Stability of Adsorbents for Direct Air Capture: Experimental and Modeling Approach

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Salar Fakhraddinfakhriazar, Grégoire Léonard
Department of Chemical Engineering, University of Liège, Belgium

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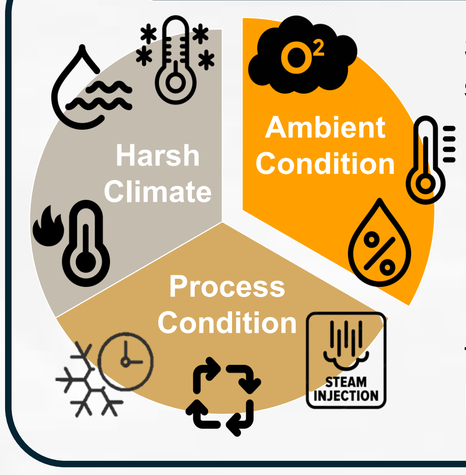
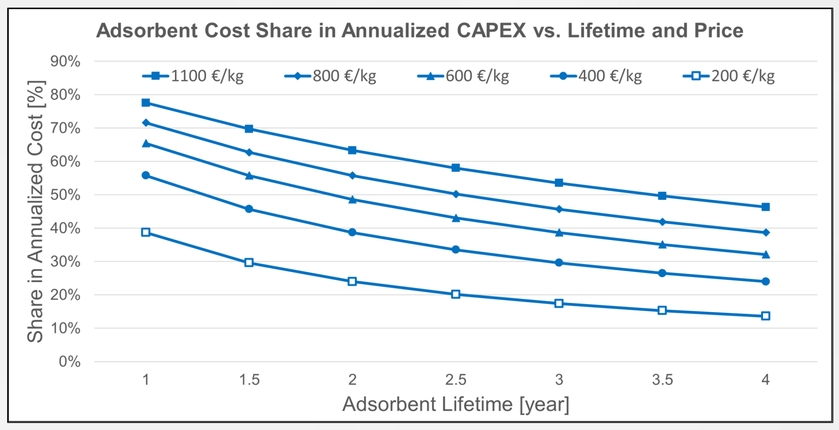
Motivation and Background



Stability of solid sorbents is a critical factor in adsorption-based separation processes, including direct air capture (DAC).

- Lifetime directly impacts **cost**, **downtime**, and **net CO_2 removal**.
- Results in **undesired emissions**, and additional material **waste**.
- While most studies focus on capacity and selectivity, **real operating conditions** (temperature, humidity, O_2) can significantly degrade sorbents.

The impact of sorbent stability on CAPEX is evaluated using the DAC model of Kim and Léonard [1] (Climeworks Hinwil, 2460 kg CO_2/day).

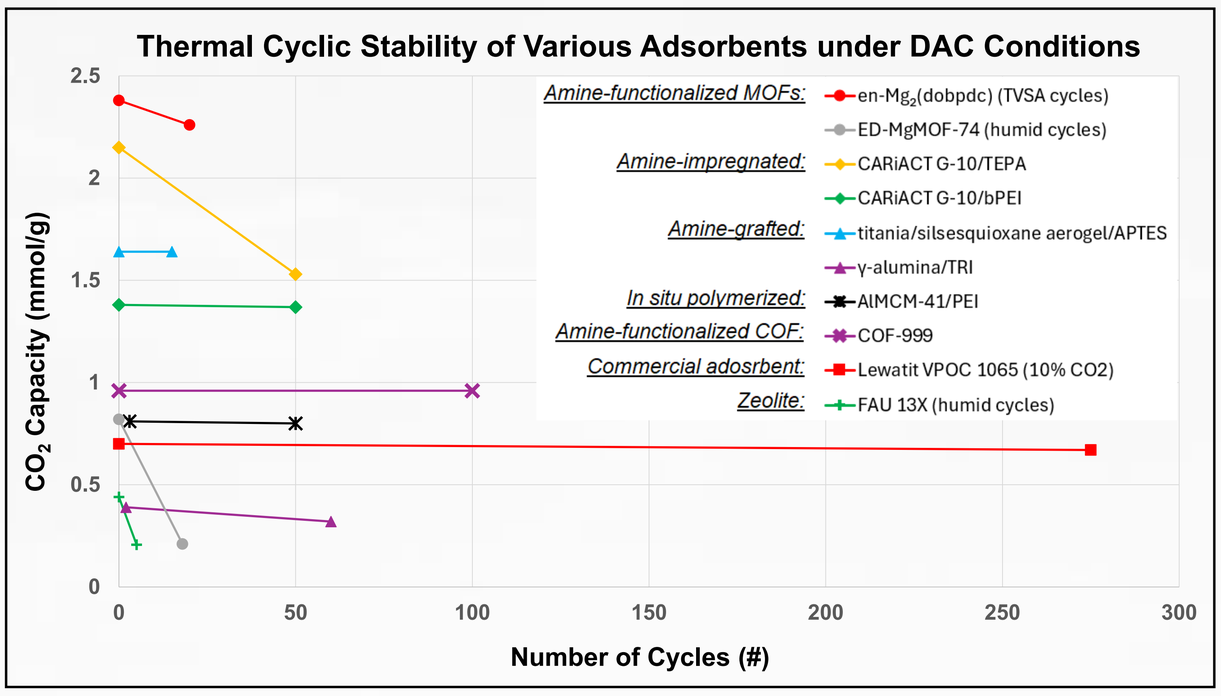


Objectives

Develop a framework integrating adsorption modeling and adsorbent degradation to predict long-term performance

1. Conduct a **literature review** to identify DAC adsorbents, major degradation mechanisms, and experimental methodologies
2. Design and build a dedicated **experimental test bench** to evaluate sorbent stability under different operating conditions
3. Develop an **adsorption process model** for DAC to predict adsorbent performance over time **considering deactivation**

Edith Flanigen (1929–2026)
"Without stability, you have nothing" ...

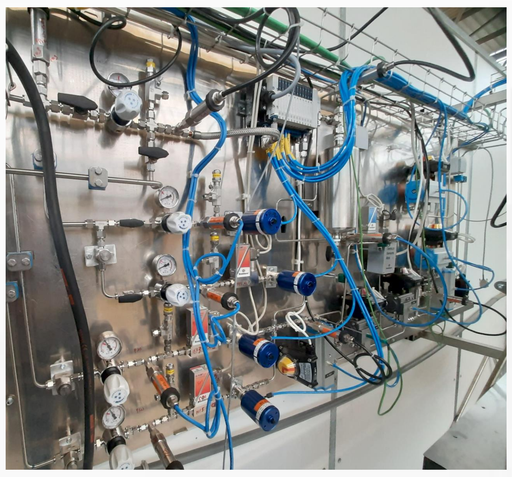


	Adsorbent Types	Advantages	Disadvantages
Physisorbents	**Zeolite**	High thermal/chemical stability High CO_2 capacity at sub-ambient conditions	Strong moisture sensitivity Low CO_2 capacity at ambient temperature
	Metal–Organic Frameworks (MOFs)	High thermal stability High CO_2 selectivity	Moisture instability for some MOFs Low capture capacity at high CO_2 pressure
Chemisorbents	**Amine-impregnated**	Effective under humid conditions Relatively simple synthesis	Low thermal stability (evaporation/leaching) Oxidatively sensitive
	Aminosilane-grafted	High thermal stability High humidity tolerance	Oxidatively sensitive More complex synthesis
	Amine-appended MOFs	High uptake at low CO_2 pressure High selectivity	Synthetic complexity Oxidative/moisture degradation
	Amine-functionalized Covalent Organic Frameworks (COFs)	Promising stability High CO_2 selectivity	Early-stage development Limited scalability Uncertain long-term stability
	Carbonate-based	Low-cost materials High chemical stability	Low regeneration temperature Slow kinetics at ambient conditions

Setup for Stability Assessment

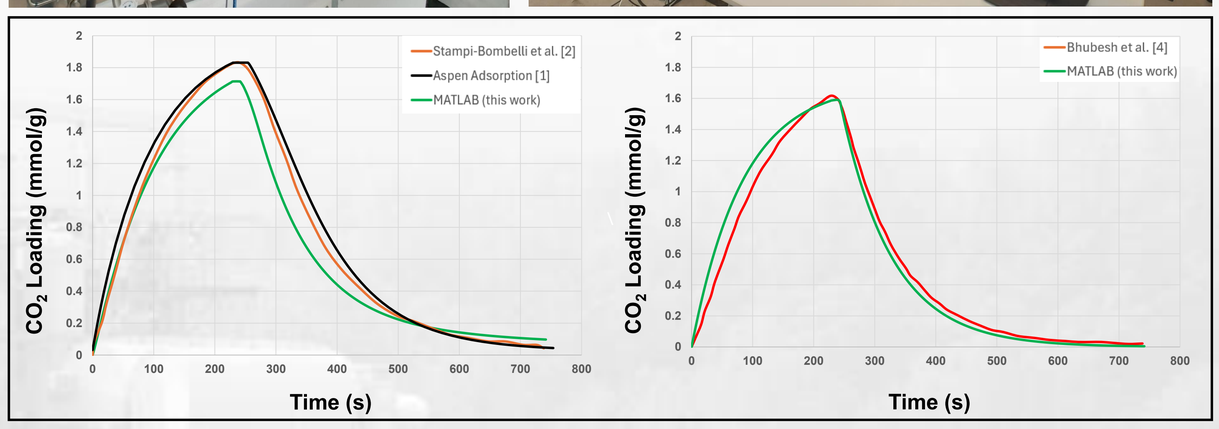
To evaluate the long-term stability of adsorbents, a dedicated automated test bench has been developed to perform repeated adsorption–desorption cycles. The setup enables stability testing of solid sorbents under controlled operating conditions:

- Temperature: −20 to 180 °C
- Gas composition: N_2/CO_2 (400–20000 ppm)/O_2
- Relative humidity: 10–90%
- Flow rate: 100–5000 Nml/min
- Adsorbent mass: ≥ 1 g



Modeling

A 1D adsorption model for amine-functionalized Nanofibrillated cellulose (TVSA and S-TVSA) was developed in MATLAB and validated using experimental data, [2,3] with additional comparison to Aspen Adsorption simulations. [1] The model includes gas-phase component mass balances with linear driving force (LDF) mass transfer and a column energy balance. Water co-adsorption is incorporated using a modified Toth isotherm model.



Next Steps

Approaches to include sorbent degradation in adsorption models:

1. Constant capacity decay factor → large prediction errors
2. Degradation rate equations integrated into the model → complex degradation phenomena
3. Cycle-dependent isotherm parameters → selected approach

In this work, degradation will be evaluated by performing 50–200 adsorption–desorption cycles. Isotherms of aged adsorbents will then be measured, and the resulting parameters will be expressed as a function of cycle number and incorporated into the adsorption model.

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References

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