Lab-pilot Scale CO_2 Capture Vacuum Pessure Swing Adsorption using MOFs

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Nowadays, power generation and carbon-intensive industries are at the origin of a large part of anthropogenic CO_2 emissions (in the order of 50%) to the atmosphere that contributes to global warming. So, the reduction of CO_2 emissions from industries is crucial. CO_2 capture technologies are a potential solution that are investigated to envisage CO_2 storage (CCS) or reuse (CCU). Absorption-regeneration amine-based process, the benchmark solution, suffers from high energy penalties that leads adsorption process a promising alternative thanks to improvement of process design and development of new materials. Among these materials, MOFs appears as very promising materials for both gas separation and purification. However, the performances of these hybrid materials in carbon capture technologies have not been fully evaluated and fine-tuning is still needed for adsorption processes at large scale in real industrial conditions.

In this context, the H2020-MOF4AIR project (https://www.mof4air.eu/) aims to develop adsorption processes of CO_2 capture with MOFs from the material synthesis to an industrial pilot scale.

27 MOFs have been studied to be used in a Vacuum Pressure Swing Adsorption (VPSA) process. MIL-160(Al) [1,2] was the first selected for its interesting selectivity (30-35) of CO_2 over N_2, its ease of regeneration (moderate heat of adsorption (32-33 kJ/mol)), and its stability against water and other pollutants as NOx or SO_2. The performance of this MOF in a VPSA process was studied by simulation using Aspen Adsorption, confirming the potential of this MOF for CO_2 capture in an industrial process (at least 95% of recovery and 90% of purity). So, MIL-160(Al) was the first selected MOF of the H2020-MOF4AIR project to be produced at 3-5 kg scale and shaped in 2mm-pellets with 3% of PVB by wet granulation.

To confirm the simulation results, a VPSA lab-pilot was designed and assembled at UMONS to test the upscaled MOFs. This apparatus can perform and assess three different VPSA configurations *i.e.,* 2-bed 5-step[3,4], 3-bed 5 step[4], and 3-bed 6-step[5], with a feed flow rate up to 1.5 $Nm^3.h^{-1}$ with different CO_2 concentrations. The VPSA pilot is fully instrumented allowing to record temperature, pressure, flow rate and CO_2 concentrations for comparison with simulations. The shaped MIL-160(Al) was then tested in operating conditions with a 3-bed 6-step configuration (the sole configuration allowing to reach good performances in terms of recovery and purity according to the simulations performed previously to study the impact of several operating parameters (step's time, step's flowrate and pressure level, …), and to find the optimum conditions allowing to reach the targets.

Results obtained from VPSA lab-pilot will be used to refine the simulation models developed. Thanks to the numerous recordings of the laboratory pilot, some uncertain parameters (heat transfer coefficients, kinetics, …) will be adjusted to fit the experimental results.

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References

[1] A. Cadiau et al., "Design of Hydrophilic Metal Organic Framework Water Adsorbents for Heat Reallocation," *Adv. Mater.* **2015**, 27(32), 4775–4780.
[2] D. Damasceno Borges et al., "Gas Adsorption and Separation by the Al-Based Metal–Organic Framework MIL-160," *J. Phys. Chem. C*. **2017,** 121 (48), 26822–26832.
[3] C. A. Grande, "Advances in Pressure Swing Adsorption for Gas Separation, *Chem. Eng.* **2012**, 1–13.
[4] L. Wang, Z. Liu, P. Li, J. Wang, and J. Yu, "CO_2 capture from flue gas by two successive VPSA units using 13XAPG," Adsorption **2012**, 18 (5–6) ,445–459.
[5] S. Krishnamurthy et al, "Post combustion carbon capture with supported amine sorbents: From adsorbent characterization to process simulation and optimization," *Chem. Eng. J.* **2021,** 406,127121