“How process engineering can enable the screening and discovery of adsorbents”

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Adsorption is a mature process used in the H2 purification, air separation, CH4 upgrading etc. In the last 20 years, significant efforts have been invested in developing these processes also for CO2 capture. The explosion in the area of adsorbent synthesis and molecular simulations have resulted in the generation of hundreds of thousands of (hypothetical & real) adsorbents, e.g., Zeolites, Metal-Organic Frameworks (MOFs). This excitement seems to have led to an implicit assumption that the key bottleneck in developing large-scale adsorption processes lies in the discovery of the right adsorbent. Recent work that focuses on the development of processes has highlighted the fact that the performance of an adsorbent is intimately linked to the process in which it is deployed, and any meaningful screening should consider the complexity of the process. Hence, screening these large databases to identify suitable candidates for scale-up is a challenging problem.

Simulation of cyclic adsorption processes is computationally intensive: they constitute the simultaneous propagation of heat and mass transfer fronts; there are no straightforward design tools, and their cyclic nature requires the calculation of the transient in order to evaluate the cyclic-steady state performance. This talk will focus on recent developments in modelling and machine-learning that have allowed us to screen large databases of adsorbents and to also develop achievable separation/cost targets that allow comparing adsorption with other technologies. These techniques have allowed us not only to understand the interplay between processes and materials, but also to explore some interesting questions about the properties of an adsorbent that will be suitable for a particular separation. The talk will focus on Pressure-Vacuum Swing Adsorption for post-combustion CO2 capture and will be based on our recent work related to the screening of adsorbents [1,2], machine-learning models for process optimization [3,4] scale-up and costing [5].

1. Burns, Thomas D., et al. "Prediction of MOF Performance in Vacuum Swing Adsorption Systems for Post-combustion CO2 Capture Based on Integrated Molecular Simulations, Process Optimizations, and Machine Learning Models." Env. Sci. Technol. 54.7 (2020): 4536-4544.

2. Balashankar, V, and Rajendran, A "Process Optimization-Based Screening of Zeolites for Post-Combustion CO2 Capture by Vacuum Swing Adsorption." ACS Sus. Chem. Engg 7.21 (2019): 17747-17755.

3. Pai, K.N., Prasad, V., and Rajendran, A. "Generalized, adsorbent-agnostic, artificial neural network framework for rapid simulation, optimization and adsorbent-screening of adsorption processes." Ind. Engg. Chem. Res (2020), in Press.

4. Pai, K. N., Prasad, V. and Rajendran, A. "Experimentally validated machine learning frameworks for accelerated prediction of cyclic steady-state and optimization of pressure swing adsorption processes." Sep Purif. Technol. 241 (2020): 116651.

5. Subraveti, S. G. , et al. "Techno-economic Assessment of Optimised Vacuum Swing Adsorption for Post-Combustion CO2 Capture from Steam-Methane Reformer Flue Gas." Sep. Purif. Technol (2020), in Press