

# Design of a flexible reactor to couple carbon capture and carbon utilization in the sorption-enhanced methanol synthesis.

Emanuele Moioli<sup>1\*</sup>, Tilman Schildhauer<sup>1</sup>

*1 Paul Scherrer Institute, Forschungstrasse 111, 5232 Villigen, Switzerland*

*\*Corresponding author: Emanuele.moioli@psi.ch*

## **Highlights**

- A system for combined CCS and CCU in biogas upgrading was designed.
- The system operates as a PSA unit for CCS and as a sorption-enhanced methanol synthesis for CCU.
- The system is optimized in terms of sorbent ration to maximize the economic output.
- This new system paves the way for a new class of flexible CCS/CCU processes.

## **1. Introduction**

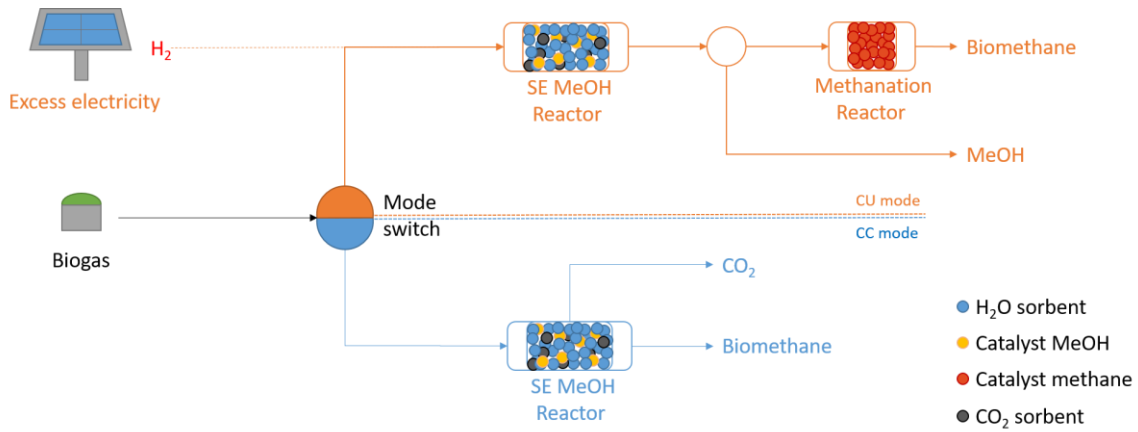
The electrification of chemical processes poses important challenges to the development of new reactive systems that can adapt to the seasonal variation in feedstock availability. As CO<sub>2</sub> converting reactions require large amount of electrolytical H<sub>2</sub>, the economic performance of these reactions is sustainable only in the limited times where electricity is cheap. For this reason, the abatement of point source CO<sub>2</sub> emissions via carbon utilization is a difficult pathway in the current market conditions. To avoid this challenge, it would be convenient to design process units that flexibly treat the CO<sub>2</sub> emission source, alternatively removing or converting CO<sub>2</sub>. In this way, the point emission could be completely mitigated, yielding a chemical product when the market conditions are favorable or simply separating CO<sub>2</sub> when electricity is expensive. This system could operate during the entire year, extending the amortization of CAPEX over a larger number of operating hours.

## **2. Methods**

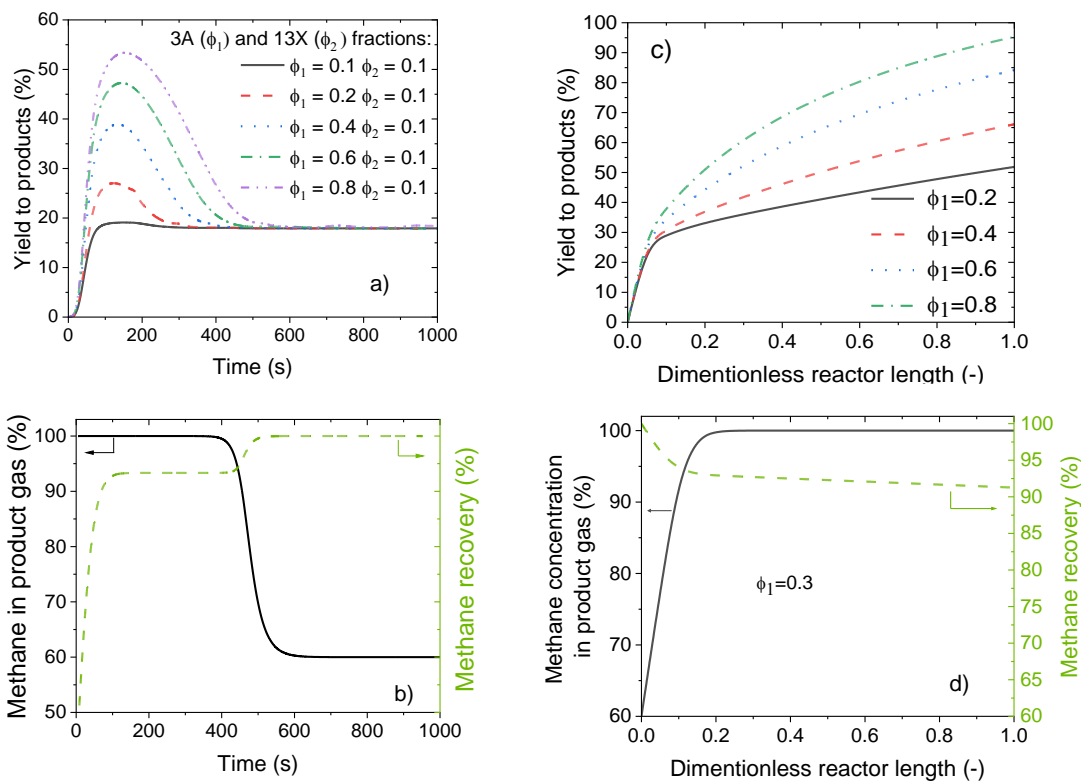
In the current market conditions (no clear CO<sub>2</sub> trade market), the best performance could be achieved when CO<sub>2</sub> should be separated from streams containing other valuable products. This is the case of biogas. Biogas upgrading through adsorption-based methods is a commercially available technology [1]. A relevant adsorbent to this scope is the zeolite 13X, which is employed in this work. The presence of an adsorbent can be exploited also in the carbon utilization mode, to perform a sorption-enhanced synthesis. In this work, the chosen carbon utilization mode is the methanol synthesis, enhanced by the presence of zeolite 3A, which selectively adsorbs water at the methanol synthesis conditions [2]. The concept of the integrated CCS/CCU system is shown in figure 1. The system is designed both for a fixed and a fluidized bed reactor.

## **3. Results and discussion**

In the fixed bed reactor, both sorbents are present in the reactor. Thanks to the higher capacity of zeolite 13X, the amount of this latter in the reactor can be 5 times less than the water adsorption zeolite (3A). The system is operated with 4 reactors in parallel, to form a temperature swing adsorption unit. The system is optimized to have similar time-on-stream in both operation modes. The calculated profiles are shown in figure 2a-b. In a fluidized bed reactor, the sorbent can be shaped to be entrained and continuously replaced in the reactor. In this case, the optimization is simpler because the CCS and CCU mode are decoupled, as shown in figure 2c-d. The economic analysis showed that both configurations can outperform the standard CO<sub>2</sub> utilization approaches, by realizing a continuous CO<sub>2</sub> abatement in a simple plant configuration.



**Figure 1.** The proposed flexible CCS/CCU process



**Figure 2.** The results of the reactor simulation in the CCU and CCS mode. a-b) fixed-bed; c-d) fluidized bed.

#### 4. Conclusions

The proposed reactor configuration is an optimal solution to minimize the OPEX required to capture CO<sub>2</sub> all over the year, maximizing the economic output of the system. The integration of CCS and CCU in the same process unit appears as an ideal case of process flexibilization, which can unlock significant potential in the application of renewable energy conversion strategies.

#### References

- [1] R. Kapoor et al., *Environ. Sci. Pollut. Res.* **2019**, *26*, 11631–11661. DOI: 10.1007/s11356-019-04767-1.
- [2] P. Maksimov, et al. *Chem. Eng. J.* **2021**, *418*, 129290. DOI: 10.1016/j.cej.2021.129290.

#### Keywords

CCS, CCU, process flexibilization, multifunctional reactors