# CO<sub>2</sub> hydrogenation through direct Fischer-Tropsch Synthesis including methane reforming as a novel scenario

Khashayar Yaghoubi<sup>1</sup>\*, Tuomas Koiranen<sup>2</sup>

1,2 Lappeenranta-Lahti University of Technology, LUT School of Engineering Science, Mukkulankatu 19, FI-15210 Lahti, Finland

\*Corresponding author:khashayar.yaghoubi@lut.fi

#### Highlights

- Reactors cofiguration investigation
- Products selectivity and distribution investigation
- Adding DMR and WGS reactor to the system as a novel scenario

# 1. Introduction

The escalating global demand for fuels alongside the imperative to diminish greenhouse gas levels has sparked significant interest among researchers in converting  $CO_2$  into hydrocarbons through hydrogenation processes. This conversion, particularly into liquid fuel range hydrocarbons, can be achieved using either a methanol-mediated pathway or Fischer-Tropsch Synthesis (FTS). In the methanol mediated process,  $CO_2$  is first turned into methanol and subsequently processed into hydrocarbons [1, 2, 3]. For converting  $CO_2$  through the Fischer-Tropsch (FT) process two primary approaches have been explored: the direct route and the indirect route. The indirect route involves two separate reactors, initially converting  $CO_2$  into CO via the RWGS reaction and subsequently employing the produced CO in the traditional FT synthesis. Alternatively, a more challenging route involves the direct conversion of  $CO_2$  with  $H_2$  into hydrocarbons. However, this method is considerably more intricate due to various constraints, necessitating a catalyst capable of facilitating both  $CO_2$  into CO conversion and the FT reactions [4]. The direct approach involves merging  $CO_2$  reduction into syngas using the reverse water gas shift (RWGS) Reaction Eq.1 and the subsequent hydrogenation of CO to hydrocarbons (HCs) via Fischer-Tropsch Synthesis (FTS) Eq.2 and 3 in the same reactor system [5, 6, 7].

1) 
$$CO_2 + H_2 \rightleftharpoons CO + H_2O$$
 (1)

2) 
$$nCO + (2n+1)H_2 \rightarrow C_nH_{2n+2} + nH_2O$$
 (2)

3) 
$$nCO + 2nH_2 \rightarrow C_nH_{2n} + nH_2O$$
 (3)

This study is focused on the direct route despite its many challenges. The reasons are increasing of energetic efficiency, elimination of the cooling system in the whole process and specially its cost-effectiveness compared to the indirect route [8, 9]. In addition, there is a lot of room for innovation in this pathway compared to indirect. This paper is supposed to present a novel approach to solve the problem of the main unwanted byproduct, methane.

# 2. Methods

All the simulations will be done by Aspen Plus.

# 3. Results and discussion

The results of this study would be a comparison between different  $CO_2$  FTS process routes and configurations to realize that which route with which configuration will lead to lower methane selectivity and higher fuel yields. In each process concept the selectivity of main products and by-products such as methane will be investigated to see how the selectivity and yield of main products will be enhanced. Also, the in-situ and ex-situ water removal system for increasing the process efficiency will be studied. In addition, to solve the problem of the produced methane (unwanted byproduct), a new scenario will be studied. In this scenario the produced methane is separated and converted to CO and H<sub>2</sub> through Dry Methane Reforming (DMR) process. The produced H<sub>2</sub> is recycled as a part of the feed and the DMR is

followed by a WGS reactor to produce  $CO_2$  and  $H_2$ . The required water for WGS reaction is provided from water removal system. Finally, the produced  $CO_2$  and  $H_2$  are recycled to the beginning of the process as feed (Figure 1). The obtained results of this study will be compared with the results from Kamkeng and Wang's work to justify this scenario. They studied three different process configurations for direct  $CO_2$  FTS [10].

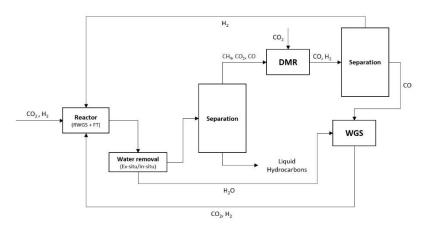


Figure 1. Direct FTS process configuration with additional DMR and WGS reactor.

#### 4. Conclusions

From the results comparison, it will be concluded that in which route with which operating conditions and configurations the best products selectivity and distribution will be obtained. Also, the best way for water removal can be determined. The investigation of the mentioned scenario in this study (adding DMR and WGS) will show if utilization of the unwanted produced methane can be feasible and affordable or not.

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# Keywords

Fischer-Tropsch, CO<sub>2</sub> Hydrogenation, Direct CO<sub>2</sub> Fischer-Tropsch