cu/ZnO/Al2O3 |
| Catalyst mass (kg) | 15 054 |
| Catalyst volumic mass ($kg/m^3$) | 1 775 |

Consequently, the utility of the reactor is modelled to obtain an outlet temperature of the reactor equal to

540K. The evolution of temperature and heat transfer inside the final model of reactor is presented figure 3 while the final reactor design parameters are presented in table 4. All the parameters listed in Table 4 influence the final conversion, and their optimal values were determined through univariate analysis. However, an additional assessment considering their interdependencies could improve the optimization process.

### Heat Integration

The cumulative heats are presented in figure 5. As no pinch point exists, the heat exchangers are combined freely if heat is transferred from warm streams to cold streams (with threshold set to $\Delta T_{min}$ = 10K). The resulting optimization of cost after Heat Integration is presented in table 5.

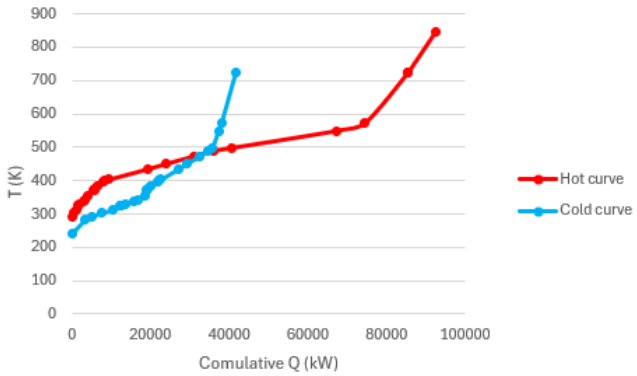


**Figure 5.** Cumulative heat of the hot and cold streams

**Table 5:** Reduction of duties and cost after HI

| | Duty reduction (kW) | Cost reduction ($million/year) |
|---|---|---|
| Cooling | 39 701 | 0.43 |
| Heating | 39 701 | 2.33 |
| **Total** | **79 401** | 2.76 |

## Economic Analysis

The economical analysis is performed for the overall process from the purchase of $H_2$ and $CO_2$ to the retailing of kerosene and its co-products. The mean value of the input parameters for the Monte-Carlo simulation are presented in table 5. The resulting distribution is plotted in figure 6 and 7 and matches with the expected distribution from table 2 for all 7 inputs parameters.

Figure 8 and Table 6 show the results of the economic assessment. The value of MSEP ($2.46/kg) fits with previously published values [11-13] but remain however higher than $0.68/kg the current price of fossil-based kerosene in Denmark [16]. Additionally, the purchase of hydrogen accounts for 78% of the total OPEX with an extremely wide range of price values (see Table 1). This results in a high standard deviation of all the output parameters.

**Table 6:** Mean Value of the input parameters for the economic assessment

| | $million | $million/year |
|---|---|---|
| FCI | 144.9 | |
| Working Capital | 22.6 | |
| **Total CAPEX** | 167.5 | |
| Utility | | 15.3 |
| Raw materials | | 249.1 |
| **Total OPEX** | | **264.4** |
| **Sales** | | **304.2** |

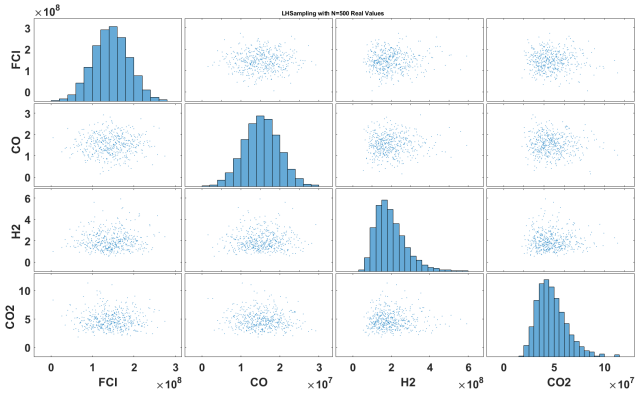


**Figure 6.** Real value distribution of the first 5 input parameters for the Monte-Carlo simulation

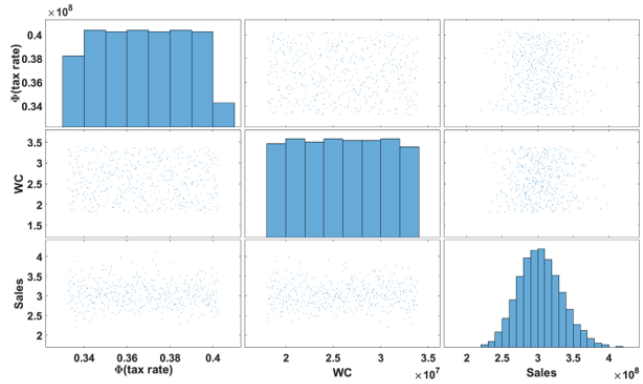


**Figure 7.** Real value distribution of the last 5 input parameters for the Monte-Carlo simulation

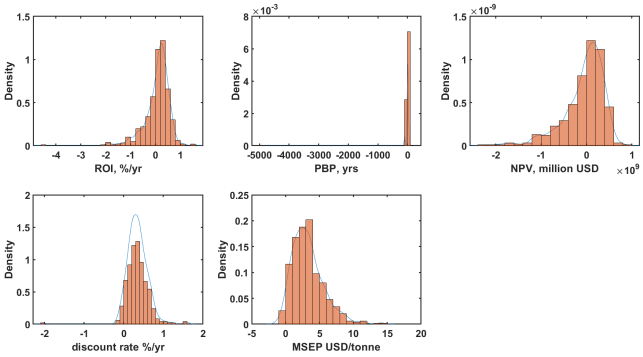


**Figure 8.** Density value of the ouput parameters of the Monte-Carlo simulation (N=500)

**Table 7:** Avearge and Standard Deviation of the ouput parameters of the Monte-Carlo simulation (N=500)

| | Average | Standard deviation |
|---|---|---|
| ROI (%/year) | 0.09 | 0.47 |
| PBP (years) | 5.87 | 50.52 |
| NPV ($million) | -50.5 | 448.2 |
| MSEP ($/kg) | 2.46 | 2.30 |

## CONCLUSION

The process design of SAF from $H_2$ and $CO_2$ appears to be a promising process for the development of alternative fuels. As the quantity of raw materials mainly impacts the final price of SAF, the conversion into methanol must be the subject of an in-depth study. A boiling-water reactor with V=17m³, P=110bara and $T_{out}$=540K is chosen for the final design.

While the Minimum Selling Price of the produced kerosene ($2.46/kg) falls into the range of previous techno-economic assessments, it remains non-competitive against fossil-based aviation fuels. Additionally, a significant sensitivity to the price of hydrogen leads to considerable uncertainty on the result. Hence, the economic viability of SAF is highly dependent on innovations in performance, cost-breakdown electrolyzer technologies along with governmental regulation on fossil-based kerosene usage. Finally, novel concepts for Sustainable Aviation Fuel (SAF) synthesis could potentially reduce aviation fuel production costs, opening pathways for more sustainable air transportation in the future.

## ACKNOWLEDGEMENTS

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