INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study : Ph.D.

Thesis Title: Performance of Selected Adsorbents for CO_2 Capture: Equilibrium and Column Dynamics Study

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Thesis Submitted to the Department/ Center : Chemical Engineering

Date of completion of Thesis Viva-Voce Exam : 18-january-2021

Key words for description of Thesis Work : Gas adsorption, Metal Organic Frameworks, Pressure Swing Adsorption

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SHORT ABSTRACT

In the last two decades, metal organic frameworks (MOFs) have emerged as promising materials for gas separation and storage. Majority of the literature on MOF materials for gas separation is limited to equilibrium measurements due to the complexity associated in dynamic measurements such as the column break through studies and development of process cycles. Other reasons contributing to this trend include, the challenges involved in scale up of the synthesis procedure and that in pelletization of the synthesized MOF powders.

In this work, the metal organic frameworks UiO-66, MIL-101(Cr), Cu-BTC and MIL-53(Al) are systematically investigated for CO_2/N_2 separation. In the first part of work, the chosen MOFs are synthesized in 10 g level. Then the synthesized MOF powders are shaped into pellets using poly vinyl alcohol (PVA) as the binder. The effect of shaping on structural and functional characteristics of MOF are examined through the BET, FESEM, FTIR, TGA and XRD analysis.

The pure component isotherms of CO_2, N_2 are measured on MOF powders and pellets. About 14-20% decrease in CO_2 adsorption capacity is observed after pelletization. Although, a reduction in specific loadings is observed, the change in volumetric capacity is lower, due to the increase in bulk density after pelletization.

A single column PVSA experimental set up is developed and experimentally validated using zeolite 13X adsorbent. The breakthrough experiments conducted using synthetic dry flue gas (15% CO_2, balance N_2) as feed in a column containing about 8 to 12g of the MOF pellets (at 1.3 bar and 300 K) reveal preferential adsorption of CO_2 over N_2 and the CO_2 separation. The process performance of MOF pellets is evaluated in three different PVSA cycles using the single column. The inclusion of purge and rinse step result in an increase of N_2 product purity and CO_2 product purity respectively. The best performance achieved with the employed 5-step (pressurization, adsorption, CO_2 rinse, blowdown and N_2 purge along with evacuation) PVSA cycle on the four chosen MOFs is CO_2 purity (35%-68%), CO_2 recovery (54%-61%) and CO_2 productivity (0.075-0.269 $kgCO_2/(kgads \cdot h)$). The findings from PVSA suggest that these MOF materials are promising for CO_2/N_2 separation at low CO_2 concentrations, however a multi-bed PVSA may be needed to meet the process performance parameters for industrial requirement (CO_2 purity >95%, CO_2 recover >95%).