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Dynamic Simulations of a Novel CCU Process Through Temperature-Swing Chemical Looping

Aim

- Development of process model for integrated CO_2 sorption-regeneration & methanation.
- Sensitivity analysis of the CO_2 sorbent and methanation catalyst properties and the sorption/methanation reaction kinetics through dynamic simulations.
- Optimize process operation and cycle design of sorption-regeneration & methanation.

Justification

The European Green Deal has highlighted the need to reach climate neutrality in the EU by 2050. In the wake of this climate crisis, Europe faces a challenging transition to a sustainable, affordable and secure energy system. The large injection of intermittent renewable energy sources (RES) raises concerns about the security of energy supply and grid stability. In the future energy system, energy molecules take on an important role to eliminate these concerns. Energy molecules such as green hydrogen can be derived from power-to-X (P2X) technologies. This green hydrogen can be utilized as is, or can be converted into synthetic methane (syn-methane) with the help of smart CCU processes. In this process, CO_2 is reduced via the Sabatier reaction (methanation).

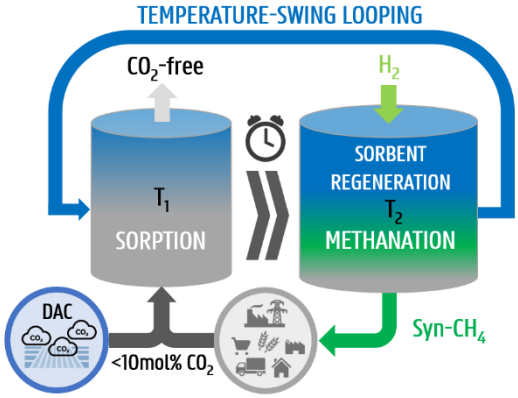

Figure 1: Schematic of potential configuration for integrated capture-regeneration & methanation.

CCU applications are often hampered by high energy costs (100-200 kJ/mol) to capture and separate CO_2 from dilute point sources (<10 mol% CO_2). For most sorbents, temperature-swing cycles are needed to sequentially adsorb and desorb CO_2. Interestingly, exothermic CO_2 methanation releases 165 kJ/mol. Integrating endothermic regeneration of a CO_2 sorbent with exothermic CO_2 methanation may decrease the overall energy penalty of this temperature-swing looping process significantly. CO_2 sorbents must display a low heat of decarbonation and thermal heat capacity [1], and decarbonate under the right temperature and pressure conditions in order for the methanation catalyst to remain sufficiently active and selective [2]. Novel Ni-based methanation catalysts display an excellent activity, CH_4-selectivity and stability at 300°C.

Aspen Adsorption™ is a useful modelling tool to study the dynamic behaviour of a packed-bed under simulated process conditions. Previous models of dynamic pressure-swing chemical looping processes have already been developed, for example to recover CO from blast-furnace gas [3]. Using these principles, a new model will be developed by implementing a kinetic model for CO_2 sorption, and simultaneous desorption and methanation.

Program

1. Literature review: investigate the kinetics/thermodynamics/material properties of CO_2 methanation on Ni-based catalysts and carbonation on suitable CO_2 sorbents.
2. Development of a temperature-swing model for selected sorbent-catalyst system.
3. Sensitivity analysis of material properties on process performance.
4. Optional: update model with experimentally-validated data (see other thesis topic: **Methanation Catalysts for Novel Sorption-Regeneration & Methanation Process**)
5. Optimization of process conditions: pressure, temperature, cycling, bed composition, etc.

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References

1. McQueen, N., et al., *Ambient weathering of magnesium oxide for CO2 removal from air.* Nat Commun, 2020. **11**(1): p. 3299.
2. Mesters, C., et al., *Direct Reduction of Magnesium Carbonate to Methane.* ACS Sustainable Chemistry & Engineering, 2021. **9**(33): p. 10977-10989.
3. Flores-Granobles, M. and M. Saeys, *Dynamic pressure-swing chemical looping process for the recovery of CO from blast furnace gas.* Energy Conversion and Management, 2022. **258**.