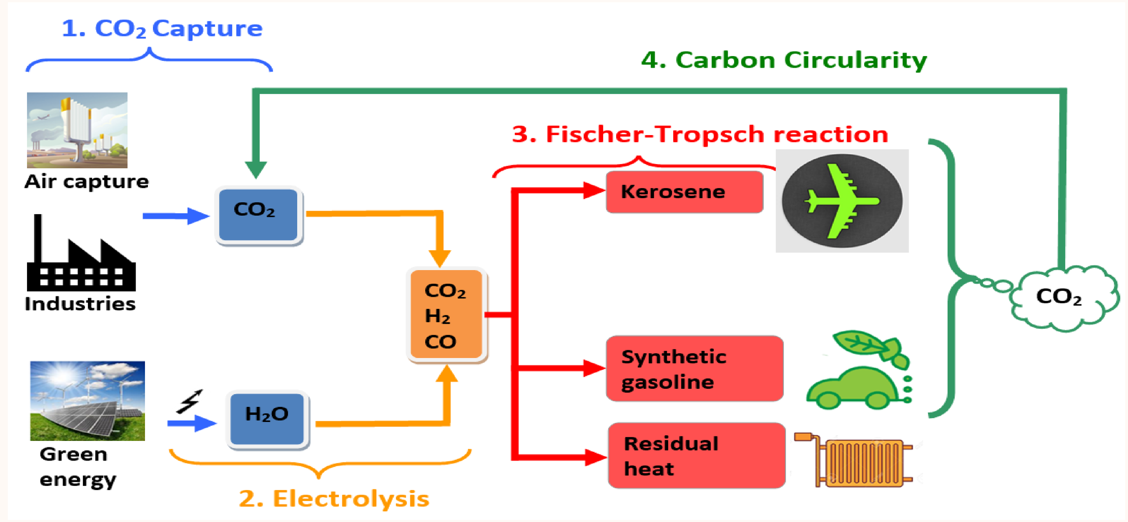
Design of a Fischer-Tropsch installation for jet fuel production using water-assisted vinylene mechanism for cobalt catalyst kinetics

A. Morales, G. Léonard
University of Liège, Department of Chemical Engineering – PEPs
www.chemeng.uliege.be

Introduction

Fischer-Tropsch (FT) technologies can contribute towards a sustainable world energy transition by transforming captured CO_2 and green hydrogen into a wide array of hydrocarbon chains, including jet fuel. Thus, difficult to electrify sectors of the economy such as the aviation sector could be defossilized. In this context, the present study simulates the FT reaction and designs a FT reactor serving as core of a future Power-to-Jet Fuel pilot-scale facility at the University of Liège (ULiège).



Power to Jet fuel diagram

Fischer-Tropsch model

- A reactor model was developed using Aspen Custom Modeler (ACM). It was then exported to Aspen Plus.
- The model improves upon the Pandey et al. (2021) FT model, which in turn adapted the kinetics model proposed by Rytter and Holmen (2018) and the stoichiometry proposed by Hillestad et al. (2015) for Re-promoted, Al_2O_3-supported cobalt catalyst.
- The model was validated at 230°C, 20 bar, a GHSV of 30 NmL/g*min and 1.6 H_2/CO. This test run achieved a conversion of 70% and selectivity towards C_{5+} of 83%. With our model, a conversion of 71% (error of 1.4%) and a selectivity of 80.1% (error of 3.75%) was attained.

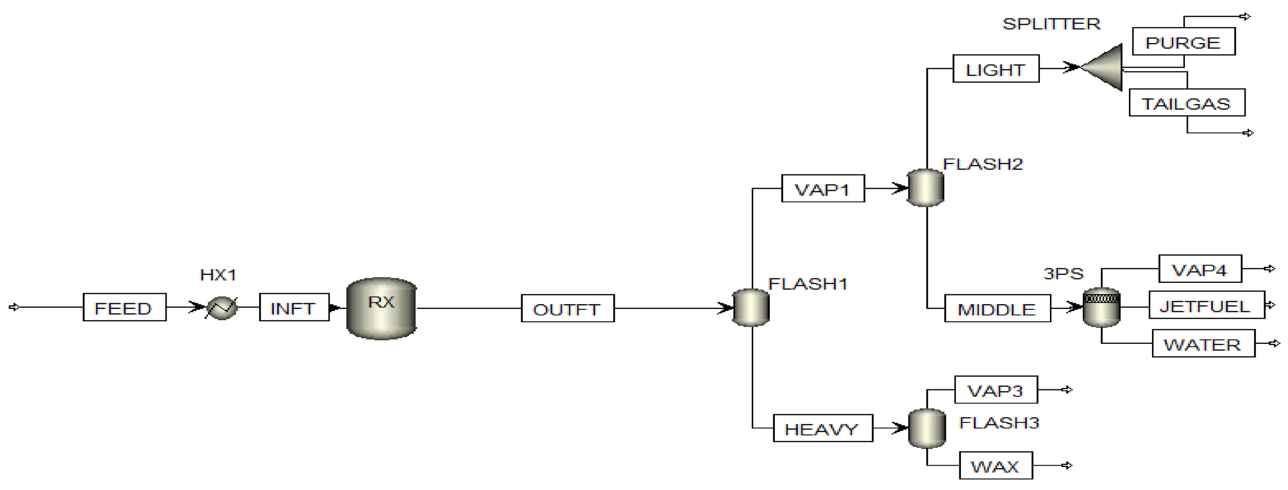
Main reactions:

FT reaction (Olefins):

$$U'H_2 + CO \rightarrow v'_n C_n H_{2n} + H_2O$$

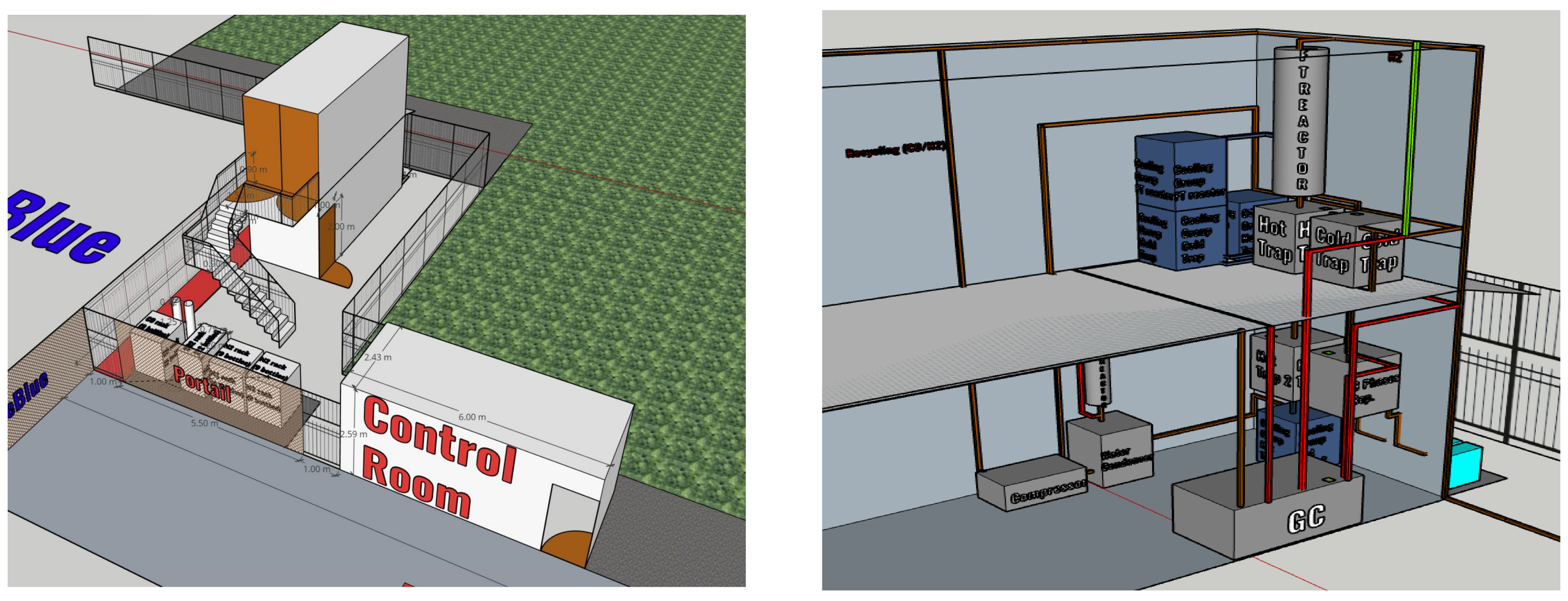
FT reaction (Parafins):

$$U''H_2 + CO \rightarrow v''_n C_n H_{2n+2} + H_2O$$



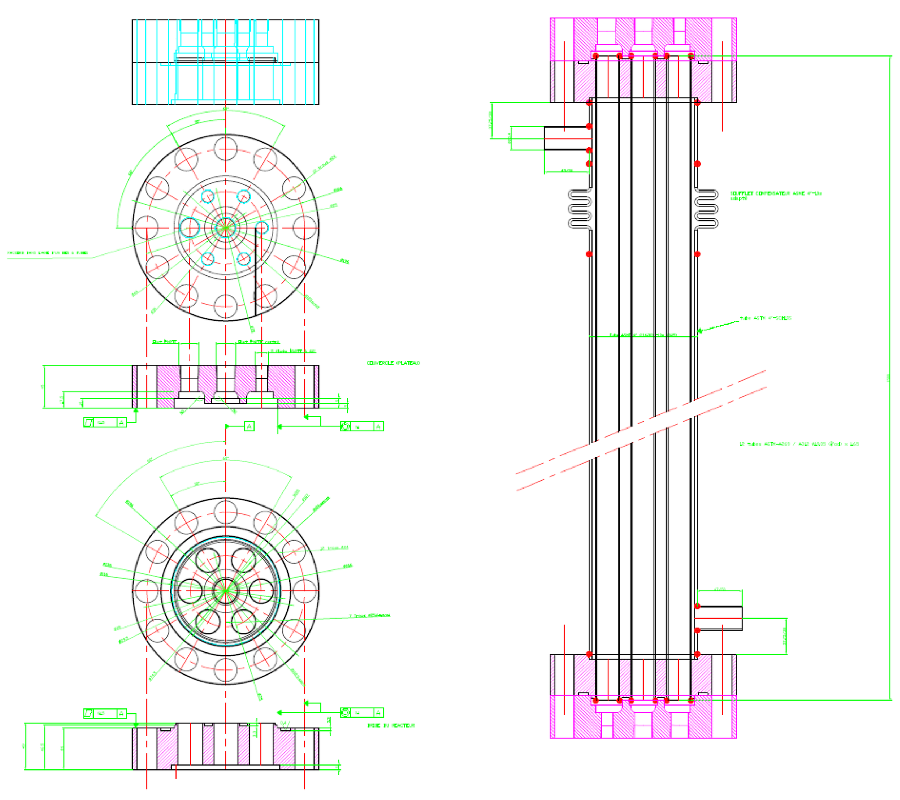
ACM + Aspen Plus simulation

- The installation has a hydrogen feed based on the total capacity of the 3 electrolysers at ULiège, 1.5 Nm³/h. The same conditions as the validation were chosen for the design of the reactor. Results are compared to a similar capacity cobalt-catalysed FT pilot plant from the Soletair project (Vidal, 2018).



Pilot plant layout

Results of the simulation



Parameter	Value	Units
Cata. Mass	1.5	kg
Cata. Diam.	1	mm
Length	1.50	m
Tube Diam.	20	mm
# Tubes	7	kg/hr

Technical drawing of the reactor and dimensions

Parameter	ULiège	Vidal (2018)	Units
Feed	2.2	3	Nm³/hr
Wax	0.16	0.148	kg/hr
Jet fuel	0.17	0.108	kg/hr
Gas	0. 57	0.656	kg/hr
Aq. Phase	0.45	0.429	kg/hr
Conversion	71	60	%
Carbon eff.	67.6	59.5	%
Hydrogen eff.	49.7	30.8	%

Single-pass model results

Conclusions

A model was developed showcasing a FT pilot-scale reactor achieving high conversion of CO and jet fuel selectivity. When compared to the Soletair project, results are in a similar order of magnitude thus validating the scale up. The performance of the future ULiège installation is overall better, due to the our focus on conversion and jet fuel maximization and potentially due to mass diffusion limitations that have yet to be integrated in the model. Future work will focus on validating our model with the results from the installation and on studying the integration of other sub-processes such as: carbon capture, electrolysis, RWGS, recycling, hydrocracking, among others.

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References: Hillestad, M., Modelling the Fischer-Tropsch distribution and model implementation. Chem. Prod. Process Model. 2015; 10: 147-159.
Pandey, U., Runningen, A., Gavrilović, L., et al. Modeling Fischer–Tropsch kinetics and product distribution over a cobalt catalyst. AIChE Journal. 2021; 67: e17234.
Rytter, E., Holmen, A., Consorted vinylene mechanism for cobalt Fischer–Tropsch synthesis encompassing water or hydroxyl assisted CO-activation. Topics in Catalysis. 2018; 61(9): 1024-1034.
Vidal, F., et al., Power-to-X technology using renewable electricity and carbon dioxide from ambient air: SOLETAIR proof-of-concept and improved process concept. Journal of CO2 Utilization. 2018; 228: 235 – 246.