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Study of the Base Case in a Comparative Analysis of Recycling Loops for Sustainable Aviation Fuel Synthesis from CO_2

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ABSTRACT

This study investigates a low-temperature cobalt-based Fischer-Tropsch (FT) process integrated with a high-temperature reverse water-gas shift (RWGS) reaction unit for CO production, with the aim of synthesizing kerosene-like hydrocarbons. Specifically, the paper focuses on the base case of a comparative analysis of various recycling loop configurations for this process. Two reaction unit models, one for each reaction, previously developed in Aspen Custom Modeler (ACM), are combined in a single Aspen Plus (AP) process simulation. The base case involves the recycling of unreacted gases and light hydrocarbons back to the inlet of the FT reactor, as typically found in the literature. Simulation results demonstrate a carbon efficiency of 42.3% toward kerosene, highlighting the need for further treatment steps and by-products valorization.

Keywords: Fischer-Trospch, reverse water-gas shift, process modelling, recycling loop, kinetics

INTRODUCTION

Amid global efforts to combat climate change, sustainable aviation fuels are recognized as a key solution for reducing hard-to-abate CO_2 emissions. Power-to-fuel processes have emerged as a promising approach to fuel synthesis by substituting crude oil with captured CO_2 as the carbon source. The conversion of CO_2 into the desired fuel relies on the FT reaction, preceded by the transformation of CO_2 into CO through the RWGS reaction. Although this process has been extensively studied in the literature, existing studies propose varying process configurations, driven by differences in recycling strategies. Specifically, the point where recycled gases are reintegrated into the loop varies, with some studies recycling to the inlet of the RWGS reactor [1], others to the inlet of the FT reactor [2], and some to both inlets simultaneously [3]. Some studies include a conversion step in the recycling loop to convert light gases into reactants, using partial oxidation or steam reforming [2,3].

However, a comprehensive comparison of these different recycling configurations remains absent from the literature. This paper addresses this gap by presenting the first scenario of a broader study that aims to compare various recycling configurations on a consistent basis. This scenario focuses on recycling unreacted gases and light hydrocarbons exclusively at the FT reactor inlet.

MATERIALS AND METHODS

Two reaction unit models, developed in ACM, serve as the core components of the process simulation. The first reaction unit models the RWGS reaction, where CO_2 is converted into CO through its reaction with H_2:

$$CO_2 + H_2 \rightleftharpoons CO + H_2O \tag{1}$$

This model incorporates specific kinetics for the RWGS reaction as well as for methanation side reactions, which are further detailed in previous work [4]. The second model simulates the FT reaction, where the CO yielded in the RWGS unit polymerizes to form hydrocarbon chains, represented as follows:

$$n\,CO + (2n+1)\,H_2 \rightleftharpoons C_nH_{2n+2} + n\,H_2O \tag{2}$$

$$n\,CO + 2n\,H_2 \rightleftharpoons C_nH_{2n} + n\,H_2O \tag{3}$$

The kinetics implemented in the FT model capture deviations from the ideal Anderson-Schulz-Flory FT product distribution, accounting for side reactions [5].

These two ACM models are integrated into an AP process model, illustrated in Figure 1. The separation section consists of flash separators designed to maximize the yield of kerosene-like hydrocarbons (C_8-C_{16}).

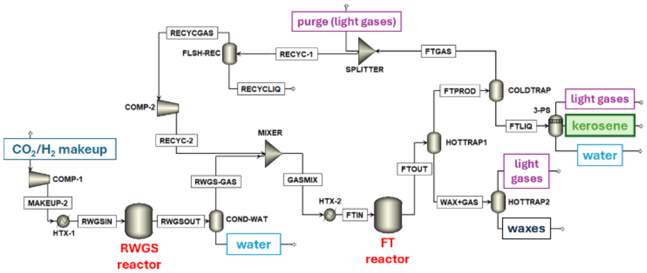

Figure 1. Aspen Plus process flowsheet

RESULTS AND PERSPECTIVES

The process scale in this study is based on the pilot project currently under development at ULiège, designed for an H_2 makeup flow rate of 1.5 Nm³/h. The H_2/CO_2 ratio is set to 2.22 to achieve an H_2/CO ratio of 2.1 at the FT reactor inlet, as this ratio maximizes the selectivity toward kerosene-like hydrocarbons. The RWGS unit operates at 850 °C and 20 bar, achieving a CO_2 conversion of 70% with a CO selectivity exceeding 97%. Figure 2 shows the distribution of FT products at the FT reactor outlet (220 °C, 20 bar), with a significant proportion of light gases due to a large recycle stream induced by a low purge ratio (5%). Figure 2 also illustrates the FT product distribution in the kerosene stream leaving the process, highlighting that over 84% of the kerosene from the FT reactor exits through this stream. Further conversion of other fractions into kerosene could enhance its purity.

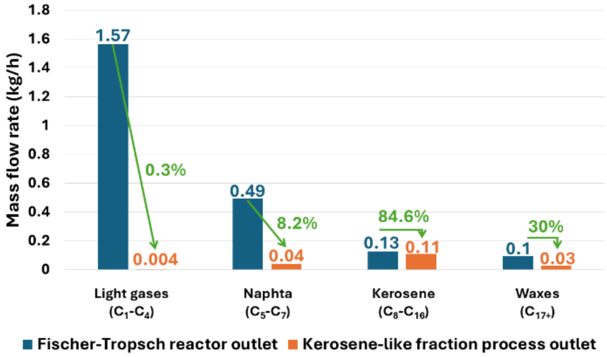

Figure 2. FT product distribution in the FT reactor outlet stream and the kerosene-like stream at the process outlet. The percentages indicate the ratio of each product fraction's flow rates between the two streams.

Under these conditions, the carbon efficiency, defined as the ratio of carbon mass entering the process to carbon mass contained in the kerosene-like fraction leaving the process, reaches 42.3%, emphasizing the need for more advanced treatment steps and by-products valorization. These results represent the first scenario in a comparative study based on carbon and energy efficiency metrics. Alternative recycling options will be explored starting from the simulation derived for this initial case, ensuring a consistent basis for comparison. Further details on this study and the comparison methodology will be provided in a forthcoming article.

ACKNOWLEDGEMENTS

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REFERENCES

1. Stefan B., Bullerdiek N., Voß S., and Kaltschmitt M. Kerosene Production from Power-Based Syngas – A Technical Comparison of the Fischer-Tropsch and Methanol Pathway. Fuel 366 (2024) https://doi.org/10.1016/j.fuel.2024.131269
2. Boilley J.H., Berrady A., Bin Shahrel H., Gürbüz E., and Gallucci F. Energy Analysis of a Power-to-Jet-Fuel Plant. International Journal of Hydrogen Energy 58 (2024) https://doi.org/10.1016/j.ijhydene.2024.01.262
3. Adelung S., Maier S., and Dietrich R-U. Impact of the Reverse Water-Gas Shift Operating Conditions on the Power-to-Liquid Process Efficiency. Sustainable Energy Technologies and Assessments 43 (2021) https://doi.org/10.1016/j.seta.2020.100897.
4. Rouxhet A., and Léonard G. The Reverse Water-Gas Shift Reaction as an Intermediate Step for Synthetic Jet Fuel Production: A Reactor Sizing Study at Two Different Scales'. In Computer Aided Chemical Engineering, 53:685–90. Ed: Elsevier (2024)
5. Pandey U., Runningen A., Gavrilović L., Jørgensen E. A., Putta K. R., Rout K. R., Rytter E., Blekkan E. A., and Hillestad M. Modeling Fischer–Tropsch Kinetics and Product Distribution over a Cobalt Catalyst'. AIChE Journal 67 (2021). https://doi.org/10.1002/aic.17234.