The Reverse Water-Gas Shift Reaction as an Intermediate Step for Synthetic Jet Fuel Production: A Reactor Sizing Study at Two Different Scales

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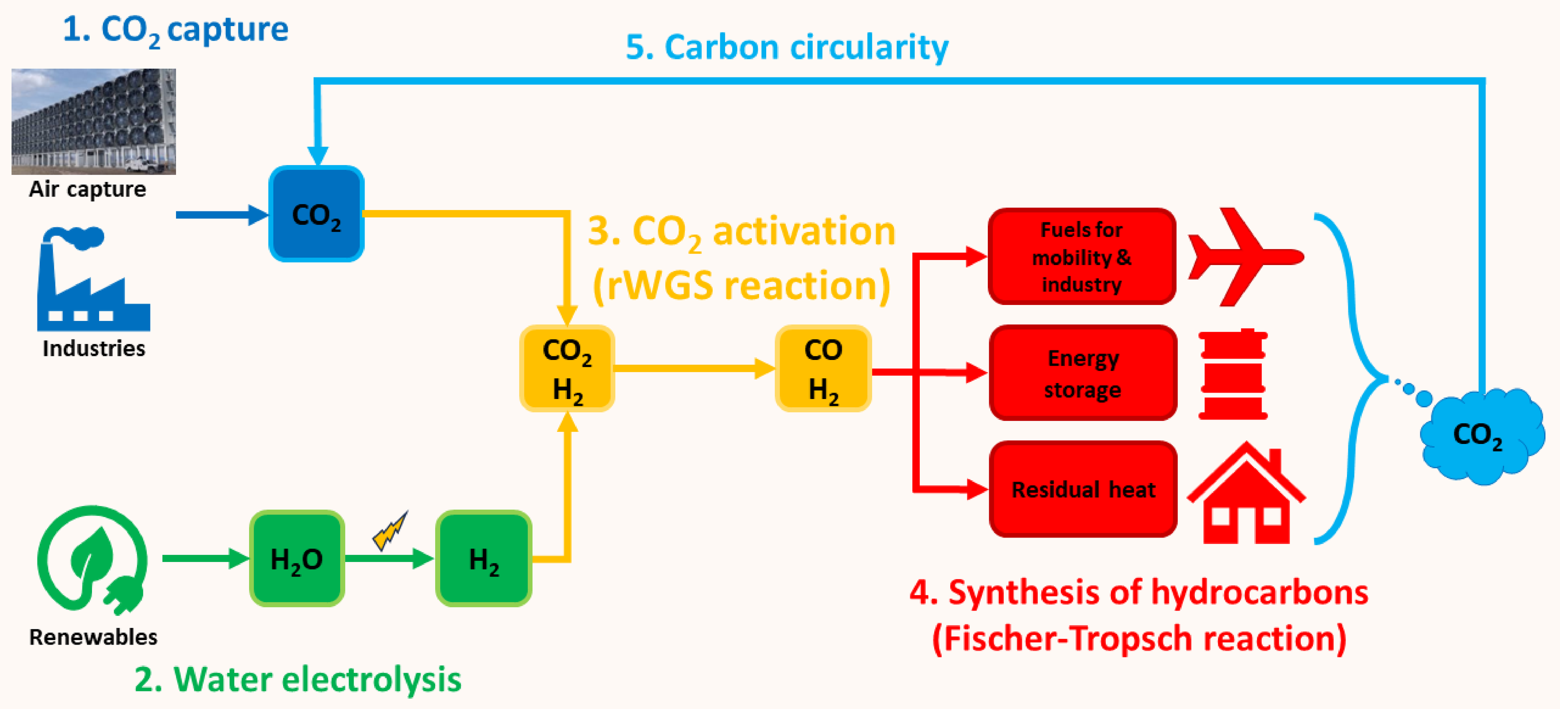
General Context and Objectives

In the context of the energy transition and the growing imperative to develop decarbonised solutions for the transportation sector, our team is investigating the conversion of CO_2 to kerosene via a Power-to-kerosene process. Given the high stability of the CO_2 molecule, an activation step is essential to convert it into more complex molecules. The reverse water-gas shift (rWGS) reaction is a promising solution to achieve this conversion. A primary objective of this project is to design and construct a small pilot facility that synthesises kerosene from CO_2 and H_2, calibrated to an available electrolysis capacity of 1.5 Nm^3/h. This study focuses on the sizing of the rWGS section for this scale and further compares it to a larger system with an electrolysis capacity 1,000 times greater.



Materials and Methods

- Complete kinetic model developed in **Aspen Custom Modeler**
- Kinetics developed by Vidal Vázquez et al. (2017)
  - LHHW-based kinetic model (**2 wt-% Ni/Al_2O_3**)
  - Validated between **550 and 800 °C** and **1 and 30 bar**

rWGS

$$CO_2 + H_2 \rightleftharpoons CO + H_2O \quad \Delta H^\circ_{298.15\,K} = +41.2 \text{ kJ/mol}$$

$$CO_2 + 4\,H_2 \rightleftharpoons CH_4 + 2\,H_2O \quad \Delta H^\circ_{298.15\,K} = -165.0 \text{ kJ/mol}$$

$$CO + 3\,H_2 \rightleftharpoons CH_4 + H_2O \quad \Delta H^\circ_{298.15\,K} = -206.2 \text{ kJ/mol}$$

Side reactions

Model Validation

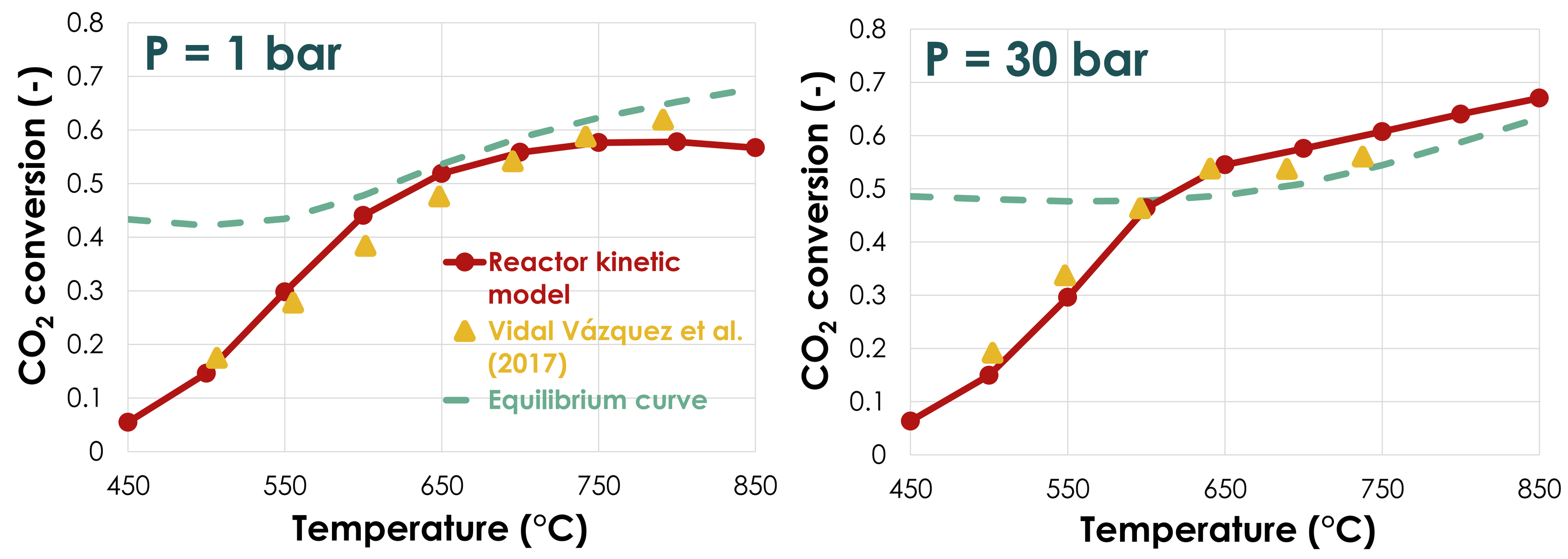


Figure 1 – CO_2 conversion at different temperatures, for an inlet H_2/CO_2 = 2 and a catalyst mass of 0.25 g, at 1 bar (left) and 30 bar (right)

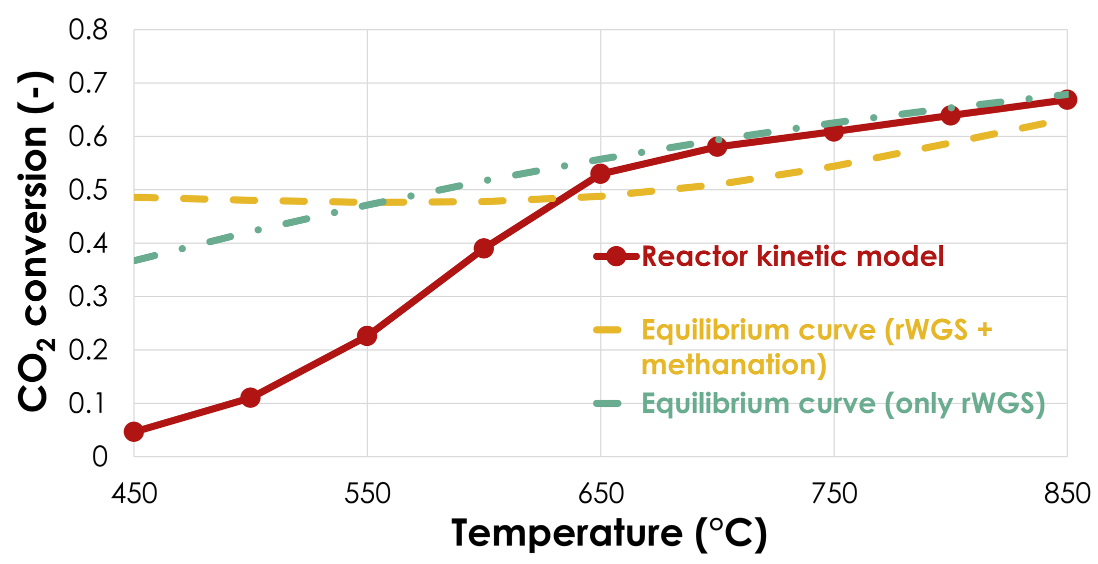


Figure 2 – Kinetic model comparison with two different equilibria (30 bar, inlet H_2/CO_2 = 2, cat. mass = 0.25 g)

How can the kinetic curve go **beyond the equilibrium** at 30 bar?

- **Competition** between three different equilibria

Sizing Study Comparison - Results

- Small-scale reactor = **isothermal**, inlet of **1.5** Nm^3/h of H_2
- Large-scale reactor = **adiabatic**, inlet of **1,500** Nm^3/h of H_2
- **Constraint** = outlet syngas ratio (H_2/CO) of **2.1**

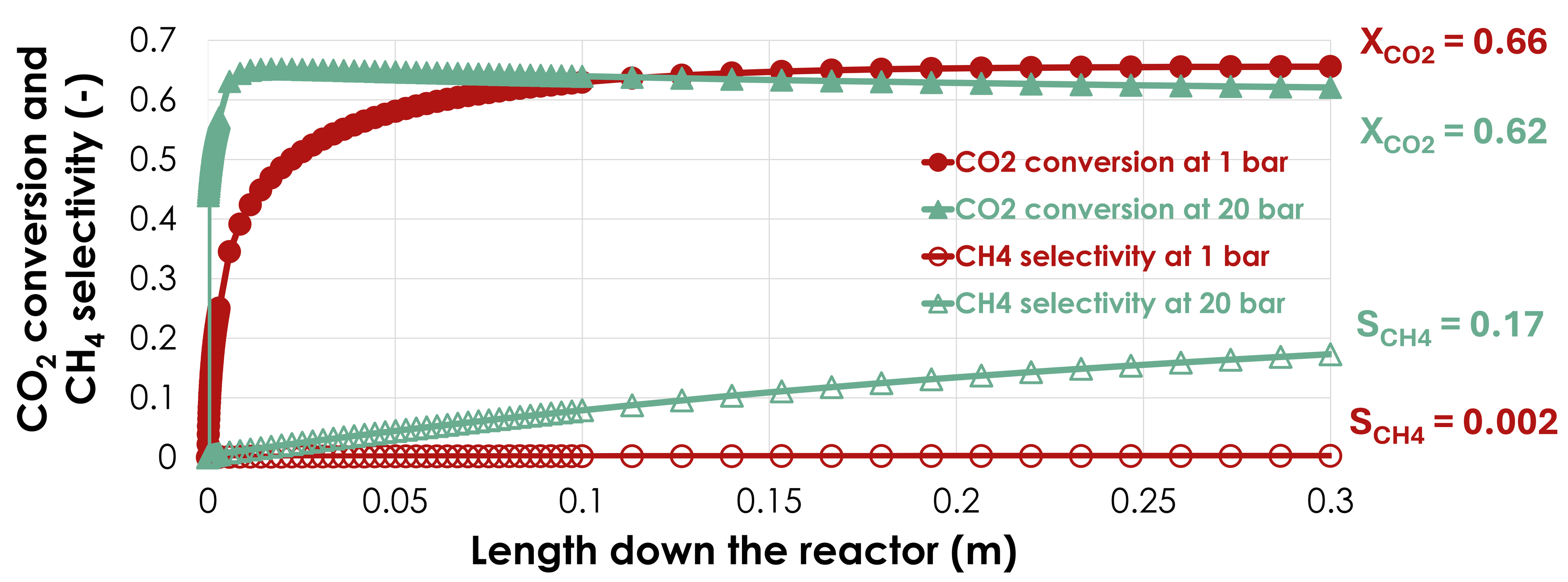


Figure 3 – Small-scale **isothermal** reactor sizing at **1** and **20** bar and 800 °C

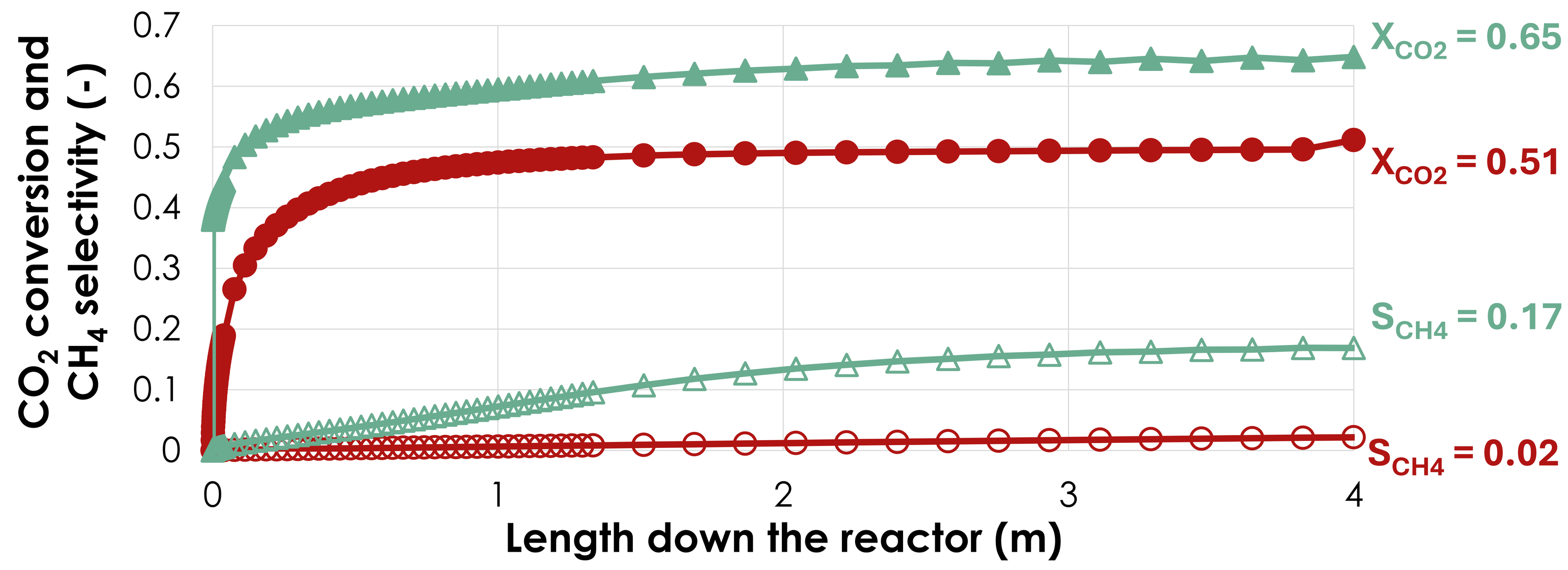


Figure 4 – Large-scale **adiabatic** reactor sizing at **1** and **20** bar and an inlet temperature of 800 °C

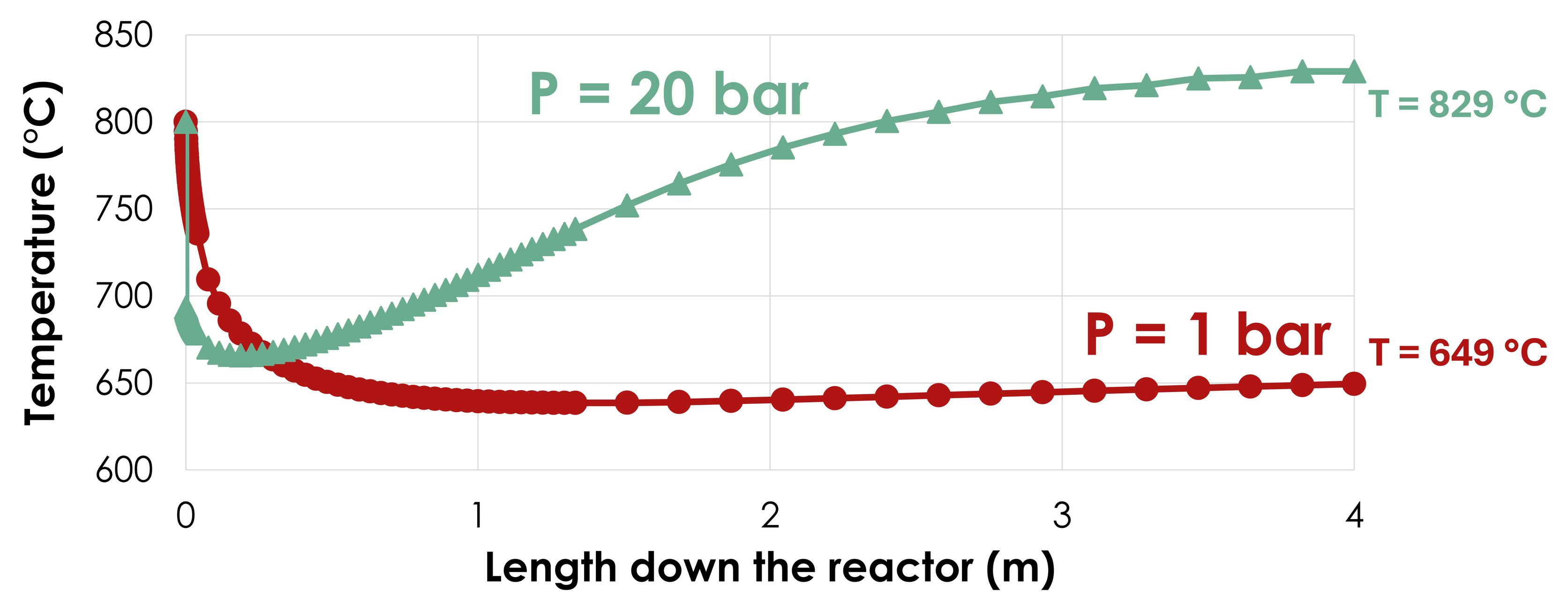


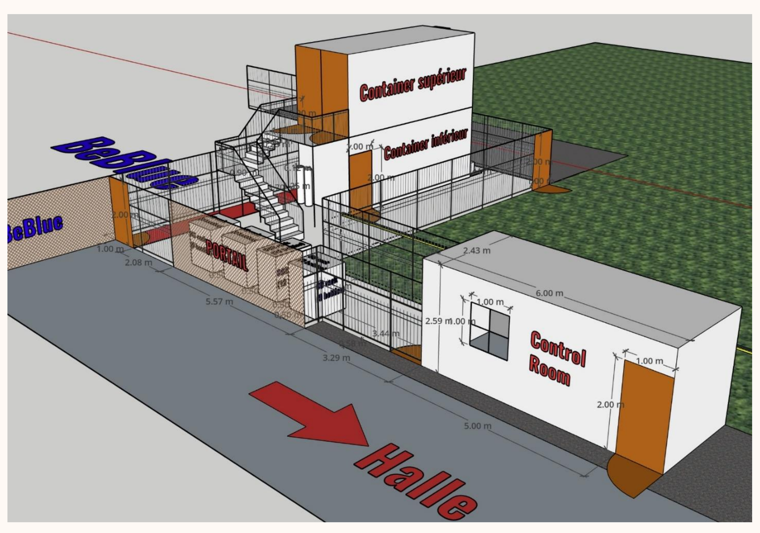
Figure 5 – Temperature profiles along the **adiabatic** reactor at **1** and **20** bar and an inlet temperature of 800 °C

Main conclusions:

- **Isothermal reactor** : optimal **size** is highly **dependent** on the operating **pressure**
- **Adiabatic reactor** : optimal **size** seems **independent** of the operating **pressure**, but better **performance** at high **pressure**

Conclusions and Perspectives

This paper investigates the sizing of an rWGS reactor in two different configurations. It is shown that the operating pressure significantly influences the optimal size of an isothermal reactor. Conversely, in an adiabatic configuration, pressure appears to improve CO_2 conversion while having minimum impact on the optimal design. The next steps include integrating this reactor model into a complete process model to further explore process optimisation aspects, rather that focusing solely on single unit optimisation.



References

F. Vidal Vázquez, P. Pfeifer, J. Lehtonen, P. Piermartini, P. Simell, and V. Alopaeus, 2017, 'Catalyst Screening and Kinetic Modeling for CO Production by High Pressure and Temperature Reverse Water Gas Shift for Fischer–Tropsch Applications', *Industrial & Engineering Chemistry Research*, 56 (45): 13262–72.

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