Study of a Reverse Water-Gas Shift Reaction Unit for Integration in a Power-to-X Process

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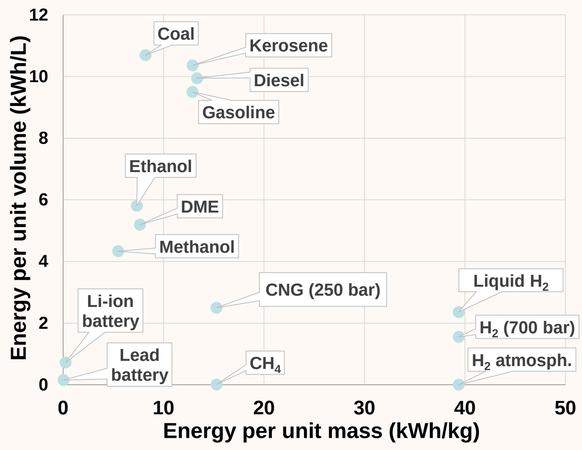
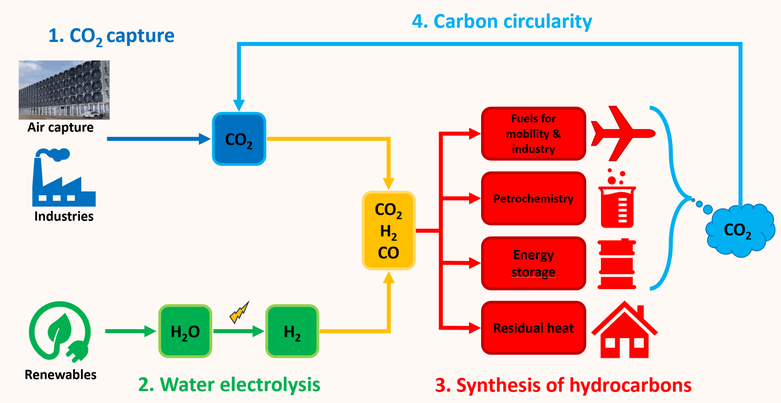
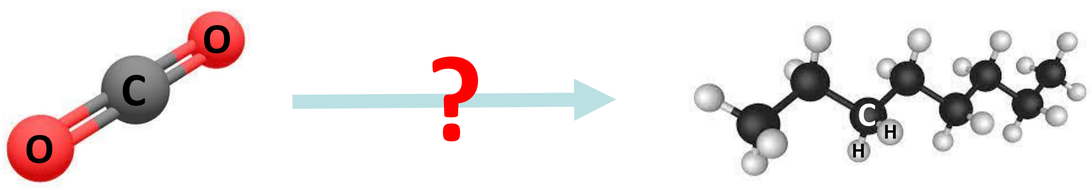
General Context

The energy sector is the largest contributor to global greenhouse gas emissions, with transportation accounting for 25% of energy-related emissions. Road vehicles are mainly responsible for these CO_2 releases into the atmosphere; great efforts are thus engaged to mitigate this issue. One part of the solution consists in increasing the share of electrified vehicles on the market and developing hydrogen-based transport. Although these solutions might be promising for road transportation, they seem to be limited options for long-freight ships and aircraft because of too low energy density reasons. Power-to-X processes offer the possibility to produce carbon-based fuels while being independent of fossil resources.

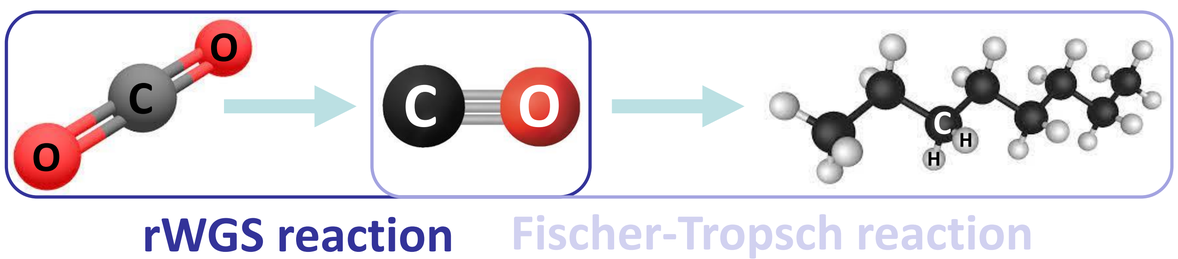




General Principle



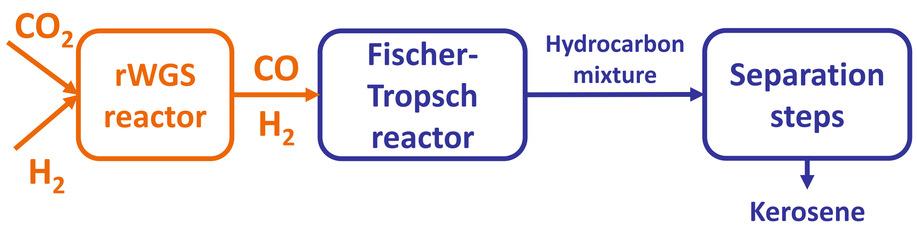
- **One-step synthesis** of long hydrocarbon chains from CO_2 is **challenging**
- CO_2 molecule is highly **stable**
- **C-C bonds** are difficult to form (**high energy barrier** to cross)
- Hydrocarbon **indirect synthesis** through the formation of an **intermediate**



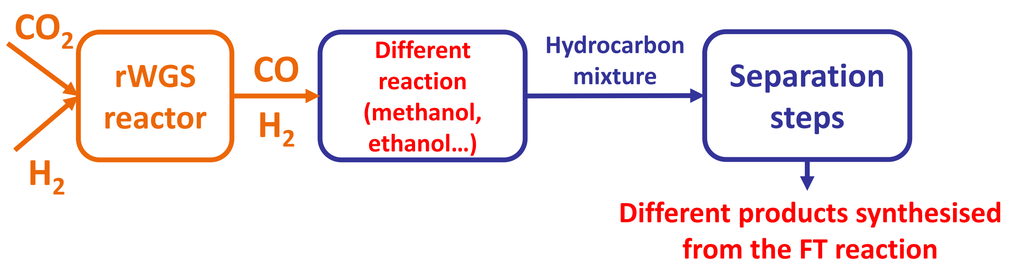
rWGS reaction Fischer-Tropsch reaction

Objectives

I. Design and optimisation



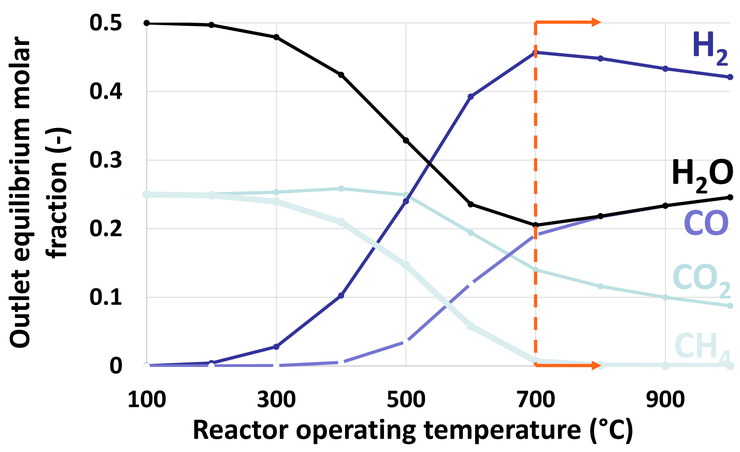
II. Study of a potential standardisation



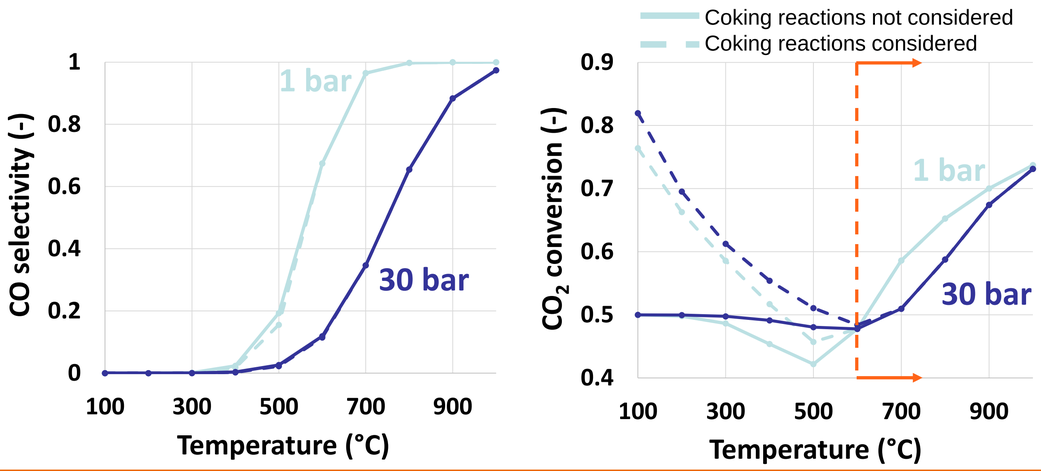
III. Study of the rWGS unit in dynamic mode (reaction to disturbances, adaptation to input/output variations…)

Results

Equilibrium-based model

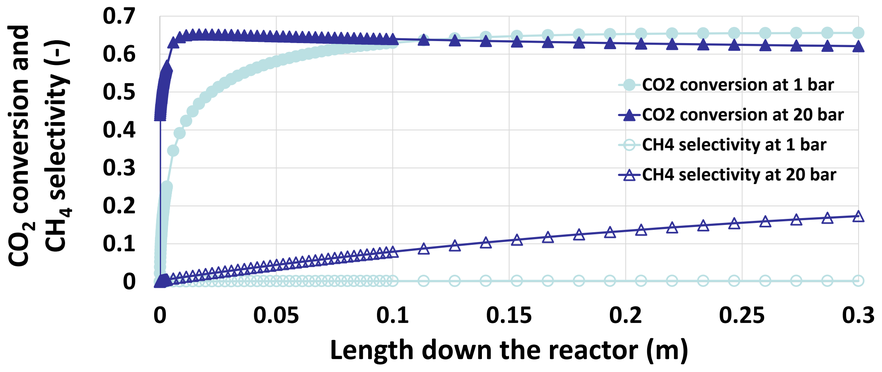


- Operating temperature **above 700°C** to limit CH_4 production at 1 bar
- Coking reactions can be neglected **above 600°C** at 1 bar

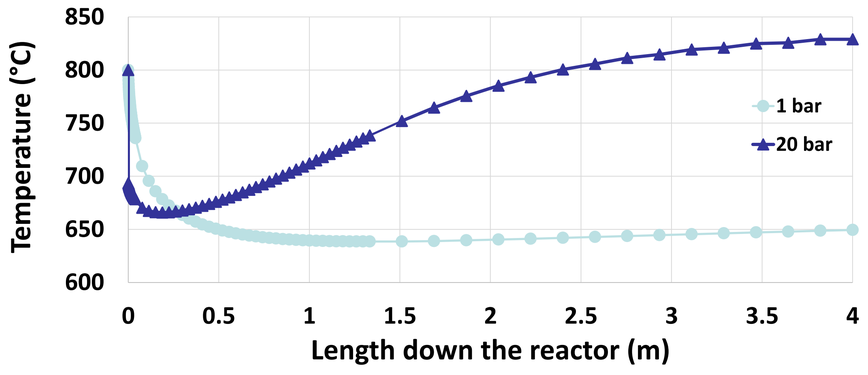


Kinetic model – Reactor sizing

Small-scale **isothermal** (800°C) reactor – Inlet H_2 of **1.5 Nm³/h**



Large-scale **adiabatic** (T_0 = 800°C) reactor – Inlet H_2 of **1500 Nm³/h**



Conclusions

Power-to-X processes are an appealing solution to produce high-density fuels with a low carbon footprint. The indirect synthesis approach is investigated in this work, more specifically its first step, i.e. the rWGS reaction. This reaction activates the highly stable CO_2 molecule by converting it to CO, which can be combined with H_2 in the Fischer-Tropsch synthesis to produce a mixture of hydrocarbon chains. This project aims to study the upgrading of this mixture to kerosene.

An equilibrium-based model was developed in Aspen Plus to get the first insights into modelling an rWGS reaction unit. The results show that the temperature must lie above 700°C to limit the production of the main by-product, CH_4. It is also shown that coking reactions can be neglected at these temperatures. Another model, based on kinetics, was also built. This kinetic model serves for the rWGS unit design, which will be included in the Power-to-kerosene pilot plant soon to be installed at ULiège. Furthermore, this model will be part of a complete process model to study the integration of a rWGS reaction unit in this kind of process.

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