Project

In recent years, carbon capture and sequestration (CCS) presented itself as the ultimate solution to mitigate climate change. No wonder, it gained tremendous support from the scientific community [1]. Scientists around the world ought to model efficient adsorption technologies and develop new materials for CO_2 capture. Depending on the CO_2 source, some technologies do better than others. In general, Pressure Swing Adsorption/Vacuum Swing Adsorption (PSA/VSA) is considered one of the promising options [2]. In this project, the PSA/VSA process will be implemented to capture CO_2 from post-combustion power plant flue gas. A preliminary process flow diagram is shown in Figure 1. The flue gas coming in at atmospheric pressure is cooled down to 25°C prior to adsorption. Once the adsorbent is saturated with CO_2, the pressure is dropped to 0.2 bar, keeping the same temperature, and CO_2 is desorbed. Finally, the CO_2 rich stream is compressed to 100-150 bars to be stored in geological formations.

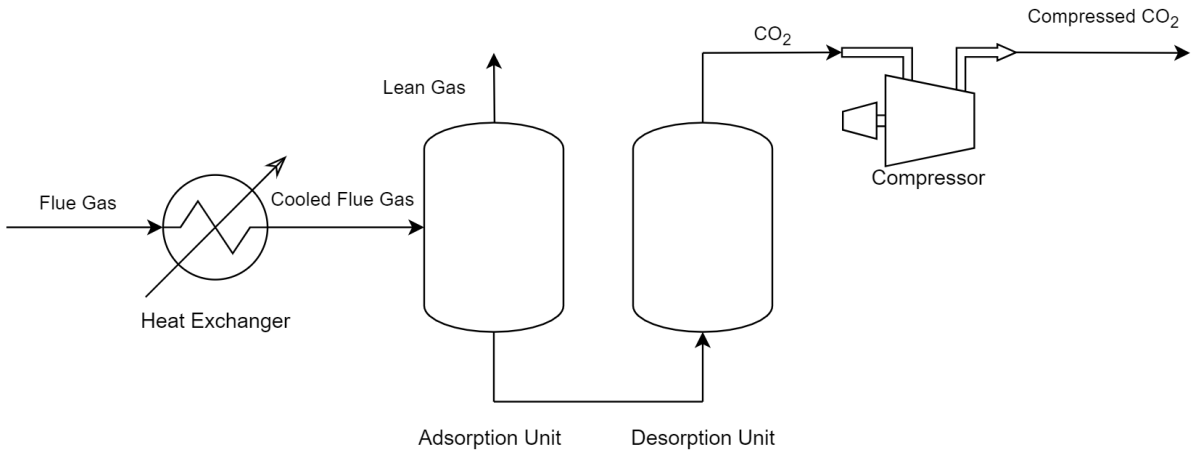

Figure 1: Flow diagram of the PSA/VSA process

Metal Organic Frameworks (MOFs) are crystalline nanoporous materials that have emerged as good sorbents for post-combustion CO_2 capture due to their high CO_2 capacity and CO_2/N_2 selectivity [3]. Assuming that the flue gas contains only CO_2 (~15%) and N_2 (~85%), you need to rank a given group of materials based on some basic properties:

1. Compute the density ($g.cm^{-3}$), accessible surface area - ASA (A^2), accessible probe-occupiable volume - POAV (A^3) and porosity of the different structures by running pore analysis. Use a probe radius of 1.525Å (4 each structure)
2. Compute the henry coefficients for CO_2 and N_2 at 25°C (2 each structure). Rank the structures based on their affinity for CO_2 (5)
3. Compute CO_2 and N_2 pure component isotherms at 25°C for the given structures (3 each structure). Plot the pure isotherms per molecule (3)
4. Calculate the CO_2 working capacity (WC) for the different structures (4 each structure)
5. Calculate the CO_2/N_2 selectivity (S) for the different structures (2 each structure)
6. Rank the structures using a WC vs. S plot (10)
7. Is the screening model conclusive as to which material performs best in a PSA/VSA process for post-combustion CO_2 capture ? Discuss the level at which the screening was performed and come up with more complex key performance indicators (10)
8. Organization of the report (6)

Hints

1. For the material structures, please refer to the Moodle page. These structures were already optimized and their charges were calculated. Use the following simulation parameters:
    - Zeo++ volpo samples: 10,000
    - Number of samples for block calculation: 100
    - Number of Widom cycles: 50,000
    - Number of GCMC initialization cycles: 500
    - Number of GCMC production cycles: 5,000
    - Maximum distance between pressure points: 0.6
    - Pressure range: 0.2 to 10.2 bars

2. The working capacity measures how much CO_2 can be theoretically recovered, i.e. the maximum recoverable amount of CO_2 given the process conditions:

$$WC = q_{adsorption} - q_{desorption}$$

   Where q is the binary loading of CO_2 in mmol.g^{-1} obtained from IAST calculations.

3. The ideal selectivity gives an indication on the competitiveness of adsorption between the different components of a gas mixture:

$$S_{CO_2/N_2} = \frac{q_{CO_2}}{q_{N_2}} \frac{y_{N_2}}{y_{CO_2}}$$

   Where q is the binary loading, obtained from IAST calculations, at the adsorption conditions in mmol.g^{-1}, and y is the molar fraction of the component in the flue gas.

References

[1] M. Bui *et al.*, "Carbon capture and storage (CCS): The way forward," *Energy Environ. Sci.*, vol. 11, no. 5, pp. 1062–1176, 2018.

[2] M. T. Ho, G. W. Allinson, and D. E. Wiley, "Reducing the cost of CO2 capture from flue gases using pressure swing adsorption," *Ind. Eng. Chem. Res.*, vol. 47, no. 14, pp. 4883–4890, 2008.

[3] T. D. Burns *et al.*, "Prediction of MOF Performance in Vacuum Swing Adsorption Systems for Postcombustion CO2 Capture Based on Integrated Molecular Simulations, Process Optimizations, and Machine Learning Models," *Environ. Sci. Technol.*, vol. 54, no. 7, pp. 4536–4544, 2020.

[4] A. Ajenifuja, L. Joss, and M. Jobson, "A New Equilibrium Shortcut Temperature Swing Adsorption Model for Fast Adsorbent Screening," 2020.